Deutsche Physikalische Gesellschaft DPG

DPG-Frühjahrstagung der Sektion Kondensierte Materie (SKM) 2025

DPG Spring Meeting of the Condensed Matter Section (SKM) 2025

together with the Working Groups

Equal Opportunities,
Industry and Business,
Physics, Modern IT and Artificial Intelligence,
“Young DPG”,
Young Leaders in Physics

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16 – 21 March 2025
University of Regensburg

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Deutsche Physikalische Gesellschaft DPG

2025

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- Playful Quantum Science and Quantum Science in Schools
- Quanta in Music, Philosophy, Art and Literature
- Quanta in the Professional world, Career and Society
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quantum2025.de

www.dpg-physik.de

Dear participants,

Welcome to the DPG Spring Meeting of the Condensed Matter Section on the campus of the University of Regensburg.

Our Spring Meetings are the DPG's flagship events for promoting scientific exchange — both for internal communication within the DPG and for exchange with researchers from all over the world. We expect a total of up to 10,000 guests at our Spring Meetings, which will once again make the DPG conferences the largest platform for scientific exchange in the field of physics in Europe this year. The comprehensive inclusion of presentations by young scientists in the conference program is also a unique selling point at both national and international level. This is by no means a matter of course: on the one hand, this is due to the well-coordinated cooperation of our many committed conference organisers in the DPG and the support of our DPG office in Bad Honnef. On the other hand, it is thanks to the generous support of the universities that are excellent hosts for our conferences. For a whole week, the universities are almost entirely dedicated to physics and thus become internationally visible "beacons" of physics research.

We are also working on making our conferences even more international, in the spirit of „Science bridges cultures." I am therefore very pleased that the DPG communication programme, which enables young scientists to actively participate in DPG conferences at the earliest possible stage of their scientific training, has been expanded thanks to the generous support of the Wilhelm und Else Heraeus-Stiftung: by awarding additional scholarships to young scientists from the countries supporting the electron storage ring "SESAME" in the Middle East as well as from Central and Eastern European countries to participate in our conferences. Strengthening and fostering international scientific exchange cannot be overestimated — especially in these times!

As the world's largest physics society, the DPG is also one of the main initiators of this year's "International Year of Quantum Science and Technology" (IYQ). The DPG is taking the lead in implementing the IYQ proclaimed by the UN in Germany. The formulation of quantum mechanics in 1925 created a lasting foundation for our physical understanding of nature. Quantum technologies have changed our daily lives and have become pillars of our prosperity, which is why we are celebrating their successes and highlighting future prospects. Under the motto "Quantum2025 — 100 years is just the beginning..." within the framework of IYQ, a wide variety of events and activities are being organized and coordinated by DPG (see *quantum2025.de*). I would like to thank all those who are contributing to the success of the quantum year!

The success of this Spring Meeting is only possible with the greatest commitment. I would like to express my sincere thanks to everyone involved. First of all, I would like to thank the University of Regensburg for their hospitality and support. Many thanks also to the Wilhelm und Else Heraeus Stiftung for generously supporting all DPG Spring Meetings. I would also like to thank the participating DPG Divisions and Working Groups for organising the scientific programme. My special thanks also go to the local organising committee at the University of Regensburg and its head, Prof. Christoph Strunk, Institute of Experimental and Applied Physics.

Finally, I would like to thank the DPG Head Office for its support of all Spring Meetings.

I wish you a great DPG Spring Meeting at the University of Regensburg with many new insights and excellent discussions!

Prof. Dr. Klaus Richter

President
Deutsche Physikalische Gesellschaft e. V.

Organisation

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Deutsche Physikalische Gesellschaft e.V.
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Email dpg@dpg-physik.de
Website www.dpg-physik.de

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Email regensburg25@dpg-tagungen.de

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Universität Regensburg
Universitätsstraße 31, 93040 Regensburg
Phone +49 (0) 941 943-2924
Email dpg-conference@uni-regensburg.de

Scientific Organisation

Chair of the Condensed Matter Section (SKM)
Prof. Dr. Sarah Köster
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Institut für Röntgenphysik
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Email sarah.koester@uni-goettingen.de

Chairs of the participating Divisions of the SKM:

(BP)	Biological Physics	–	Prof. Dr. Kerstin Blank (kerstin.blank@jku.at)
(CPP)	Chemical and Polymer Physics	–	Prof. Dr. Stephan Roth (stephan.roth@desy.de)
(DS)	Thin Films	–	Prof. Dr. Stefan Krischok (stefan.krischok@tu-ilmenau.de)
(DY)	Dynamics and Statistical Physics	–	Prof. Dr. Carsten Beta (carsten.beta@uni-potsdam.de)
(HL)	Semiconductor Physics	–	Prof. Dr. Alexander Holleitner (holleitner@wsi.tum.de)
(KFM)	Crystalline Solids and their Microstructure	–	J. Prof. Dr. Anna Grünebohm (anna.gruenebohm@rub.de)
(MA)	Magnetism	–	Prof. Dr. Claudia Felser (claudia.felser@cpfs.mpg.de)
(MM)	Metal and Material Physics	–	Prof. Dr. Christian Elsässer (christian.elsaesser@iwm.fraunhofer.de)
(O)	Surface Science	–	Prof. Dr. Wolf Widdra (widdra@physik.uni-halle.de)
(SOE)	Physics of Socio-economic Systems	–	Dr. Philipp Hövel (philipp.hoevel@uni-saarland.de)
(TT)	Low Temperature Physics	–	Prof. Dr. Stefan Kehrein (stefan.kehrein@theorie.physik.uni-goettingen.de)
(VA)	Vacuum Science and Technology	–	Dr. Stylianos Varoutis (stylianos.varoutis@ipp.mpg.de)

Chairs of the participating Working Groups

(AGYouLeap)	Young Leaders in Physics	–	Dr. Susanne Liese (susanne.liese@physik.uni-augsburg.de) Dr. Alexander Schlaich (alexander.schlaich@simtech.uni-stuttgart.de)
(AKC)	Equal Opportunities	–	OStR Agnes Sandner (akc@dpg-physik.de)
(AIW)	Industry and Business	–	Dr. Hans-Georg Grothues (hg.grothues@dlr.de)
(AKjDPG)	Young DPG	–	Pauleo Nimtz (nimtz@jdpg.de)
(AKPIK)	Physics, Modern IT and Artificial Intelligence	–	Dr. Tim Ruhe (tim.ruhe@tu-dortmund.de)

Symposia

SYAI	–	AI in (Bio-)Physics
SYED	–	Physics of Embryonic Development Across Scales: From DNA to Organisms
SYES	–	Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics
SYFD	–	Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning
SYIS	–	Progress and Challenges in Modelling Electron-Phonon Interaction in Solids
SYMD	–	AI-driven Materials Design: Recent Developments, Challenges and Perspectives
SYMS	–	Spins in Molecular Systems: Strategies and Effects of Hyperpolarization
SYQS	–	Nonequilibrium Collective Behavior in Open Classical and Quantum Systems
SYSD	–	SKM Dissertation Prize 2025

Organisation of the Exhibition of Scientific Instruments and Literature

DPG-Ausstellungs-, Kongreß- und Verwaltungsgesellschaft mbH
Hauptstraße 5, 53604 Bad Honnef

Phone	+49 (0)2224 9232-0
Email	info@dpg-gmbh.de
Website	www.dpg-gmbh.de

Programme

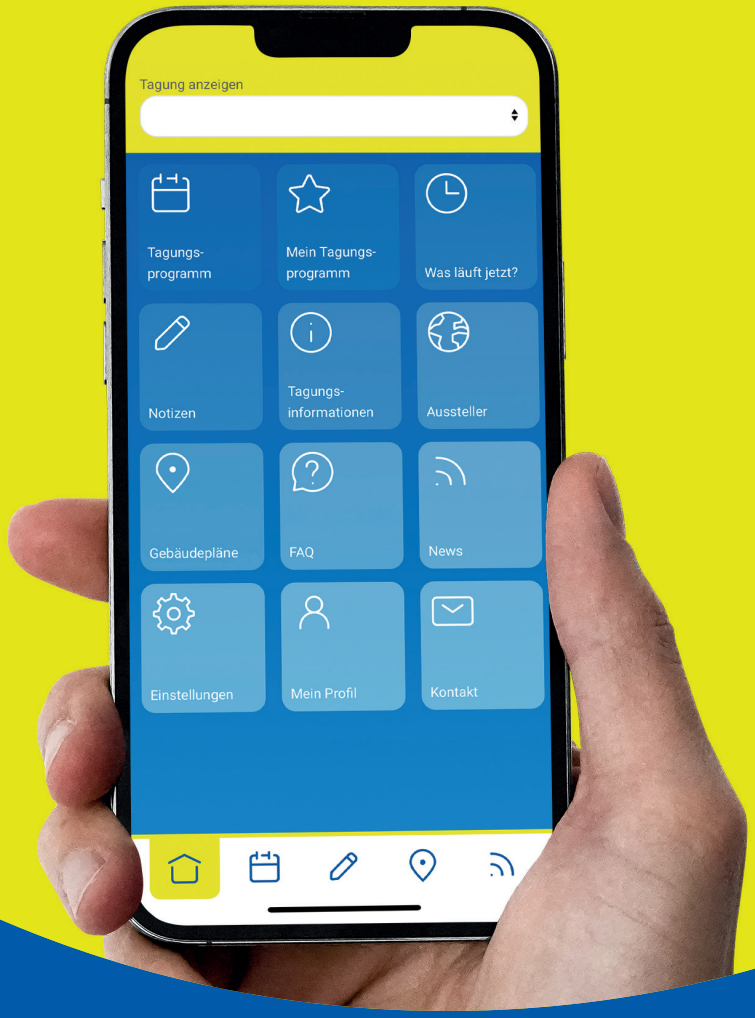
The scientific programme consists of **3,849** contributions:

11	Plenary Talks
1	Evening Talk
8	Prize Talks
1	Ceremonial Talk
5	Lunch Talks
215	Invited Talks
32	Topical Talks
2,368	Contributed Talks
14	Tutorials
1,192	Posters
2	Discussions

The programme stated in this document corresponds to the status from January 30, 2025. You will find the updated programme using the DPG App and at

www.dpg-verhandlungen.de/year/2025/conference/regensburg

DPG



Laden im App Store

JETZT BEI Google Play

Navigate the Spring Meeting with the DPG App!

The DPG app informs you about the conference programme, the venues and the exhibitors. Features such as your personal conference calendar and detailed floor plans simplify finding your way around the conference!

for iOS

for Android

Explore conference contributions on the new DPG Map.

CURRENTLY IN BETA

Dive into our network visualization and find related contributions.

Visit our platform at map.dpg-verhandlungen.de

Information for Participants

The conference will be held March 16 – 21, 2025

Conference Information

Conference Venue
University of Regensburg
Universitätsstraße 31
93053 Regensburg

The central activities will take place in the Main Lecture Hall (Audimax) of the University of Regensburg, Universitätsstraße 31, 93053 Regensburg. A detailed map of the campus and the buildings can be found at the end of this book. The location of the lecture halls on the Campus can be found in the DPG-App.

For visitors with reduced mobility and visitors with pushchairs, a detailed map with barrier-free routes and information on lifts, car parks and toilets is available: go.ur.de/barrier-free

Transportation
By car, train, plane or bus?
You will always find up-to-date directions for your journey on the website of the University of Regensburg as follows:

- Travel information of the University of Regensburg: go.ur.de/directions
- Parking at the University of Regensburg: go.ur.de/parking
- Further information and maps of the University of Regensburg: go.ur.de/maps

Conference Office / Information Desk
The conference office and information desk are located in the foyer of the Main Lecture Hall (foyer Audimax). The opening hours are:

		Registration	**Information Desk**
Sunday	March 16	15:00 – 19:00	12:00 – 20:00
Monday	March 17	07:30 – 18:00	07:30 – 22:00
Tuesday	March 18	08:00 – 17:00	08:00 – 20:00
Wednesday	March 19	08:00 – 17:00	08:00 – 22:00
Thursday	March 20	08:00 – 17:00	08:00 – 22:00
Friday	March 21	08:00 – 12:00	08:00 – 15:00

To contact the information desk during the opening hours call +49 (0)941-943 2530.

You will receive a receipt for your conference fee, the printed short programme, vouchers for food and drinks for the welcome evening, and your name tag at the conference office. **The name tag must be worn visibly during the entire conference**. Please note that the conference fee does not include a ticket for local public transport in Regensburg.

The organisers, the staff of the conference desk, and the student assistants will be identifiable by name tags and Φ-T-shirts in a uniform colour. Please contact them if you have any questions.

Do not hesitate to inquire about all necessary information concerning the conference, orientation in Regensburg, accommodation, restaurants, going out, and cultural events at the information desk located in the foyer of the Main Lecture Hall.

Allocation of the Lecture Halls

H1-H10, H22, H23	Main Lecture Hall Building
H11-H17	Law and Economy Building
H18-H20	Multi-purpose Building
H24-H25	Vielberth-Building
H31, H32	Mathematics Building
H33-H36	Physics Building
H37-H38	Pre-clinical Medicine Building
H43-H47	Chemistry and Pharmacy Building
Plenary talks, joint Symposia	H1 (Audimax), H2
Lunch Talks	H1, H2, H3, H4
Prize Ceremony, Evening Talk	H1 (Audimax)

Job Market	Kunsthalle (Foyer Audimax, 1st floor)
Registration Desk	Foyer Audimax (Main Lecture Hall)
Information Desk	Foyer Audimax (Main Lecture Hall)
Einstein Slam	H1 (Audimax)

WIFI & LAN

The University of Regensburg is member of the eduroam-network. Users from eduroam institutions, who have registered for eduroam, can use WIFI at the University of Regensburg without local registration in Regensburg. Please ask the computer center/network administration of your home institution for eduroam-registration. Eduroam in Regensburg is possible with WLAN SSID eduroam.

In addition to eduroam WIFI BayernWLAN is offered without prior registration. Furthermore you will have access with "StudiWLAN". Login required:
"RZ Account": dpg2025
"RZ Password": dpg2025

A few workstations for guests are available in the central library for emergencies. Please sign up directly at the information desk of the central library at th University of Regensburg! Opening hours: Mo-Fr 10:00 — 14:00.

Printing service

The „Print Gallery" printing company (Monday to Friday 10:00 — 18:00, Carl-Maria-von-Weber-Straße 6, 93053 Regensburg) offers prints up to DIN A0 format. You are welcome to send the data in PDF format with the exact details by email to: *info@printgallery.de*
It is not possible to print posters in DIN A0 format directly at the shop – the printing service needs 1 day in advance! The copy shop on the university forum has been closed unfortunately.

Presentations

Scientific presentations will be held either as oral presentations or posters. Presentations are held in English (preferred) or German.

Usually, presentations will have the following durations:

- For contributed talks a total of 15 minutes including discussion time and speaker change (12 min talk + 3 min discussion/speaker change).
- For invited talks a total of 30 minutes including discussion time and speaker change (25 min talk + 5 min discussion/speaker change).
- For plenary talks 45 minutes without discussion.

For further information on the language or length of the presentation, please contact the division or working group in which you have submitted your presentation.

PCs/laptops will be available in all lecture halls. **Therefore, the presentation should be recorded onto an USB stick as back-up in PDF and power point format.** Of course, you can also use your own laptop – please consider to bring your own adapter if required. All lecture rooms are equipped with projectors. The projectors mainly display in the 4:3 format. However they are compatible with the 16:9, limited to the display width. Some newer systems also work directly with 16:9. A majority of lecture halls offers radio microphone amplifiers as well. Overhead-Projectors are not available. Presenters and/or laser pointers will be available in all lecture rooms.

All lecture rooms will be opened, at the latest, 30 minutes prior to the lecture. Speakers must be in the lecture room at least 20 minutes before the sessions starts. They must report to the chairperson and the technical staff. They will receive an equipment introduction.

Poster Presentations

Sites for poster sessions are named and located as follows:

Poster area P1	Sammelgebäude (Multi-purpose Building)
Poster area P2	Physik (Physics)
Poster area P3	Exhibition tent in front of the Physics Building
Poster area P4	Chemie (Chemistry and Pharmacy)

The poster boards will be marked with the number according to the scientific programme. As there will be several different poster sessions at the poster sites every day, **authors are asked to mount their poster max. 1 hour before their session.** Each poster should display the number according to the scientific programme. Each poster should be no larger than 85 cm x 120 cm (A0 portrait format).

For the mounting of the poster please use the prepared "poster strips" (P1, P2, P4) or magnets (P3) at the poster frame (residue-free removing). You are also welcome to contact the student assistants on site.

Presenters are requested to be available at their poster for at least half of the length of their poster session. Please provide the information when you will be available at the poster. **The posters have to be removed after the session. Any posters remaining on display walls will be removed and disposed without requesting your permission.** The conference management accepts no liability for the posters.

Notice Board

The programme stated in this document is current as of 30 January 2025 and will not be updated!

All changes to the conference programme (i.e. cancellation of presentations, change of rooms, etc.) will be continuously updated on the notice board of the conference website. The information is identical to the programme updates of the scientific programme and is also available there in other formats (sorted by publication date, filterable by conference parts and as an rss-feed). Please use the form *regensburg25.dpg-tagungen.de/programm/notice-board* to notify changes or cancellations.

Cloakroom

Participants are asked to carefully watch their clothes, valuables, laptops, and other belongings. The organisers decline any liability. You will find a cloakroom in the basement of the Main Lecture Hall (Audimax). Please note that there is only limited possibility to store luggage! The opening hours are:

Sunday	March 16	14:00 — 19:30
Monday	March 17	07:00 — 22:30
Tuesday	March 18	07:30 — 19:00
Wednesday	March 19	07:30 — 21:00
Thursday	March 20	07:30 — 21:00
Friday	March 21	07:30 — 15:00

Lost and Found Property

Take your found items to the information desk in the foyer of the Audimax. You can also claim your lost property there.

Wilhelm and Else Heraeus Communication Programme

Important notes for participants who apply for a grant in the WEH Communication Programme:
At the beginning of the conference you will receive an identification form at the conference office. Your participation in the conference must be certified at the conference office. At the end of the conference, you may leave this certificate with DPG staff members at the conference office (preferably) or submit it to the DPG head office (DPG-Geschäftsstelle, Hauptstr. 5, 53604 Bad Honnef, Germany) by **April 18, 2025 at the latest.** For more detailed information refer to *weh.dpg-physik.de*.

The Deutsche Physikalische Gesellschaft thanks the Wilhelm und Else Heraeus-Stiftung for the generous financial support of young academic talents. We hope that young physicists will continue to benefit from the offered opportunity for active scientific communication at DPG meetings. A total of about 41,900 young academics were supported by this programme so far.

SAY CHEESE!

The DPG Spring Meetings are basically public to the press. Please note: On behalf of DPG, photos and videos will be recorded during the Spring Meetings. In the context of public relations, a selection of this footage will be published on our website, in social media or within printed materials of the DPG for example.

Tactfulness

All participants are requested to contribute to a successful and enjoyable conference through respect- and tactful behaviour. Please contact the conference office or the local conference organisers in the event of disturbances. §§ 9 and 12 of the DPG's Statutes are applicable.

CO_2 Compensation for the DPG Conferences

By decision of its council, the DPG will compensate for fossil CO_2 emissions resulting from mobility for DPG conferences and committee meetings.

Deutsche Physikalische Gesellschaft DPG

DPG-FRÜHJAHRSTAGUNG REGENSBURG 2025

Physik und Beruf

Jobbörse

in Kooperation mit Wiley VCH

Wo arbeiten Physiker:innen?

Di – Fr, 12:00 – 15:00 Uhr

Kunsthalle

Mehr Informationen auf Seite 15

Industrietag

Woran arbeiten Physiker:innen?

Mittwoch, 14:00 – 18:00 Uhr

H4

Mehr Informationen auf Seite 41

Industrieausstellung

Womit arbeiten Physiker:innen?

Di – Mi, 10:00 – 18:00 Uhr

ZHG-Foyer + Untergeschoss, ReWi, Zelt

Mehr Informationen auf Seite 16

Lunch Talks

Wie arbeiten Physiker:innen?

Mo – Do, 13:15 – 13:45 Uhr

H1 / H3 / H4

Mehr Informationen auf Seite 54

Bei den Angeboten von „Physik und Beruf“ sind alle Tagungsteilnehmende herzlich willkommen!

Acknowledgement
The Deutsche Physikalische Gesellschaft (DPG) and the local organisers want to thank the following institutions for supporting the conference:

- the Wilhelm and Else Heraeus Foundation, Hanau
- the University of Regensburg
- all industrial sponsors of the DPG-Frühjahrstagung (refer to page 18)
- and all staff, who make the success of the conference possible.

Disclaimer of liability
Participants are asked to look carefully after their wardrobe, valuables, laptops, and other belongings. The organisers decline any liability.

Catering
Free coffee, tea and water will be provided to all registered participants of the conference at DPG-coffee corners located near all exhibition and poster areas. All locations are displayed in the map of the campus at the end of this booklet. Please wear your name tag visibly during the entire conference.

Refreshments and snacks are also available in the cafeterias in the Multi-purpose Building and in the Buildings of Chemistry, Physics, Philosophy and Law (Monday-Friday). Please pay by your debit oder credit card. Cash Payment is not possible!

Mensa:
Lunch will be supplied in the Mensa of the University (Monday-Friday: 11:00 – 14:00). Prices: about 12.00 € including the meal, one drink and one dessert. Please pay by your EC- oder credit card. Cash Payment is not possible!

Tent
In the exhibition and poster tent in front of the physics department focaccia is offered by the Pizzeria UNIKAT at lunchtime (also vegetarian and vegan!).

Food-Truck:
In addition to the Mensa and the cafeterias, a Food truck ("Tommy's Mutzbraten") will offer hearty (= non-vegetarian) grilled food in front of the Physics Building (outside). Cash only!

Uni-Pizzeria:
The Pizzeria UNIKAT offers freshly made food. Reservation recommended!

Campus' Grocery Store
The Campus' Grocery Store "Hechtbauer" at the Forum offers food, beverages and convenience goods (Monday-Friday: 08:00 – 18:00).

Social Events

Tutorials
On Sunday, March 16, 16:00 – 18:15, there will be Tutorials on current scientific topics for interested conference participants, in particular for students and young scientists. All conference participants are welcome.

The topics of the Tutorials are:

- Hands-on Tutorial: AI Fundamentals for Research
- How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science
- Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism
- Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics
- Automated Workflows

Welcome Evening
Sunday, March 16, 18:30 – 21:30, Mensa
On Sunday evening, a Bavarian Welcome Evening will be held in the Mensa of the University of Regensburg to which all registered participants are kindly invited. Snacks and drinks will be served. "Vieraloa" (Bavarian Brass Music) will entertain you with music.

Do not miss the opportunity to register in the conference office (15:00 – 19:00) for the conference before the Welcome Evening as well as the official beginning of the conference. During check-in at the conference you will receive your badge and **food and drink vouchers** for the Welcome Evening (you will find these in the conference bag!). Please note that the cloakroom in the lecture hall basement closes on Sunday at 19:30!

Welcome Address
A short welcome address will be given by the chair of the Condensed Matter Section (SKM) on Monday, March 17 from 8:25 until 8:30 in lecture hall H1 (Audimax).

Einstein Slam
Monday, March 17, 20:00, H1 (Audimax)
Einstein Slam is the competitive art of making complex science accessible to a broad audience. There are just 10 minutes for every attendee to present his/her self-made performance. The event will finish with a public poll in order to evaluate if a particular contribution was either instructive and amusing or rather should have never been performed. All presentations will be given in English. For more information please refer to *www.einstein-slam.de*.

Climate Lounge
Tuesday, March 18, 14:00 – 16:00, H7
Following the lunchtime lecture PSV III '*The human task of climate change and the DPG: founding the Climate Working Group*', there will be the opportunity to exchange views on the topic in the 'Climate Lounge' with talks, questions and discussions.

Special Plenary Session with Award Ceremony
On Tuesday, March 18, at 16:00 the Ceremonial Session with Award Ceremony will take place in H1 (Audimax). The programme is as follows:

Music

Welcome
Prof. Dr. Christoph Strunk, Universität Regensburg
Local Organiser

Prof. Dr. Udo Hebel
President of the Universität Regensburg

Speech
Prof. Dr. Klaus Richter
President of the Deutsche Physikalische Gesellschaft

Music

Award Ceremony

Walter-Schottky-Prize 2025
to Dr. Libor Šmejkal, JGU Mainz / MPI für Physik komplexer Systeme, Dresden

Gaede-Prize 2025
to PD Dr. Wouter Jolie, Universität zu Köln

Dissertation Prize of the Condensed Matter Section 2025
(The Laureate will be announced at the award ceremony)

Ceremonial Lecture

Prof. Dr. Petra Schwille, Max-Planck-Institut für Biochemie, Martinsried
„How to build a biological cell from scratch" (PSV IV)

Prize Talks
The following prize talks will be given during the conference (in chronological order):

Gustav-Hertz-Prize 2025
Monday, March 17, 13:15 — 13:45, H2,
Dr. Anna Seiler, ETH Zürich, Switzerland
„Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene“ (PRV I)

Gustav-Hertz-Prize 2025
Tuesday, March 18, 13:15 — 13:45, H2,
Dr. Lisanne Sellies, IBM Research Europe — Zurich
„Single-molecule electron spin resonance by means of atomic force microscopy“ (PRV II)

Gentner-Kastler-Prize 2025
Wednesday, March 19, 13:15 — 13:45, H2
Prof. Dr. Regine von Klitzing, Technische Universität Darmstadt
„Complex liquids under confinement“ (PRV III)

Max-Born-Prize 2025
Wednesday, March 19, 13:15 — 13:45, H4
Prof. Michael Johnston, University of Oxford, United Kingdom
„Nanowire-based THz polarimetry“ (PVR IV)

Gaede-Prize 2025
Wednesday, March 19, 13:15 — 13:45, H4
PD Dr. Wouter Jolie, Universität zu Köln
„Confining strongly correlated quasiparticles in 2D semiconductors“ (PRV VI)

Walter-Schottky-Prize 2025
Thursday, March 20, 13:15 — 13:45, H2
Dr. Libor Šmejkal, JGU Mainz / MPI für Physik komplexer Systeme, Dresden
„Altermagnetism and spin symmetries“ (PRV V)

Georg-Simon-Ohm-Prize 2025
Thursday, March 20, 11:15, H15
Annika Janssen, Technische Hochschule Nürnberg
„Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules“

Physik: Erkenntnisse und Perspektiven — A Publication for Everyone (in German)!

The title “Physik: Erkenntnisse und Perspektiven” (Physics: Insights and Perspectives) refers to a publication, which was produced on a voluntary basis by almost 200 authors. It provides a detailed exploration of the fundamentals of physics, current research and future developments. The book offers readers an engaging and inspiring insight into the world of physics! The publication is also available at www.physik-erkenntnisse-perspektiven.de – along with exclusive video interviews. Printed copies can also be ordered by covering the shipping costs.

For interested readers: Experience the brand-new book live!
Join us for the book launch on Wednesday, 19 March 2025, from 13:15 to 13:45 (H3). You will have the opportunity to pick up a free copy – as long as stocks last!

Public Evening Lecture *(in German language)*
Wednesday, March 19, 19:00 – 20:15, Audimax (H1)
Prof. Dr. Thomas Jung, Alfred Wegener Institut, Bremerhaven, will speak about *„Leben in einer wärmer werdenden Welt: Wie der Klimawandel unser Leben beeinflusst”*.

The Public Evening Lecture is open for all conference participants and interested public. The entrance is free.

Job Market
During the conference, various companies and organisations will present their working fields and career opportunities to all interested participants. The presentations will last for about 30 minutes plus discussion and will take place in the Kunsthalle (Foyer Audimax, 1st floor). The Programme is as follows:

Tuesday, March 18

11:00 –12:00	**d-fine GmbH** *„Als Physiker:in in die Unternehmensberatung? Der Einsatz von MINT-Know-how zur Lösung komplexer Probleme in der Praxis bei d-fine.“*
13:00 – 14:00	**Carl Zeiss AG** *„Karrierechancen bei Carl Zeiss AG.“*
15:00 – 16:00	**ritzenhoefer & company** *„Transformation Consulting.“*

Wednesday, March 19

11:00 – 12:00	**Basycon Unternehmensberatung GmbH** *„Aus der Wissenschaft in die Beratung.“*

Thursday, March 20

11:00 – 12:30	**BCG – The Boston Consulting Group GmbH** *„Als Physiker:in in die Strategieberatung “*

Exhibition of Scientific Instruments and Literature

From Tuesday to Thursday there will be an exhibition of scientific instruments and literature in the Main Lecture Hall Foyer (A – Main Lecture Hall Foyer), in the Economy Building (E – “Wirtschaft und Recht”), and one tent (T – Tent in front of the Physics Building). Almost 100 companies (see list of exhibitors at the end of this booklet) will present their products. Opening hours are from 09:00 to 18:00. All conference participants are welcome to attend the exhibition. The entrance is free.

City Tours „Regensburg – Experience a Historic City“

Walking Tour
“Regensburg – Experience a Historic City“ (90 min; 14,00 € per person)
Meeting point: in front of the Tourist Information in the Old Town Hall of Regensburg
in German: daily 10:30, Tuesday March, 18 also at 16:30
in English: only on Tuesday, March 18, 16:30
Please register via e-mail *tourismus@regensburg.de*

Bus trip „CityTour“
Information and booking at *www.city-tour.info/en/regensburg/tour*

jDPG Pub Crawl

Tuesday, 18 March, 19:00 – 22:00

Meeting Point: “Kugel” (sculpture) at the Audimax (Albertus-Magnus-Straße 5)
In case you need some time to take a rest in the middle of the conference and you are looking for conversations beyond physics, the local group of the Young DPG cordially invites you to a pub crawl through the nightlife in Regensburg.

Members‘ Assemblies of the Divisions and Working Groups

During the DPG Spring Meeting, Members‘ Assemblies of the divisions and working groups take place. Please refer to the scientific programme for the time and place of the meetings.

Deutsche Physikalische Gesellschaft DPG

2nd DPG Fall Meeting

of the Deutsche Physikalische Gesellschaft

Quantum Physics

Topics:

- **Quantum Physics in Research and Technology**
- **The Path to the Modern Quantum World**
- **Applications of Quantum Technologies**

Joint Meeting of the

- **Atomic, Molecular, Quantum Optics and Photonics Section (SAMOP)**
- **Condensed Matter Section (SKM)**
- **Matter and Cosmos Section (SMuK)**

100 years ago, Göttingen played a central role in creating quantum physics as we know it today. In 1925 Werner Heisenberg, then an assistant at the Göttingen Institute for Theoretical Physics, published his famous article "Quantum-Theoretical Re-Interpretation of Kinematic and Mechanical Relations". This article marks the beginning of quantum mechanics and therefore the United Nations, the German Physical Society (DPG) and numerous Physical Societies around the world will celebrate 2025 as the "Year of Quantum Science and Technology".

The activities of the Quantum Year 2025 in Germany will culminate in an international conference in Göttingen (2nd DPG Fall Meeting, Sept. 8-12, 2025). The meeting will cover the present status and perspectives of all fields of modern physics reigned by quantum mechanics (condensed matter physics, atomic and molecular physics, quantum optics, elementary particle physics, quantum information and computing, and many others) as well as the historical roots of quantum mechanics and conceptual questions that still challenge us today.

Apart from high profile speakers covering all fields of modern physics there will be contributed sessions, all together creating a unique opportunity to look across the boundaries of individual research topics under the umbrella of quantum physics.

Save the Date!
8-12 Sep 2025

quantum25.dpg-tagungen.de

8-12 September 2025

Local and Scientific Organisers:

Prof. Dr. Stefan Kehrein
Institut für Theoretische Physik
Friedrich-Hund-Platz 1
37077 Göttingen

Prof. Dr. Thomas Weitz
I. Physikalisches Institut - Experimentalphysik
Friedrich-Hund-Platz 1
37077 Göttingen

Conference Venue:

Georg-August Universität Göttingen, Zentrales Hörsaalgebäude,
Platz der Göttinger Sieben 5, 37073 Göttingen

Abstract Submission: 31 March - 6 June 2025

Sponsors of the DPG Spring Meeting Regensburg

Premium Sponsor:

Main Sponsors (in alphabetical order):

Sponsors (in alphabetical order):

Synopsis of the Daily Programme

Sunday, March 16, 2025

TUT

			Sessions
16:00	H2	TUT 1	**Hands-on Tutorial: AI Fundamentals for Research**
16:00	H2	TUT 1.1	Introduction •Janine Graser
16:40	H2	TUT 1.2	Hands-On Session 1 – Function Approximation •Jan Bürger
17:30	H2	TUT 1.3	Hands-On Session 2 – Classification and More •Robin Msiska
16:00	H3	TUT 2	**Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science**
16:00	H3	TUT 2.1	FAIR-data management with the NOMAD infrastructure: Core functionalities •Joseph F. Rudzinski
16:30	H3	TUT 2.2	Using NOMAD's API for project management •Nathan Daelman
17:00	H3	TUT 2.3	Creating custom entries in NOMAD using yaml schema and ELN integration •Andrea Albino
17:30	H3	TUT 2.4	Creating custom workflow entries in NOMAD to link multiple uploads •Bernadette Mohr
16:00	H4	TUT 3	**Tutorial: Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism**
16:00	H4	TUT 3.1	3D Magnetic Imaging: Utilizing Synchrotron X-Ray Coherence for Nanometric Resolution in Thick Samples •Marisel Di Pietro Martinez
16:45	H4	TUT 3.2	Nanoscale Mapping of Magnetic Textures in 3D Using Vector Field Electron Tomography •Axel Lubk
17:30	H4	TUT 3.3	3D magnetic imaging: an experimental window to study 3D magnetization at the nanoscale •Aurelio Hierro-Rodriguez
16:00	H10	TUT 4	**Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics**
16:00	H10	TUT 4.1	Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange •Hiroshi Katsumoto
16:45	H10	TUT 4.2	Computing magnetic exchange interactions using DFT •Manuel dos Santos Dias
17:30	H10	TUT 4.3	Hands-on atomistic spin-dynamics simulations with Spirit •Thorben Pürling
16:00	H15	TUT 5	**Tutorial: Automated Workflows**
16:00	H15	TUT 5.1	Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations •Jörg Neugebauer

18:30	Mensa	**Welcome Evening** (for registered participants)

Monday, March 17, 2025

08:25	H1		**Welcome Address**

			Plenary Talks
08:30	H1	PLV I	Seeing dents in the atom •Franz Giessibl
14:00	H1	PLV II	High-power semiconductor lasers based on Hermitian and non-Hermitian control in photonic crystals •Susumu Noda
14:00	H2	PLV III	Physics informed artificial intelligence and data-driven design of materials •Jörg Neugebauer
			Prize Talk
13:15	H2	PRV I	Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene •Anna Seiler (Laureate of the Gustav-Hertz-Prize 2025)
			Discussion
13:15	H1	PSV I	Karriere auf Zeit: Perspektiven auf befristete Arbeitsverträge in der Wissenschaft •Carolin Wagner, •Axel Dürkop, •Raja Hoffmann

SYED

			Invited Talks
09:30	H1	SYED 1.1	Emergent crystalline order in a developing epithelium •Frank Jülicher
10:00	H1	SYED 1.2	A tissue rigidity phase transition shapes morphogen gradients •Nicoletta Petridou
10:30	H1	SYED 1.3	Building quantitative dynamical landscapes of developmental cell fate decisions •David Rand
11:15	H1	SYED 1.4	Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate •Anne Grapin-Botton
11:45	H1	SYED 1.5	Chromosomes as active communication and memory machines •Leonid A. Mirny
			Session
09:30	H1	SYED 1	Physics of Embryonic Development Across Scales: From DNA to Organisms

SYMD

			Invited Talks
15:00	H1	SYMD 1.1	Learning physically constrained microscopic interaction models of functional materials •Boris Kozinsky
15:30	H1	SYMD 1.2	GRACE universal interatomic potential for materials discovery and design •Ralf Drautz
16:00	H1	SYMD 1.3	Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction •Nong Artrith
16:45	H1	SYMD 1.4	Inverse Design of Materials •Hongbin Zhang
17:15	H1	SYMD 1.5	Data-Driven Materials Science •Miguel Marques
			Session
15:00	H1	SYMD 1	AI-driven Materials Design: Recent Developments, Challenges and Perspectives

Monday, March 17, 2025

SYSD

Invited Talks

09:30	H2	SYSD 1.1	Nanoscale Chemical Analysis of Ferroic Materials and Phenomena •Kasper Aas Hunnestad
10:00	H2	SYSD 1.2	Advanced Excitation Schemes for Semiconductor Quantum Dots •Yusuf Karli
10:30	H2	SYSD 1.3	Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors •Clemens Kuhlenkamp
11:00	H2	SYSD 1.4	Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics •Till Münker
11:30	H2	SYSD 1.5	Coherent Dynamics of Atomic Spins on a Surface •Lukas Veldman

Session

09:30	H2	SYSD 1	SKM Dissertation Prize Symposium

BP

Invited Talks

11:15	H44	BP 3.7	Killing to survive – how protein-lipid interactions drive programmed cell death •Kristyna Pluhackova
09:30	H46	BP 4.1	Spatiotemporal organization of bacterial biofilm formation and functions •Knut Drescher
15:00	H44	BP 7.1	Single-molecule dynamic structural biology with Graphene Energy Transfer •Philip Tinnefeld
16:15	H46	BP 8.6	In situ control of cells and multicellular structures at the microscale by two-photon lithography •Christine Selhuber-Unkel

Sessions

09:30	H37	BP 2	Active Matter I
09:30	H44	BP 3	Computational Biophysics I
09:30	H46	BP 4	Bacterial Biophysics
11:30	H46	BP 5	Membranes and Vesicles I
15:00	H37	BP 6	Active Matter II
15:00	H44	BP 7	Single Molecule Biophysics
15:00	H46	BP 8	Biomaterials, Biopolymers and Bioinspired Functional Materials I
17:00	H46	BP 9	Biomaterials, Biopolymers and Bioinspired Functional Materials II

CPP

Invited Talks

09:30	H34	CPP 1.1	Impact of smallest loops and composition Fluctuations on the structure of end-linked polymer model networks •Michael Lang
11:30	H38	CPP 5.1	Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via ab initio spectroscopy simulations •Daniel Sebastiani
15:00	H38	CPP 8.1	The Nanoscale Photovoltaics Laboratory on a Tip •Stefan Weber

Sessions

09:30	H34	CPP 1	Gels, Polymers Networks and Elastomers I
09:30	H37	CPP 2	Active Matter I
09:30	H38	CPP 3	Organic Electronics and Photovoltaics I
11:30	H34	CPP 4	Crystallization, Nucleation and Self-Assembly I
11:30	H38	CPP 5	Composites and Functional Polymer Hybrids
15:00	H34	CPP 6	Gels, Polymers Networks and Elastomers II

Monday, March 17, 2025

CPP

15:00	H37	CPP 7	Active Matter II
15:00	H38	CPP 8	Hybrid and Perovskite Photovoltaics I
15:00	H46	CPP 9	Biomaterials and Biopolymers
16:15	H34	CPP 10	Wetting, Fluidics and Liquids at Interfaces and Surfaces I
16:15	H38	CPP 11	Hybrid and Perovskite Photovoltaics II
17:00	H46	CPP 12	Biomaterials, Biopolymers and Bioinspired Functional Materials I
17:15	H38	CPP 13	Molecular Electronics and Excited State Properties I
17:30	H34	CPP 14	Wetting, Fluidics and Liquids at Interfaces and Surfaces II
19:00	P4	CPP 15	Poster Session I

DS

Sessions

09:30	H3	DS 1	Thin Film Properties
09:30	H14	DS 2	Layer Deposition
15:00	H3	DS 3	2D Materials and their Heterostructures I

DY

Invited Talks

10:45	H37	DY 3.6	Collective behavior of photoactive macroscopic particles •Iker Zuriguel
09:45	H43	DY 4.2	Physical application of infinite ergodic theory •Eli Barkai
11:30	H43	DY 4.7	Modelling the movements of organisms: Movement ecology meets active particles and anomalous diffusion •Rainer Klages
15:00	H43	DY 8.1	Spatio-temporal pattern formation in time-delayed optical systems •Svetlana Gurevich
16:45	H43	DY 8.6	Nonlinear dynamics and time delays in metal cutting •Andreas Otto
16:00	H47	DY 9.5	Large-deviation simulations of non-equilibrium stochastic processes •Alexander K. Hartmann

Sessions

09:30	H31	DY 2	Nonequilibrium Quantum Systems
09:30	H37	DY 3	Active Matter I
09:30	H43	DY 4	Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications I
09:30	H47	DY 5	Statistical Physics: General
11:30	H47	DY 6	Critical Phenomena and Phase Transitions
15:00	H37	DY 7	Active Matter II
15:00	H43	DY 8	Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications II
15:00	H47	DY 9	Statistical Physics far from Thermal Equilibrium
16:15	H34	DY 10	Wetting, Fluidics and Liquids at Interfaces and Surfaces I
17:30	H34	DY 11	Wetting, Fluidics and Liquids at Interfaces and Surfaces II

HL

Invited Talks

09:30	H17	HL 3.1	Alexandria Database – Improving machine-learning models in materials science through large datasets •Jonathan Schmidt
10:00	H17	HL 3.2	Generative Models on the Rise – Which one shall I pick for my Inverse Design Problem? •Hanna Türk
10:30	H17	HL 3.3	Machine-learning accelerated prediction of two-dimensional conventional superconductors •Haichen Wang

Monday, March 17, 2025

HL

11:15	H17	HL 3.4	Machine Learning for Design, Understanding, and Discovery of (Semiconducting) Materials •Pascal Friederich
11:45	H17	HL 3.5	OptiMate: Artificial intelligence for optical spectra •Malte Grunert
			Sessions
09:30	H13	HL 1	Perovskite and Photovoltaics I
09:30	H15	HL 2	2D Semiconductors and van der Waals Heterostructures I
09:30	H17	HL 3	Focus Session: Machine Learning of semiconductor properties and spectra
15:00	H3	HL 4	2D Materials and their Heterostructures I
15:00	H11	HL 5	2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction
15:00	H13	HL 6	Materials and Devices for Quantum Technology I
15:00	H14	HL 7	Semiconductor Lasers
15:00	H15	HL 8	2D Semiconductors and van der Waals Heterostructures II
15:00	H17	HL 9	Oxide Semiconductors I
15:00	H19	HL 10	Spin-Dependent Phenomena in 2D
16:00	H14	HL 11	Ultra-fast Phenomena I
16:45	H15	HL 12	Quantum Transport and Quantum Hall Effects
16:45	H17	HL 13	Heterostructures, Interfaces and Surfaces

KFM

			Invited Talk
09:30	H9	KFM 1.1	Epitaxial films of layered perovskite-based ferroelectrics: phase stability, polarization enhancement, and pathways to polar metallicity •Elzbieta Gradauskaite
			Sessions
09:30	H9	KFM 1	(Multi)ferroic States: From Fundamentals to Applications (I)
09:30	H13	KFM 2	Perovskite and Photovoltaics I
09:30	H16	KFM 3	Multiferroics and Magnetoelectric Coupling
11:30	H9	KFM 4	(Multi)ferroic States: From Fundamentals to Applications (II)
15:00	H9	KFM 5	Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons
15:00	H10	KFM 6	Invited Talk: X. Fang
17:15	H22	KFM 7	Materials for the Storage and Conversion of Energy

MA

			Invited Talks
09:30	H20	MA 5.1	Driving Coherent Phonon-Phonon Angular Momentum Transfer via Lattice Anharmonicity •Sebastian Maehrlein
10:00	H20	MA 5.2	Chiral phonons, phono-magnetism, and spin-rotation coupling •Matthias Geilhufe
10:30	H20	MA 5.3	Geometry of temporal chiral structures and photoinduced chirality-spin coupling •Olga Smirnova
11:15	H20	MA 5.4	Phonon thermal Hall effect •Kamran Behnia
11:45	H20	MA 5.5	Giant effective magnetic moment of chiral phonons •Swati Chaudhary
15:00	H16	MA 6.1	Magnetization dynamics of chiral helimagnetic insulators •Aisha Aqeel
15:00	H18	MA 7.1	Realizing Reservoir Computing with skyrmions in geometrical confinements tuned by ion irradiation •Grischa Beneke
15:20	H18	MA 7.2	Low-energy spin excitations of the Kitaev candidate material $Na_2Co_2TeO_6$ probed by high-field/high-frequency electron spin resonance spectroscopy •Luca Bischof

MA

15:40	H18	MA 7.3	Tailoring the first-order magnetostructural phase transition in Ni-Mn-Sn for caloric applications by microstructure •Johannes Puy
16:15	H18	MA 7.4	Tuning the properties of two-dimensional magnetic heterostructures via interface engineering with molecular and inorganic van der Waals crystals. •Carla Boix-Constant
16:40	H18	MA 7.5	Theoretical Prediction for Probing Magnon Topology •Robin R. Neumann
17:05	H18	MA 7.6	Multiphysics-Multiscale Simulation of Additively Manufactured Functional Materials •Yangyiwei Yang

Sessions

09:30	H16	MA 2	Multiferroics and Magnetoelectric Coupling
09:30	H18	MA 3	Magnonics I
09:30	H19	MA 4	Electron Theory of Magnetism and Correlations
09:30	H20	MA 5	Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I
15:00	H16	MA 6	Skyrmions I
15:00	H18	MA 7	INNOMAG e.V. Prizes 2025 (Diplom-/Master and Ph.D. Thesis)
15:00	H19	MA 8	Spin-Dependent Phenomena in 2D
15:00	H20	MA 9	Altermagnets I

MM

Invited Talks

09:30	H10	MM 2.1	Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations •Roger De Souza
15:00	H10	MM 5.1	Room-temperature dislocations in oxide ceramics: from understanding to active engineering •Xufei Fang

Sessions

09:30	H10	MM 2	Invited Talk: R. de Souza
10:15	H10	MM 3	Data-driven Materials Science: Big Data and Worksflows
10:15	H22	MM 4	Materials for the Storage and Conversion of Energy
15:00	H10	MM 5	Invited Talk: X. Fang
15:45	H10	MM 6	Phase Transformations
15:45	H22	MM 7	Materials for the Storage and Conversion of Energy
17:15	H22	MM 8	Materials for the Storage and Conversion of Energy
18:30	P1	MM 9	Poster

O

Invited Talks, Topical Talk

09:30	H24	O 3.1	Insights in real and electronic structure of interfaces by electron microscopy •Kerstin Volz
11:15	H11	O 7.4	Nanoimaging the electronic, plasmonic, and phononic structure and dynamics of 2D materials •Sarah King
10:30	H24	O 8.1	Chiral reactions at surfaces elucidated by machine learning and enhanced sampling •Daniele Passerone
15:00	H2	O 10.1	Probing coherent optical emission processes with ultrafast scanning electron microscopy •Albert Polman
16:15	H2	O 10.5	Ultrafast exciton dynamics in momentum space •Ralph Ernstorfer

Monday, March 17, 2025

O

15:00	H24	O 15.1	Kondo and Yu-Shiba-Rusinov resonances: transport and coupling •Laëtitia Farinacci
15:30	H24	O 15.2	Electron delocalization in a 2D Mott insulator •Amadeo L. Vazquez de Parga
16:00	H24	O 15.3	Kondo or no Kondo, that is the question •Alexander Weismann
16:30	H24	O 15.4	Evidence for spinarons in Co atoms on noble metal (111) surfaces •Artem Odobesko
17:00	H24	O 15.5	Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures •Samir Lounis

Sessions

09:30	H24	O 3	Overview Talk Kerstin Volz
10:30	H4	O 4	Solid-Liquid Interfaces: Structure
10:30	H6	O 5	Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale I
10:30	H8	O 6	Oxides and Insulator Surfaces: Structure, Epitaxy and Growth
10:30	H11	O 7	Focus Session Ultrafast Electron Microscopy at the Space-Time Limit I
10:30	H24	O 8	Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation I
10:30	H25	O 9	Surface Reactions
15:00	H2	O 10	Focus Session Ultrafast Electron Microscopy at the Space-Time Limit II
15:00	H4	O 11	Electronic Structure of Surfaces: Spectroscopy, Surface States I
15:00	H6	O 12	Nanostructures at Surfaces I
15:00	H8	O 13	Organic Molecules on Inorganic Substrates: Adsorption and Growth
15:00	H11	O 14	2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction
15:00	H24	O 15	Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond
15:00	H25	O 16	Scanning Probe Techniques: Method Development
18:00	P2	O 17	Poster Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation
18:00	P2	O 18	Poster Focus Session Ultrafast Electron Microscopy at the Space-Time Limit
18:00	P2	O 19	Poster Surface Magnetism
18:00	P2	O 20	Poster Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale
18:00	P2	O 21	Poster Heterogeneous Catalysis
18:00	P2	O 22	Poster Surface Reactions
18:00	P2	O 23	Poster Ultrafast Electron Dynamics
18:00	P2	O 24	Poster Scanning Probe Techniques: Method Development

SOE

Prize Talk, Invited Talk

15:00	H45	SOE 1.1	Interplay between multiscaling and rough volatility •Tiziana Di Matteo
16:30	H45	SOE 2.1	Higher-order network science •Federico Battiston (Laureate of the Young Scientist Award for Socio- and Econophysics2025)

Sessions

15:00	H45	SOE 1	Econophysics
16:15	H45	SOE 2	Award Session: Young Scientist Award for Socio- and Econophysics (YSA)
17:30	P4	SOE 3	Poster

TT

Sessions

09:30	H20	TT 1	Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I
09:30	H31	TT 2	Nonequilibrium Quantum Systems

Monday, March 17, 2025

O

09:30	H32	TT 3	Correlated Magnetism – General
09:30	H33	TT 4	Topological Insulators
09:30	H36	TT 5	Superconductivity: Properties and Electronic Structure I
15:00	H24	TT 6	Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond
15:00	H31	TT 7	Correlated Electrons: Electronic Structure Calculations
15:00	H32	TT 8	Measurement Technology and Cryogenics
15:00	H33	TT 9	Correlated Magnetism – Low-Dimensional Systems
15:00	H36	TT 10	Topological Semimetals
15:00	P4	TT 11	Superconductivity: Poster
16:45	H15	TT 12	Quantum Transport and Quantum Hall Effects

20:00	H1		**Einstein Slam**

Tuesday, March 18, 2025

Plenary Talk

08:30	H1	PLV IV	Some new aspects of unconventional superconductivity in layered materials •Irina Grigorieva

Prize Talk

13:15	H2	PRV II	Single-molecule electron spin resonance by means of atomic force microscopy •Lisanne Sellies (Laureate of the Gustav-Hertz-Prize 2025)

Lunch Talks

13:15	H1	PSV II	Research Funding by the DFG – Funding of Coordinated Programmes •Christian Hahn
13:15	H4	PSV III	Menschheitsaufgabe Klimawandel und die DPG: Gründung der AG Klima •Gregor Schaumann

Ceremonial Session with Award Ceremony and Ceremonial Talk

16:00	H1	PSV IV	How to build a biological cell from scratch •Petra Schwille

SYIS

Invited Talks

09:30	H1	SYIS 1.1	Electron-phonon and exciton-phonon coupling in advanced materials •Claudia Draxl
10:00	H1	SYIS 1.2	Exciton-phonon dynamics from first principles •Enrico Perfetto
10:30	H1	SYIS 1.3	Polarons and exciton polarons from first principles •Feliciano Giustino
11:15	H1	SYIS 1.4	Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors •Alexander Steinhoff
11:45	H1	SYIS 1.5	Phonon influence on (cooperative) photon emission from quantum dots •Erik Gauger

Session

09:30	H1	SYIS 1	Progress and Challenges in Modelling Electron-Phonon Interaction in Solids

BP

Invited Talks

09:30	H44	BP 11.1	Network connectivity determines the mechanisms responsible for cytoskeletal elasticity •Martin Lenz
11:45	H44	BP 15.1	Does Oncology Need Physics of Cancer? •Josef Käs

Sessions

09:30	H43	BP 10	Focus Session: Nonlinear Dynamics in Biological Systems I
09:30	H44	BP 11	Cytoskeleton
09:30	H46	BP 12	Biomaterials, Biopolymers and Bioinspired Functional Materials III
09:30	H47	BP 13	Active Matter III
10:00	P3	BP 14	Poster Session I
11:45	H44	BP 15	Cell Mechanics I
14:00	H43	BP 16	Focus Session: Nonlinear Dynamics in Biological Systems II
18:00	P4	BP 17	Poster Session II

Tuesday, March 18, 2025

CPP

Invited Talks

09:30	H34	CPP 16.1	Multifunctional structural batteries •Göran Lindbergh
09:30	H38	CPP 17.1	Continuum models for water's peculiar behavior on the nanoscale •Alexander Schlaich
09:30	H46	CPP 18.1	Hybrid materials from colloidally stable nanocellulose and nanoparticles – scattering techniques are needed for characterization •Eva Malmström
11:30	H38	CPP 20.1	Tailored polymer thin films enabled by initiated chemical vapor deposition (iCVD): From fundamentals to functional applications •Stefan Schröder

Sessions

09:30	H34	CPP 16	Energy Storage and Batteries I
09:30	H38	CPP 17	Modeling and Simulation of Soft Matter I
09:30	H46	CPP 18	Biomaterials, Biopolymers and Bioinspired Functional Materials II
09:30	H47	CPP 19	Active Matter III
11:30	H38	CPP 20	Interfaces and Thin Films I
14:00	H34	CPP 21	Modeling and Simulation of Soft Matter II
14:00	H38	CPP 22	Organic Electronics and Photovoltaics II

DS

Invited Talk

09:30	H3	DS 4.1	Graphene-based epitaxial 2D heterosystems: making graphene great again •Christoph Tegenkamp

Sessions

09:30	H3	DS 4	2D Materials and their Heterostructures II
14:00	H3	DS 5	Thin Oxides and Oxide Layers

DY

Invited Talks

09:30	H43	DY 14.1	Robust signal amplification and information integration via self-tuned proximity to bifurcation points •Isabella Graf
11:30	H43	DY 14.7	Beyond the connectionist view: (De-)synchronizing neural networks via cell-intrinsic dynamics •Susanne Schreiber
10:45	H47	DY 15.6	Beyond spheres – active matter in new shapes •Juliane Simmchen
12:30	H47	DY 15.11	Emergent correlations and boundary fluctuations in epithelial cell sheets •Silke Henkes
14:00	H43	DY 17.1	Mechanistic origins of temperature scaling in the early embryonic cell cycle •Lendert Gelens

Sessions

09:30	H31	DY 12	Quantum Coherence and Quantum Information Systems
09:30	H37	DY 13	Many-body Quantum Dynamics I
09:30	H43	DY 14	Focus Session: Nonlinear Dynamics in Biological Systems I
09:30	H47	DY 15	Active Matter III
14:00	H37	DY 16	Many-body Systems: Equilibration, Chaos, and Localization
14:00	H43	DY 17	Focus Session: Nonlinear Dynamics in Biological Systems II
14:00	H47	DY 18	Pattern Formation

Tuesday, March 18, 2025

HL

Invited Talks

09:30	H17	HL 18.1	Ultrafast Nano-Spectroscopy of Photo-Induced Dynamics in Low-Dimensional Materials •Takashi Kumagai
10:00	H17	HL 18.2	Landau level Nanoscopy of charge and heat transport in low-dimensional heterostructures •Mengkun Liu
10:30	H17	HL 18.3	Real space mapping of electrically tunable anisotropic THz plasmon polaritons in hBN encapsulated black phosphorus •Eva Pogna
11:15	H17	HL 18.4	Ultra-confined THz hyperbolic phonon polaritons in a transition metal dichalcogenide •Alexander Paarmann
11:45	H17	HL 18.5	Programmable polariton nanophotonics using phase-change materials •Thomas Taubner

Sessions

09:30	H3	HL 14	2D Materials and their Heterostructures II
09:30	H13	HL 15	Quantum Dots and Wires: Growth and Properties
09:30	H14	HL 16	Organic Semiconductors
09:30	H15	HL 17	2D Semiconductors and van der Waals Heterostructures III
09:30	H17	HL 18	Focus Session: Nanoscale Light-matter Interaction I
09:30	H36	HL 19	Focus Session: Strongly Correlated Quantum States in Moire Heterostructures
10:00	P3	HL 20	Poster I
10:30	H6	HL 21	Graphene: Electronic Structure and Excitations
10:30	H8	HL 22	2D Materials: Electronic Structure and Exitations I
11:15	H13	HL 23	Quantum Dots and Wires: Transport
12:15	H14	HL 24	Thermal Properties
13:30	P3	HL 25	Poster 2D Materials: Electronic Structure and Exitations
13:30	P3	HL 26	Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction
13:30	P3	HL 27	Poster 2D Materials: Stacking and Heterostructures
14:00	H16	HL 28	Topological Insulators
18:00	P1	HL 29	Poster II

KFM

Invited Talk

09:30	H9	KFM 8.1	Ferrolectric bubble currents •Hugo Aramberri

Sessions

09:30	H9	KFM 8	(Multi)ferroic States: From Fundamentals to Applications (III)
11:45	H9	KFM 9	(Multi)ferroic States: From Fundamentals to Applications (IV)
14:00	H22	KFM 10	Materials for the Storage and Conversion of Energy

MA

Sessions

09:30	H16	MA 10	Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II
09:30	H18	MA 11	Spin Transport and Orbitronics, Spin-Hall Effects I
09:30	H19	MA 12	Magnetization Dynamics and Damping
09:30	H20	MA 13	Altermagnets II
09:30	H36	MA 14	Focus Session: Strongly Correlated Quantum States in Moire Heterostructures
10:00	P1	MA 15	Poster I
14:00	H16	MA 16	Topological Insulators
14:00	H18	MA 17	Micro- and Nanostructured Magnetic Materials
14:00	H19	MA 18	Functional Antiferromagnetism
14:00	H20	MA 19	Magnetic Imaging and Sensors

Tuesday, March 18, 2025

MM

Topical Talks

09:30	H10	MM 10.1	Understanding the impact of disconnection flow on microstructure evolution •Marco Salvalaglio
10:15	H10	MM 11.1	The role of disconnections in the shear-migration coupling of grain boundaries •Marc Legros
11:30	H10	MM 11.4	Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics •Fadi Abdeljawad
12:30	H10	MM 11.7	Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling •Helene Zapolsky
14:00	H10	MM 13.1	Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles •Eugen Rabkin

Sessions

09:30	H10	MM 10	Topical Talk: M. Salvalaglio
10:15	H10	MM 11	Topical Session: Defects of Defects
10:15	H22	MM 12	Materials for the Storage and Conversion of Energy
14:00	H10	MM 13	Topical Session: Defects of Defects
14:00	H22	MM 14	Materials for the Storage and Conversion of Energy

O

Invited Talks, Topical Talk

09:30	H24	O 25.1	Exploring quantum physics with scanning probe methods •Jörg Kröger
10:30	H2	O 26.1	Attosecond Electron Microscopy •Peter Baum
12:00	H4	O 27.7	Ultrafast electrochemistry beyond the RC time constant •Yujin Tong
11:30	H11	O 30.5	Resonant molecular transitions in femtosecond second harmonic generation spectroscopy of Fe-porphyrin/Cu(001) •Andrea Eschenlohr
11:00	H24	O 31.3	Single molecule machines on surface •Francesca Moresco

Sessions

09:30	H24	O 25	Overview Talk Jörg Kröger
10:30	H2	O 26	Focus Session Ultrafast Electron Microscopy at the Space-Time Limit III
10:30	H4	O 27	Solid-Liquid Interfaces: Reactions and Electrochemistry I
10:30	H6	O 28	Graphene: Electronic Structure and Excitations
10:30	H8	O 29	2D Materials: Electronic Structure and Exitations I
10:30	H11	O 30	Surface Magnetism
10:30	H24	O 31	Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II
10:30	H25	O 32	Heterogeneous Catalysis I
13:30	P3	O 33	Poster Graphene: Electronic Structure and Excitations
13:30	P3	O 34	Poster Solid-Liquid Interfaces: Reactions and Electrochemistry
13:30	P3	O 35	Poster Solid-Liquid Interfaces: Structure
13:30	P3	O 36	Poster 2D Materials: Electronic Structure and Exitations
13:30	P3	O 37	Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction
13:30	P3	O 38	Poster 2D Materials: Stacking and Heterostructures
14:00	H4	O 39	Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules I
14:00	H6	O 40	Surface Dynamics
14:00	H8	O 41	Heterogeneous Catalysis II
14:00	H11	O 42	Electron-driven Processes
14:00	H24	O 43	Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale II
18:00	P2	O 44	Poster Oxides and Insulator Surfaces: Structure, Epitaxy and Growth

Tuesday, March 18, 2025

O

18:00	P2	O 45	Poster Spins on Surfaces at the Atomic Scale
18:00	P2	O 46	Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties
18:00	P2	O 47	Poster Electron-driven Processes
18:00	P2	O 48	Poster Surface Dynamics
18:00	P2	O 49	Poster Nanostructures at Surfaces
18:00	P2	O 50	Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth
18:00	P2	O 51	Poster Electronic Structure of Surfaces: Spectroscopy, Surface States
18:00	P2	O 52	New Methods: Experiment
18:00	P2	O 53	Poster Electronic Structure Theory
18:00	P2	O 54	Poster New Methods: Theory
18:00	P2	O 55	Poster Topology and Symmetry-protected Materials

SOE

Invited Talks

09:30	H45	SOE 4.1	Urban scaling and conflicting goals •Diego Rybski
14:00	H45	SOE 6.1	Analyzing Political Regime Stability Through the Diffusion Equation: Insights from V-Dem Data (1900-2021) •Karoline Wiesner

Sessions

09:30	H45	SOE 4	Urban systems, Scaling, and Social Systems
12:15	H45	SOE 5	Agent-Based Modeling
14:00	H45	SOE 6	Political Systems and Conflicts

TT

Invited Talk, Topical Talks

09:30	H31	TT 15.1	Solving Many-Body Problems on Quantum Computers •Benedikt Fauseweh
09:30	H36	TT 18.1	The Thermoelectric Effect and Its Natural Heavy Fermion Explanation in Twisted Bilayer and Trilayer Graphene •Bogdan Andrei Bernevig
10:00	H36	TT 18.2	Angle-Tuned Chiral Phase Transition in Twisted Bilayer Graphene •Laura Classen
10:30	H36	TT 18.3	Quantum Optics of Semiconductor Moire Materials •Atac Imamoglu
11:15	H36	TT 18.4	Probing the Band Structures of Multilayer Graphene Using the Quantum Twisting Microscope •Martin Lee
11:45	H36	TT 18.5	Gate-Tunable Bose-Fermi Mixture in a Strongly Correlated Moiré Bilayer Electron System •Nathan Wilson

Sessions

09:30	H16	TT 13	Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II
09:30	H18	TT 14	Spin Transport and Orbitronics, Spin-Hall Effects I
09:30	H31	TT 15	Quantum Coherence and Quantum Information Systems
09:30	H32	TT 16	Superconductivity: Properties and Electronic Structure II
09:30	H33	TT 17	Correlated Electrons: Method Development
09:30	H36	TT 18	Focus Session: Strongly Correlated Quantum States in Moiré Heterostructures
09:30	H37	TT 19	Many-body Quantum Dynamics I
10:30	H8	TT 20	2D Materials: Electronic Structure and Exitations I
11:15	H13	TT 21	Quantum Dots and Wires: Transport
14:00	H37	TT 22	Many-body Systems: Equilibration, Chaos, and Localization
14:15	H33	TT 23	Members' Assembly

Tuesday, March 18, 2025

AKPIK

			Invited Talks
11:00	H5	AKPIK 3.1	3D Integration Towards Autonomous Optical Neural Networks •Adrià Grabulosa
14:00	H5	AKPIK 4.1	The Scaling of Intelligence: From Transformers to Agentic AI •Oliver Mey
14:30	H5	AKPIK 4.2	Inverse Design in Electromagnetics with Artificial Intelligence •Willie Padilla
15:00	H5	AKPIK 4.3	Inverse design of lateral hybrid metasurfaces with machine learning •Rui Fang
			Sessions
09:30	H5	AKPIK 2	Machine Learning Prediction and Optimization Tasks
11:00	H5	AKPIK 3	Research with AI: Hardware, Software, Tools
14:00	H5	AKPIK 4	Focus: Applications of Deep Neural Networks

09:00	Foyer Audimax, H6, Economy Bldg., Tent	**Exhibition of Scientific Instruments and Literature** (free entrance)

		Job Market
11:00	Kunsthalle	d-fine GmbH: *"Von der Kosmologie in die Beratung"*
13:00	Kunsthalle	Carl Zeiss AG: *„Karrierechancen bei Carl Zeiss AG"*
15:00	Kunsthalle	ritzenhoefer & company: *"Transformation Consulting"*

19:00	"Kugel" am Audimax	**jDPG Pub Crawl**

Wednesday, March 19, 2025

Plenary Talks

08:30	H1	PLV V	Ultrafast magnetism – terra incognita beyond the classical approximations •Alexey Kimel
14:00	H1	PLV VI	Topological spin-textures – from domain walls to Hopfions: Current innovations and future challenges •Stefan Blügel
14:00	H2	PLV VII	Variance sum rule for dissipative systems •Felix Ritort

Prize Talks

13:15	H2	PRV III	Complex liquids under confinement •Regine von Klitzing (Laureate of the Gentner-Kastler-Prize 2025)
13:15	H4	PRV IV	Nanowire-based THz polarimetry •Michael Johnston (Laureate of the Max-Born-Prize 2025)

Lunch Talk, Discussion

13:15	H1	PSV V	Career Paths: Academia or Industry? •Adelind Elshani, •Jan Wilhelm, •Valentin Kahl
13:15	H3	PSV VI	Book Launch – Physik: Erkenntnisse und Perspektiven (in German) •Sarah Köster, •Lutz Schröter

SYFD

Invited Talks

09:30	H1	SYFD 1.1	Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight •Astrid Schneidwind
10:00	H1	SYFD 1.2	Establishing Workflows of Experimental Solar Cell Data into NOMAD •Eva Unger
10:30	H1	SYFD 1.3	Building up the EOSC Federation •Ute Gunsenheimer
11:15	H1	SYFD 1.4	Data-Driven Materials Science for Energy-Sustainable Applications •Jacqueline Cole
11:45	H1	SYFD 1.5	Machine Learning and FAIR Data in X-ray Surface Science •Stefan Kowarik

Session

09:30	H1	SYFD 1	Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights

SYMS

Invited Talks

15:00	H1	SYMS 1.1	Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer •Christoph Boehme
15:30	H1	SYMS 1.2	The puzzle of spin and charge transport in the chirality induced spin selectivity effect •Bart van Wees
16:00	H1	SYMS 1.3	Nano- and Microscale NMR spectroscopy with spin qubits in diamond •Nabeel Aslam
16:45	H1	SYMS 1.4	Spin effects in adsorbed organometallic complexes •Richard Berndt
17:15	H1	SYMS 1.5	Quantum Computing with Molecules •Mario Ruben

Session

15:00	H1	SYMS 1	Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Wednesday, March 19, 2025

BP

Invited Talks

09:30	H44	BP 18.1	Mechanical Imprints of Cell Competition •Benoit Ladoux
11:30	H46	BP 19.8	Rolling vesicles: From confined rotational flows to surface-enabled motion •Laura R. Arriaga
16:30	H44	BP 20.6	Centrosome positioning in cell migration and immune response •Heiko Rieger
15:00	H46	BP 22.1	From DNA Nanotechnology to biomedical insight: Towards single-molecule spatial omics •Ralf Jungmann

Sessions

09:30	H44	BP 18	Tissue Mechanics
09:30	H46	BP 19	Membranes and Vesicles II
15:00	H44	BP 20	Statistical Physics of Biological Systems I
15:00	H45	BP 21	Networks, From Topology to Dynamics
15:00	H46	BP 22	Bioimaging
18:00	P2	BP 23	Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure
18:15	H46	BP 24	Members' Assembly

CPP

Invited Talks

09:30	H34	CPP 23.1	Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties •Manfred Wilhelm
11:30	H34	CPP 26.1	Polyelectrolytes in the confined space of mesopores for transport regulation •Annette Andrieu-Brunsen
16:15	H34	CPP 30.1	Challenges and Opportunities in Bringing Machine Learning to a Synchrotron •Alexander Hexemer
16:15	H38	CPP 31.1	Moving with minimum effort – Optimal work protocols for systems with memory •Sarah Loos

Sessions

09:30	H34	CPP 23	Polymer and Molecular Dynamics, Friction and Rheology
09:30	H38	CPP 24	Hybrid and Perovskite Photovoltaics III
10:00	P3	CPP 25	Poster: Active Matter, Soft Matter, Fluids
11:30	H34	CPP 26	Nanostructures, Nanostructuring and Nanosized Soft Matter I
11:30	H38	CPP 27	Molecular Electronics and Excited State Properties II
15:00	H34	CPP 28	Modeling and Simulation of Soft Matter III
15:00	H38	CPP 29	Organic Electronics and Photovoltaics III
16:15	H34	CPP 30	Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I
16:15	H38	CPP 31	Responsive and Adaptive Polymers

DS

Invited Talk

09:30	H14	DS 7.1	Enhancing Organic Spin Valves Through Spinterface Engineering •Shuaishuai Ding

Sessions

09:30	H3	DS 6	Thin Film Application
09:30	H14	DS 7	Spins in Molecular Systems: Strategies and Effects of Hyperpolarization
12:00	H3	DS 8	Optical Analysis of Thin Films I

DY

Invited Talks

15:00	H43	DY 24.1	Dynamics of odd and chiral active systems •Hartmut Löwen

DY

16:45	H43	DY 24.7	Odd dynamics and universal flows of passive objects in a chiral active fluid •Cory Hargus
18:00	H43	DY 24.11	How to model frictional contacts in sheared and active colloids •Friederike Schmid

Sessions

09:30	H17	DY 19	Focus Session: Quantum Emission from Chaotic Microcavities
09:30	H37	DY 20	Many-body Quantum Dynamics II
09:30	H43	DY 21	Granular Matter
10:00	P3	DY 22	Poster: Statistical Physics
10:00	P3	DY 23	Poster: Active Matter, Soft Matter, Fluids
15:00	H43	DY 24	Focus Session: Broken Symmetries in Statistical Physics – Dynamics of Odd Systems
15:00	H44	DY 25	Statistical Physics of Biological Systems I
15:00	H45	DY 26	Networks, From Topology to Dynamics
15:00	P4	DY 27	Poster: Nonlinear Dynamics, Pattern Formation, Granular Matter
15:00	P4	DY 28	Poster: Machine Learning, Data Science
15:00	P4	DY 29	Poster: Quantum Dynamics and Many-body Systems

HL

Invited Talks

09:30	H13	HL 30.1	Exploring semiconducting epigraphene grown by polymer-assisted sublimation growth •Teresa Tschirner
10:00	H13	HL 30.2	Huge Enhancement of the Giant Negative Magnetoresistance with Decreasing Electron Density •Lina Bockhorn
10:30	H13	HL 30.3	Ultrafast quantum optics with single-photon emitters in 2D materials •Steffen Michaelis de Vasconcellos
11:15	H13	HL 30.4	Realistic simulation of quantum emitter dynamics made easy •Moritz Cygorek
11:45	H13	HL 30.5	Data-driven Design of Next Generation 2D Materials and Their Heterostructures •Rico Friedrich
09:30	H17	HL 34.1	From complex internal dynamics to emission characteristics control in quantum billiards •Martina Hentschel
10:00	H17	HL 34.2	Positioning of microcavities around single emitters •Tobias Huber-Loyola
10:30	H17	HL 34.3	Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities •Jan Wiersig
11:15	H17	HL 34.4	Correlations and statistics in cavity embedded quantum dot sources of quantum light •Ana Predojevic
11:45	H17	HL 34.5	Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum •Dario Ballarini
16:45	H17	HL 42.1	Quantum key distribution with single photons from quantum dots •Jingzhong Yang

Sessions

09:30	H13	HL 30	Focus Session: Young Semiconductor Forum
12:15	H13	HL 31	Focus Session: Young Semiconductor Forum Poster
09:30	H15	HL 32	Nitrides: Preparation and Characterization I
11:15	H15	HL 33	Nitrides: Devices
09:30	H17	HL 34	Focus Session: Quantum Emission from Chaotic Microcavities
10:30	H11	HL 35	2D Materials: Electronic Structure and Exitations II
15:00	H13	HL 36	Materials and Devices for Quantum Technology II

Wednesday, March 19, 2025

HL

15:00	H15	HL 37	Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I
15:00	H17	HL 38	Nanomechanical systems
15:00	P3	HL 39	Poster III
15:30	H15	HL 40	2D Semiconductors and van der Waals Heterostructures IV
15:45	H17	HL 41	Spin Phenomena in Semiconductors
16:45	H17	HL 42	Quantum Dots and Wires: Optics I
17:00	H31	HL 43	Twisted Materials / Systems
18:00	H13	HL 44	Focus Session: Quantum Technologies in Deployed Systems I

KFM

Invited Talks

09:30	H9	KFM 11.1	Towards 3D nanoscale chemical mapping with atom probe tomography •Kasper Hunnestad
11:00	H9	KFM 12.1	Model-assisted Insight into Degradation of Li-Ion Batteries during Thermal Abuse •Ulrike Krewer

Sessions

09:30	H9	KFM 11	(Multi)ferroic States: From Fundamentals to Applications (V)
11:00	H9	KFM 12	Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Modelling of Battery Materials and Degradation)
15:00	H9	KFM 13	Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Experimental Characterisation and Safety Testing)
17:00	P1	KFM 14	Poster

MA

Invited Talks

09:30	H20	MA 23.1	Magneto-transport effects in crystalline magnetic films •Sebastian T. B. Goennenwein
10:00	H20	MA 23.2	Cubic magneto-optic Kerr effect in thin films depending on structural domain twinning and crystal orientation •Robin Silber
11:15	H20	MA 23.5	electrical and optical detection of the multipolar structure in the magnetization space •Dazhi Hou
12:30	H20	MA 23.9	Ultrafast Néel order dynamics detected by time-resolved magneto-optical Voigt effect •Haibin Zhao
16:00	H18	MA 30.1	Boosting Coercivity in Additively Manufactured Magnets Through Nano-Functionalization of NdFeB Powder •Anna Ziefuss

Sessions

09:30	H16	MA 20	Magnonics II
09:30	H18	MA 21	Frustrated Magnets I
09:30	H19	MA 22	Caloric Effects in Ferromagnetic Materials
09:30	H20	MA 23	Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization I
09:30	H36	MA 24	Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets
15:00	H15	MA 25	Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I
15:00	H16	MA 26	Ultrafast Magnetization Effects I
15:00	H18	MA 27	Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization II
15:00	H19	MA 28	Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions
15:00	H20	MA 29	Skyrmions II
16:00	H18	MA 30	Bulk Materials: Soft and Hard Permanent Magnets
17:00	P1	MA 31	Poster II
17:30	H19	MA 32	Spin Transport and Orbitronics, Spin-Hall Effects II

Wednesday, March 19, 2025

MM

Invited Talks, Topical Talks

09:30	H10	MM 15.1	Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties •Christina Scheu
10:15	H10	MM 16.1	Microstructure and transport in model isotropic amorphous solids •Peter Derlet
11:45	H10	MM 16.5	Structural relaxation and deformation of bulk metallic glasses •Gerhard Wilde
15:00	H10	MM 19.1	Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys •Laure Bourgeois
15:45	H10	MM 20.1	Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting •Paola Tiberto
17:15	H10	MM 20.5	Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations •Thomas Voigtmann
18:00	H10	MM 20.7	The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys •Ralf Busch

Sessions

09:30	H10	MM 15	Invited Talk: C. Scheu
10:15	H10	MM 16	Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids
10:15	H22	MM 17	Development of Calculation Methods
10:15	H23	MM 18	SYMD contributed
15:00	H10	MM 19	Invited Talk: L. Bourgeois
15:45	H10	MM 20	Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids
15:45	H22	MM 21	Interface Controlled Properties, Nanomaterials and Microstructure Design
15:45	H23	MM 22	Materials for the Storage and Conversion of Energy
17:15	H23	MM 23	Phase Transformations
18:45	H10	MM 24	Members' Assembly

O

Invited Talks, Topical Talk

09:30	H24	O 56.1	trends and perspectives in on-surfece UHV synthesis •Pavel Jelínek
11:00	H2	O 57.3	Floquet engineering in black phosphorus •Changhua Bao
11:00	H11	O 61.3	Polaritons in two-dimensional materials and hybrids probed by electron beams •Nahid Talebi
11:30	H24	O 62.5	On-Surface Synthesis with Hydrogen Atoms •Szymon Godlewski
15:00	H2	O 64.1	Topological spin structures in two-dimensional van der Waals magnets and heterostructures •Stefan Heinze
15:30	H2	O 64.2	Ferromagnetic Order in 2D Layers of Transition Metal Dichlorides •Martina Corso
16:00	H2	O 64.3	Tailoring spin lattice in van der Waals monolayer crystals •Ying-Shuang Fu
16:30	H2	O 64.4	Spin excitations in 2D heterostructures from realistic fermionic models •António Costa
15:00	H8	O 66.1	Unveiling the crucial role of kinetic modeling of gas flows in vacuum and fusion technologies •Christos Tantos

Wednesday, March 19, 2025

O

15:30	H8	O 66.2	Advances in traceable vacuum and outgassing rate measurements •Matthias Bernien
17:00	H24	O 68.9	On-Surface Synthesis of Porphyrins and BN-Substituted Carbon Scaffolds •Willi Auwärter

Sessions

09:30	H24	O 56	Overview Talk Pavel Jelinek
10:30	H2	O 57	Ultrafast Electron Dynamics I
10:30	H4	O 58	Solid-Liquid Interfaces: Reactions and Electrochemistry II
10:30	H6	O 59	Spins on Surfaces at the Atomic Scale I
10:30	H8	O 60	Plasmonics and Nanooptics: Fabrication, Characterization and Applications I
10:30	H11	O 61	2D Materials: Electronic Structure and Exitations II
10:30	H24	O 62	Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation III
10:30	H25	O 63	Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules II
15:00	H2	O 64	Focus Session Atomic Scale Investigation of Magnetic 2D Materials
15:00	H6	O 65	Solid-Liquid Interfaces: Reactions and Electrochemistry III
15:00	H8	O 66	Vacuum Science Technology: Theory and Applications
15:00	H11	O 67	Ultrafast Electron Dynamics II
15:00	H24	O 68	Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation IV
15:00	H25	O 69	Nanostructures at Surfaces II
18:00	P2	O 70	Poster Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules
18:00	P2	O 71	Poster Plasmonics and Nanooptics: Fabrication, Characterization and Applications
18:00	P2	O 72	Poster Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy
18:00	P2	O 73	Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules
18:00	P2	O 74	Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth
18:00	P2	O 75	Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure
18:00	P2	O 76	Poster Focus Session Atomic Scale Investigation of Magnetic 2D Materials
18:00	P2	O 77	Poster Vacuum Science Technology: Theory and Applications

SOE

Invited Talk, Topical Talk

09:30	H45	SOE 7.1	When networks can think: The meaning of self-regulation in the presence of humans •Alina Herderich
11:15	H45	SOE 7.6	Self-organization in neural systems •Philipp Hövel

Sessions

09:30	H45	SOE 7	Focus Session: Self-Regulating and Learning Systems: from Neural to Social Networks
15:00	H45	SOE 8	Networks, From Topology to Dynamics
18:00	H45	SOE 9	Members' Assembly

TT

Invited Talks, Topical Talks

09:30	H31	TT 24.1	Possible Origin of High-Field Reentrant Superconductivity in UTe_2 •Toni Helm
11:30	H31	TT 24.7	Unconventional Superconductivity in Epitaxial $KTaO_3$-Based Heterostructures •Denis Maryenko
09:30	H36	TT 27.1	Detecting Anyons Using Nonlinear Pump-Probe Spectroscopy •Max McGinley

Wednesday, March 19, 2025

TT

10:00	H36	TT 27.2	Two-Dimensional Nonlinear Dynamic Response of Frustrated Magnets •Wolfram Brenig
10:30	H36	TT 27.3	Imaging Magnetization Dynamics and Collective Spin Excitations in Compensated Magnets on Ultrafast Timescales •Benjamin Stadtmüller
11:15	H36	TT 27.4	Revealing Dynamics of Hidden Sectors with Nonlinear Spectroscopy •Yoshito Watanabe
11:45	H36	TT 27.5	Theory of Nonlinear Spectroscopy of Quantum Magnets •Stefan Birnkammer
15:00	H31	TT 31.1	Quantum Skyrmion Hall Effect •Ashley Cook
17:00	H33	TT 33.8	Emergent Dynamical Gauge Fields in Generic Kitaev Spin Liquids: From Monolayer to Multilayers •Aprem Joy

Sessions

09:30	H31	TT 24	Unconventional Superconductors
09:30	H32	TT 25	Superconductivity: Supercurrent Diode Effect
09:30	H33	TT 26	Correlated Magnetism – Frustrated Systems
09:30	H36	TT 27	Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets
09:30	H37	TT 28	Many-body Quantum Dynamics II
10:30	H11	TT 29	2D Materials: Electronic Structure and Exitations II
15:00	H17	TT 30	Nanomechanical systems
15:00	H31	TT 31	Topology: Quantum Hall Systems
15:00	H32	TT 32	Superconductivity: Yu-Shiba-Rusinov and Andreev Physics
15:00	H33	TT 33	Correlated Magnetism – Spin Liquids
15:00	H36	TT 34	Superconductivity: Theory
15:00	P3	TT 35	Topology: Poster
15:00	P3	TT 36	Nanotubes, BEC, Cryocoolers: Poster
15:00	P4	TT 37	Correlated Electrons: Poster
16:45	H32	TT 38	Superconducting Electronics: SQUIDs, Qubits, Circuit QED I
17:00	H31	TT 39	Twisted Materials / Systems
17:30	H19	TT 40	Spin Transport and Orbitronics, Spin-Hall Effects II

AIW

Sessions

14:00	H4	AIW 1	Quantencomputing
15:55	H4	AIW 2	Quantenkommunikation
17:20	H4	AIW 3	Get Together bei Bier und Brezeln

09:00	Foyer Audimax, H6, Economy Bldg., Tent	**Exhibition of Scientific Instruments and Literature** (free entrance)

Job Market

11:00	Kunsthalle	Basycon Unternehmensberatung GmbH: *"Aus der Wissenschaft in die Beratung"*

Public Evening Talk (free entrance)

19:00	H1	PSV VII	Leben in einer wärmer werdenden Welt: Wie der Klimawandel unser Leben beeinflusst •Thomas Jung

AIW Verbunden durch Physik

Deutsche Physikalische Gesellschaft DPG

Industrietag 2025

Quantentechnologien in Wirtschaft und Gesellschaft

Der Industrietag, an dem rund 200 Personen (meist Studierende und Promovierende) teilnehmen, wird durch den Arbeitskreis Industrie und Wirtschaft (AIW) der Deutschen Physikalischen Gesellschaft (DPG) organisiert und durchgeführt. Ziel der Veranstaltungen ist es, Studierende und Promovierende für Berufe in Wirtschaft und Industrie zu begeistern.

Ablauf der Veranstaltung

14:00 Uhr Willkommen und Grußwort durch AIW und AKPIK
Dr. Hans-Georg Grothues, Dr. John Kettler, Dr. Tim Ruhe

Themenblock 1 Quantencomputing

14:10 Uhr Von Quantenwinter bis Quantensprung – Wo stehen Quantentechnologien heute?
Carina Kiessling, Roland Berger

14:30 Uhr Der Weg zum praktischen Quantencomputing – Potenziale und Use-Cases
Dr. Nico Piatkowski – Fraunhofer-Institut für Intelligente Analyse- und Informationssysteme

14:50 Uhr Wie verbinden wir die Quanten- mit unserer klassischen Welt?
Dr. Claudius Riek – Zurich Instruments Germany

15:10 Uhr Podiumsdiskussion: Quantencomputing – Perspektiven für die Industrie

15:30 Uhr Kaffeepause

15:55 Uhr Finde deinen Weg: Berufliche Orientierung und Unterstützung durch die DPG
Gabriele Becker – Referentin des Vorstandes der DPG

Themenblock 2 Quantenkommunikation

16:00 Uhr Introduction to quantum cryptography and related use-cases
Dr. Mathieu Bozzio – Universität Wien

16:20 Uhr Quantenkommunikation in der Raumfahrt
Dr. Stephan Seidel – Airbus Defense & Space

16:40 Uhr Small is beautiful: Leading innovation in miniaturizing quantum sensors
Dr. Binh Tran – Bosch Quantum Sensing

17:00 Uhr Podiumsdiskussion: Quantenkommunikation – Chancen für globale Anwendungen

17:20 Uhr Get-Together bei Bier und Brezeln bis 18:30 Uhr

Veranstaltungsort:
Universität Regensburg
Zentrales Hörsaalgebäude, H4
Universitätsstr. 31
93053 Regensburg

Datum und Uhrzeit:
19.03.2025
14:00 Uhr – 18:30 Uhr

Thursday, March 20, 2025

			Plenary Talks
08:30	H1	PLV VIII	Learning how biomolecules move and undergo chemical reactions •Frauke Gräter
14:00	H1	PLV IX	Tunable Ultrafast Dynamics of Antiferromagnetic Vortices in Nanoscale Dots •Jelena Klinovaja
14:00	H2	PLV X	Process-directed formation of nonequilibrium structures in copolymer materials •Marcus Müller
			Prize Talks
13:15	H2	PRV V	Altermagnetism and spin symmetries •Libor Šmejkal (Laureate of the Walter-Schottky-Prize 2025)
13:15	H4	PRV VI	Confining strongly correlated quasiparticles in 2D semiconductors •Wouter Jolie (Laureate of the Gaede-Prize 2025)
			Lunch Talks
13:15	H1	PSV VIII	Let's talk about science communication! •Nicolas Wöhrl
13:15	H3	PSV IX	From PhD to Head of Product Management at a Biotech Company •Judith Stolwijk

SYAI

			Invited Talks
09:30	H1	SYAI 1.1	Predicting interaction partners and generating new protein sequences using protein language models •Anne-Florence Bitbol
10:00	H1	SYAI 1.2	Realizing Schrödinger's dream with AI-enabled molecular dynamics •Alexandre Tkatchenko
10:30	H1	SYAI 1.3	Emergent behavior of artificial intelligence •Steffen Rulands
11:15	H1	SYAI 1.4	AI in medical research – navigating complexity with AI •Daniel Truhn
11:45	H1	SYAI 1.5	Computational Modelling of Morphogenesis •Dagmar Iber
			Session
09:30	H1	SYAI 1	AI in (Bio-)Physics

SYQS

			Invited Talks
15:00	H1	SYQS 1.1	Active quantum flocks •Markus Heyl
15:30	H1	SYQS 1.2	Robust dynamics and function in stochastic topological systems •Evelyn Tang
16:00	H1	SYQS 1.3	Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases •Artur Widera
16:45	H1	SYQS 1.4	Topological classification of driven-dissipative nonlinear systems •Oded Zilberberg
17:15	H1	SYQS 1.5	Learning dynamical behaviors in physical systems •Vincenzo Vitelli
			Session
15:00	H1	SYQS 1	Nonequilibrium Collective Behavior in Open Classical and Quantum Systems

Thursday, March 20, 2025

BP

Invited Talks

09:30	H44	BP 25.1	Oncogenic signaling and stiffness sensing •Johanna Ivaska
11:00	H46	BP 26.6	Theory for sequence selection via phase separation and oligomerization •Christoph Weber
15:00	H44	BP 29.1	Community-driven software and data training for computational biology •Toby Hodges
16:00	H46	BP 30.5	Topology in biological matter – are there double knots in proteins or maybe even more complicated knots? Prediction and in vitro verification. •Joanna I Sulkowska

Sessions

09:30	H44	BP 25	Cell Mechanics II
09:30	H46	BP 26	Synthetic life-like systems and Origins of Life
15:00	H24	BP 27	Focus Session Chemical Imaging for the Elucidation of Molecular Structure I
15:00	H37	BP 28	Microswimmers and Microfluidics
15:00	H44	BP 29	Focus Session: Innovations in Research Software Engineering
15:00	H46	BP 30	Protein Structure and Dynamics

CPP

Invited Talks

15:00	H34	CPP 34.1	Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials •Valentina Guccini
16:15	H34	CPP 37.1	Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level •Malin Wohlert
16:15	H38	CPP 38.1	Adsorption and Interaction of Amino Acids on Titanium Oxide Photocatalyst •Heshmat Noei

Sessions

09:30	P3	CPP 32	Poster Session II
11:45	H34	CPP 33	Modeling and Simulation of Soft Matter IV
15:00	H34	CPP 34	Focus Session: Interactions Between Water and Cellulose I
15:00	H37	CPP 35	Microswimmers and Microfluidics
15:00	H38	CPP 36	Organic Electronics and Photovoltaics IV
16:15	H34	CPP 37	Focus Session: Interactions Between Water and Cellulose II
16:15	H38	CPP 38	Interfaces and Thin Films II
18:00	H38	CPP 39	Members' Assembly

DS

Invited Talks

09:30	H3	DS 9.1	Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces •Sebastian Heidenreich
10:00	H3	DS 9.2	Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces •Bernd Bodermann
16:15	H3	DS 12.1	Probing the Electronic Structure of Halide Perovskites •Selina Olthof
16:45	H3	DS 12.2	Quantum Science with Single Atoms and Molecules on Surfaces •Philip Willke
17:30	H3	DS 12.3	Gallium Nitride Technology – the second pillar of microelectronics •Andreas Waag
18:00	H3	DS 12.4	Ultrafast X-ray photoelectron spectroscopy and photoelectron diffraction •Philip Hofmann

Thursday, March 20, 2025

DS

Sessions

09:30	H3	DS 9	Optical Analysis of Thin Films II
11:30	H14	DS 10	Transport Properties
15:00	H3	DS 11	Thermoelectric and Phase Change Materials
16:15	H3	DS 12	Gaede-Jubiläumssitzung
18:00	P1	DS 13	Poster
18:30	H3	DS 14	Members' Assembly

DY

Invited Talks

10:45	H37	DY 31.6	Strong coupling and coherence in quantum thermodynamics •Janet Anders
09:30	H43	DY 32.1	Fluctuation-Response Relations for Non-equilibrium Systems •Benjamin Lindner
15:00	H37	DY 36.1	Light-Driven Manipulation of Passive and Active Microparticles •Svetlana Santer

Sessions

09:30	H31	DY 30	Quantum-Critical Phenomena
09:30	H37	DY 31	Focus Session: Nonequilibrium Collective Behavior in Open Classical and Quantum Systems
09:30	H43	DY 32	Nonlinear Stochastic Systems
09:30	H47	DY 33	Machine Learning in Dynamics and Statistical Physics I
11:30	H43	DY 34	Nonlinear Dynamics, Synchronization, and Chaos
15:00	H31	DY 35	Fluctuations, Noise and Other Transport Topics
15:00	H37	DY 36	Microswimmers and Microfluidics
15:00	H43	DY 37	Brownian Motion and Anomalous Diffusion
15:00	H44	DY 38	Focus Session: Innovations in Research Software Engineering
15:00	H47	DY 39	Machine Learning in Dynamics and Statistical Physics II
18:00	H43	DY 40	Members' Assembly

HL

Prize Talk, Invited Talks

09:30	H15	HL 46.1	Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System •Alex Greilich
11:15	H15	HL 46.6	Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules •Annika Janssen (Laureate of the Georg-Simon-Ohm-Prize 2025)
09:30	H17	HL 47.1	Quantum-Dot Quantum Light Sources in Deployed Systems •Peter Michler
10:00	H17	HL 47.2	Field test of semiconductor quantum light sources •Fei Ding
10:30	H17	HL 47.3	Quantum dot based quantum communication in urban networks •Rinaldo Trotta
11:15	H17	HL 47.4	Quantum communication protocols over a 14-km urban fiber link •Jürgen Eschner

Sessions

09:30	H13	HL 45	Perovskite and Photovoltaics II
09:30	H15	HL 46	Optical Properties
09:30	H17	HL 47	Focus Session: Quantum Technologies in Deployed Systems II
09:30	H36	HL 48	Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides
10:30	H11	HL 49	2D Materials: Electronic Structure and Exitations III
15:00	H6	HL 50	2D Materials: Stacking and Heterostructures

Thursday, March 20, 2025

HL

15:00	H13	HL 51	Transport Properties
15:00	H14	HL 52	Oxide Semiconductors II
15:00	H15	HL 53	2D Semiconductors and van der Waals Heterostructures V
15:00	H17	HL 54	Ultra-fast Phenomena II
15:00	H33	HL 55	Graphene and 2D Materials
17:30	H17	HL 56	Members' Assembly

KFM

Invited Talks

09:30	H9	KFM 15.1	Is CVD diamond now ready to become an electronic material? •Philippe Bergonzo
15:30	H9	KFM 18.1	Domain gratings of sub-micrometer period for quantum technologies •Carlota Canalias

Sessions

09:30	H9	KFM 15	Crystal Structure Defects / Real Structure / Microstructure
09:30	H13	KFM 16	Perovskite and Photovoltaics II
11:45	H23	KFM 17	Functional Materials: Performance, Reliability and Degradation; and Complex Materials
15:30	H9	KFM 18	Materials Research in Polar Oxides: Perspectives for Optics & Electronics
18:00	H9	KFM 19	Members' Assembly

MA

Invited Talks

09:35	H20	MA 35.1	Artificial Intelligence for Materials Science: Critical Importance of Rare Events, Active Learning, and Uncertainties •Matthias Scheffler
10:05	H20	MA 35.2	Physics meets data: decoding magnetic inhomogeneities through latent analysis •Karin Everschor-Sitte
10:35	H20	MA 35.3	AI used for micromagnetic simulations •Thomas Schrefl
11:15	H20	MA 35.4	Future method for estimating parameters in magnetic films using machine learning •Kenji Tanabe
15:00	H18	MA 38.1	Liquid-mediated surface-surface interactions investigated by close-to-surface magnetic particle transport •Rico Huhnstock
15:00	H19	MA 39.1	Voltage control of magnetism using hydrogen •Markus Gößler

Sessions

09:30	H16	MA 33	Non-Skyrmonic Magnetic Textures I
09:30	H18	MA 34	Molecular Magnetism
09:30	H20	MA 35	PhD Focus Session: Using Artificial Intelligence Tools in Magnetism
09:30	H36	MA 36	Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides
15:00	H16	MA 37	Magnetic Imaging Techniques
15:00	H18	MA 38	Magnetic Particles / Clusters & Biomagnetism
15:00	H19	MA 39	Magnetic Thin Films
15:00	H20	MA 40	Frustrated Magnets II
15:00	P3	MA 41	Poster III
18:00	H20	MA 42	Members' Assembly

MM

Invited Talk

09:30	H10	MM 25.1	Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments •David Rodney

Thursday, March 20, 2025

MM

Sessions

09:30	H10	MM 25	Invited Talk: D. Rodney
10:15	H10	MM 26	Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids
10:15	H22	MM 27	Transport in Materials: Diffusion, Charge or Heat Conduction
10:15	H23	MM 28	Mechanical properties
12:00	H10	MM 29	Liquid and Amorphous Materials
11:45	H23	MM 30	Functional Materials: Performance, Reliability and Degradation; and Complex Materials
15:00	H10	MM 31	Data-driven Materials Science: Big Data and Worksflows
15:00	H22	MM 32	Transport in Materials: Diffusion, Charge or Heat Conduction

O

Invited Talks, Topical Talk

09:30	H24	O 78.1	Imaging Electronic and Atomic Motion in Molecules •Manish Garg
15:00	H24	O 91.1	Infrared Nanoscopy and Tomography of Intracellular Structures •Emmanuel Pfitzner
15:30	H24	O 91.2	Coherent Raman Imaging •Michael Schmitt
16:00	H24	O 91.3	Sum Frequency Generation Microscopy of Electrochemical Interfaces •Steven Baldelli

Sessions

09:30	H24	O 78	Overview Talk Manish Garg
10:30	H2	O 79	Ultrafast Electron Dynamics III
10:30	H4	O 80	Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I
10:30	H6	O 81	Heterogeneous Catalysis III
10:30	H8	O 82	Plasmonics and Nanooptics: Fabrication, Characterization and Applications II
10:30	H11	O 83	2D Materials: Electronic Structure and Exitations III
10:30	H24	O 84	Gerhard Ertl Young Investigator Award Competition
10:30	H25	O 85	New Methods: Theory
15:00	H2	O 86	Electronic Structure of Surfaces: Spectroscopy, Surface States II
15:00	H4	O 87	Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy I
15:00	H6	O 88	2D Materials: Stacking and Heterostructures
15:00	H8	O 89	Metal and Semiconductor Substrates: Structure, Epitaxy and Growth
15:00	H11	O 90	Spins on Surfaces at the Atomic Scale II
15:00	H24	O 91	Focus Session Chemical Imaging for the Elucidation of Molecular Structure I
15:00	H25	O 92	Electronic Structure Theory
19:00	H1	O 93	Members' Assembly
19:30	H1	O 94	Post Deadline Session

SOE

Invited Talk

15:00	H45	SOE 10.1	Emergent Behaviors in LLMs-Populated Societies •Giordano De Marzo

Session

15:00	H45	SOE 10	Focus Session: Large Language Models, Social Dynamics, and Assessment of Complex Systems

TT

Invited Talk, Topical Talks

09:30	H36	TT 44.1	Evidence of Unconventional Superconductivity in Monolayer and Bulk van der Waals Material TaS_2 •Somesh Chandra Ganguli

Thursday, March 20, 2025

TT

10:00	H36	TT 44.2	Signatures of Unconventional Superconductivity in Transition Metal Dichalcogenides •Miguel Ugeda
10:30	H36	TT 44.3	Friedel Oscillations and Chiral Superconductivity in Monolayer $NbSe_2$ •Magdalena Marganska
11:15	H36	TT 44.4	Unconventional Pairing in Ising Superconductors •Andreas Kreisel
11:45	H36	TT 44.5	High-Field Study of Ising Superconductivity in TMDs •Oleksandr Zheliuk
15:00	H32	TT 48.1	Optical Conductivity as a Probe for Chiral Majorana Edge Modes •Lina Johnsen Kamra

Sessions

09:30	H31	TT 41	Quantum-Critical Phenomena
09:30	H32	TT 42	Superconductivity: Tunneling and Josephson Junctions
09:30	H33	TT 43	Correlated Electrons: Other Theoretical Topics
09:30	H36	TT 44	Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides
10:30	H11	TT 45	2D Materials: Electronic Structure and Exitations III
15:00	H13	TT 46	Transport Properties
15:00	H31	TT 47	Fluctuations, Noise and Other Transport Topics
15:00	H32	TT 48	Topology: Majorana Physics
15:00	H33	TT 49	Graphene and 2D Materials
15:00	H36	TT 50	Superconducting Electronics: SQUIDs, Qubits, Circuit QED II
16:45	H32	TT 51	Topological Superconductors

AKPIK

Sessions

15:00	P2	AKPIK 5	Poster
16:30	H5	AKPIK 6	AI Methods for Materials Science

09:00	Foyer Audimax, H6, Economy Bldg., Tent	**Exhibition of Scientific Instruments and Literature**

Job Market

11:00	BCG – The Boston Consulting Group GmbH: *„Als Physiker:in in die Strategieberatung “*

Friday, March 21, 2025

Plenary Talk

08:30	H1	PLV XI	Exploring correlated phases and topology in van der Waals platforms •Roser Valenti

SYES

Invited Talks

09:30	H1	SYES 1.1	Ab-initio Design of superconductors •Lilia Boeri
10:00	H1	SYES 1.2	Topological superconductivity from first principles •László Szunyogh
10:30	H1	SYES 1.3	First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe •Myrta Grüning
11:15	H1	SYES 1.4	Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects. •Thomas Olsen
11:45	H1	SYES 1.5	Spin-phonon and magnon-phonon interactions from first principles •Marco Bernardi

Session

09:30	H1	SYES 1	Electronic Structure Theory for Quantum Technology

BP

Invited Talks

09:30	H44	BP 31.1	Wave propagation in systems of active filaments •Kirsty Y. Wan
13:15	H2	BP 35.1	Active control of forces, movement and shape: from biological to non-living systems •Ulrich S. Schwarz

Sessions

09:30	H44	BP 31	Active Matter IV
09:30	H46	BP 32	Computational Biophysics II
10:30	H24	BP 33	Focus Session Chemical Imaging for the Elucidation of Molecular Structure II
11:30	H43	BP 34	Statistical Physics in Biological Systems II
13:15	H2	BP 35	Closing Talk Ulrich Schwarz

CPP

Invited Talk

09:30	H38	CPP 41.1	Simulations of reaction equilibria in macromolecular systems •Peter Košovan

Sessions

09:30	H34	CPP 40	Energy Storage and Batteries II
09:30	H38	CPP 41	Charged Soft Matter, Polyelectrolytes and Ionic Liquids I
09:30	H44	CPP 42	Active Matter IV
09:30	H47	CPP 43	Droplets, Wetting, Complex Fluids, and Soft Matter
11:30	H34	CPP 44	2D Materials
11:30	H38	CPP 45	Charged Soft Matter, Polyelectrolytes and Ionic Liquids II
13:15	H2	CPP 46	Closing Talk Ulrich Schwarz

DS

Invited Talk

09:30	H3	DS 15.1	Structure formation and growth at the metal-organic interface •Peter Zeppenfeld

Friday, March 21, 2025

DS

Session

09:30	H3	DS 15	Organic Thin Films, Organic-Inorganic Interfaces

DY

Invited Talks

09:30	H47	DY 44.1	From Cavitation in Soft Matter to Erosion on Hard Matter •Claus-Dieter Ohl
11:30	H43	DY 46.1	Equilibrium and non-equilibrium dynamics of biological systems with memory •Roland Netz

Sessions

09:30	H37	DY 41	Quantum Dynamics, Decoherence, and Quantum Information
09:30	H43	DY 42	Stochastic Thermodynamics
09:30	H44	DY 43	Active Matter IV
09:30	H47	DY 44	Droplets, Wetting, Complex Fluids, and Soft Matter
11:30	H37	DY 45	Quantum Chaos
11:30	H43	DY 46	Statistical Physics of Biological Systems II
13:15	H2	DY 47	Closing Talk Ulrich Schwarz

HL

Invited Talks

09:30	H17	HL 60.1	Constructing Artificial Matter in the Electron Microscope – Atomic Fabrication at Scale in CrSBr •Julian Klein
10:00	H17	HL 60.2	Tuning the structure and magnetism in CrSBr via external pressure •Ece Uykur
10:30	H17	HL 60.3	A theoretical perspective on exciton-magnon coupling and its implications •Akashdeep Kamra
11:15	H17	HL 60.4	Exciton and valley properties of monolayer transition metal dichalcogenides on the van der Waals magnetic semiconductor CrSBr •Yara Galvao Gobato
12:30	H17	HL 60.8	Electric field control of intra- and interlayer excitons in CrSBr •Nathan Wilson

Sessions

09:30	H13	HL 57	Quantum Dots and Wires: Optics II
09:30	H14	HL 58	Nitrides: Preparation and Characterization II
09:30	H15	HL 59	2D Semiconductors and van der Waals Heterostructures VI
09:30	H17	HL 60	Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II
10:45	H14	HL 61	THz and MIR physics in semiconductors
11:45	H15	HL 62	2D Semiconductors and van der Waals Heterostructures VII
12:00	H14	HL 63	Focus Session: Nanoscale Light-matter Interaction II

MA

Sessions

09:30	H16	MA 43	Skyrmions III / Non-Skyrmionic Magnetic Textures II
09:30	H17	MA 44	Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II
09:30	H18	MA 45	Computational Magnetism
09:30	H19	MA 46	Surface Magnetism
09:30	H20	MA 47	Altermagnets III
11:15	H20	MA 48	Ultrafast Magnetization Effects II

Friday, March 21, 2025

MM

Invited Talk

09:30	H10	MM 33.1	Fatigue in steels: Micromechanical modelling of cyclic damage •Petra Sonnweber-Ribic

Sessions

09:30	H10	MM 33	Invited Talk: P. Sonnweber-Ribic
10:15	H10	MM 34	Development of Calculation Methods
10:15	H22	MM 35	Transport in Materials: Diffusion, Charge or Heat Conduction
10:15	H23	MM 36	Mechanical Properties
12:00	H22	MM 37	Functional and Complex Materials

O

Invited Talks, Topical Talks

09:30	H24	O 95.1	A quantum sandwich world and how we can explore it with soft x-rays •Kai Rossnagel
10:30	H24	O 100.1	Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things •Steven Lee
11:00	H24	O 100.2	MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research •Andreas Römpp
13:15	H1	O 102.1	Quantum sensing with atomic-scale spatial resolution •Andreas Heinrich

Sessions

09:30	H24	O 95	Overview Talk Kai Rossnagel
10:30	H4	O 96	Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy II
10:30	H6	O 97	Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties II
10:30	H8	O 98	Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules
10:30	H11	O 99	Ultrafast Electron Dynamics IV
10:30	H24	O 100	Focus Session Chemical Imaging for the Elucidation of Molecular Structure II
10:30	H25	O 101	Topology and Symmetry-protected Materials
13:15	H1	O 102	Closing Talk Andreas Heinrich

TT

Sessions

09:30	H31	TT 52	Nickelates and Other Complex Oxides
09:30	H32	TT 53	Topology: Other Topics
09:30	H33	TT 54	Correlated Electrons: Charge Order
09:30	H36	TT 55	Superconducting Electronics: SQUIDs, Qubits, Circuit QED III
09:30	H37	TT 56	Quantum Dynamics, Decoherence, and Quantum Information
10:30	H25	TT 57	Topology and Symmetry-protected Materials
11:30	H31	TT 58	f-Electron Systems and Heavy Fermions
11:30	H37	TT 59	Quantum Chaos

AKC

Invited Talks

10:45	H2	AKC 1.1	Reshaping the History of Quantum Physics: Paths to Gender Equality •Andrea Reichenberger
11:15	H2	AKC 1.2	Prevention and protection against sexual harassment, discrimination and violence (SBDG): A private matter or how much does it concern us as a university? •Michael Tunç

Sessions

10:45	H2	AKC 1	AKC
12:15	H2	AKC 2	Women in Physics Lunch

Plenary Talks

Plenary Talk PLV I Mon 8:30 H1

Seeing dents in the atom — •Franz Giessibl — Exp. and Appl. Phys., University of Regensburg, 93053 Regensburg, Germany

Explaining the emission spectra of atoms was a giant early success of quantum mechanics. Directly seeing atoms remained elusive, though. When Binnig and Rohrer imaged the atoms of the silicon 7x7 reconstructed surface with the scanning tunneling microscope (STM), it came as a surprise. STM relies on a quantum effect, electron tunneling. In 1986, Binnig, Gerber and Quate introduced atomic force microscopy (AFM), a method that also images samples by probing it with, ideally, the single front atom of a sharp tip. Feynman quoted the atomic hypothesis (attracting each other when they are a little distance apart, but repelling upon being squeezed into one another) in chapter 1 of his Lectures on Physics. The AFM uses exactly those forces between atoms to create images line by line. The force sensor needs to probe forces small enough such that neither the tips front atom nor the sample are displaced. AFM passed its acid test when it resolved the silicon 7x7 surface in a non-contact mode using the frequency shift of an oscillating cantilever. The qPlus sensor, a self-sensing quartz cantilever oscillating at sub-A amplitudes resolves molecules with a CO tip. Today, AFM even resolves structures within single atoms. The quantum corral, introduced by Crommie, Lutz and Eigler in 1993, was revisited by AFM, showing that this 2D artificial atom interacts similar with AFM tips as a natural atom. A qPlus sensor with a metal tip reunites STM with AFM and it enables us to do surface science of insulators on the atomic level.

Plenary Talk PLV II Mon 14:00 H1

High-power semiconductor lasers based on Hermitian and non-Hermitian control in photonic crystals — •Susumu Noda — Department of Electronic Science and Engineering, Kyoto University, Kyoto 615-8510, Japan

Realizing single-mode, high-power, high-beam-quality semiconductor lasers, which rival (or even replace) bulky gas and solid-state lasers, is one of the ultimate goals of photonics and laser physics. Conventional high-power semiconductor lasers, however, inevitably suffer from poor beam quality owing to the onset of many-mode oscillation. In this conference, I will review the recent progress, in which these challenges have been surmounted by developing large-scale photonic-crystal surface-emitting lasers (PCSELs) with controlled Hermitian and non-Hermitian couplings inside the photonic crystal. A CW output power exceeding 50W with purely single-mode oscillation and an exceptionally narrow divergence of 0.05˚has been achieved for PCSELs with a diameter of 3mm. The brightness, a figure of merit encapsulating both output power and beam quality, exceeds 1GWcm-2sr-1, which is over ten times larger than those of conventional semiconductor lasers and rivals those of existing bulky lasers. I will also discuss our recent efforts towards realizing even 1-kW-class PCSELs with expanded resonant diameters of 10mm and finely tuned Hermitian and non-Hermitian couplings. Such PCSELs are expected to replace conventional, bulkier lasers in the near future. Finally, I will refer to the high functionalities of PCSELs including the emission of arbitrary beam patterns, and high-peak-power short-pulse generation.

Plenary Talk PLV III Mon 14:00 H2

Physics informed artificial intelligence and data-driven design of materials — •Jörg Neugebauer — MPI für Nachhaltige Materialien, Düsseldorf, Germany

Recent advances in materials science have introduced novel compositionally and structurally complex materials, opening up a vast configuration space for discovery. These innovative materials promise to revolutionize industries related to energy storage, transportation, and medicine. However, traditional methodologies fall short in dealing with the high-dimensional configuration spaces involved. This presentation addresses the application of physics-informed artificial intelligence (PIAI) and data-driven strategies as an emerging solution. PIAI uses physical laws and advanced simulation techniques to improve the predictability of AI models, while automated digital workflows facilitate efficient exploration and material discovery. This synergy accelerates the design pipeline and effectively supports navigation of the newly opened vast material space. Real-world case studies will illustrate the potential of these methodologies.

Plenary Talk PLV IV Tue 8:30 H1

Some new aspects of unconventional superconductivity in layered materials — •Irina Grigorieva — University of Manchester, Manchester, UK

I will overview our recent work on layered superconductors where signatures of unconventional superconductivity are revealed or sometimes promoted by their response to magnetic fields. Magnetic correlations and superconductivity are usually antagonistic. However, in some situations external magnetic fields can be helpful in bringing to light new superconducting properties. One example is magnetic field induced multiphase superconductivity in an anisotropic superconductor with strong spin-orbit coupling, PdBi2. Another is an unconventional response of surface superconductivity to the applied magnetic field due to the presence of topological surface states in In2Bi. Yet another is proximity superconductivity surviving in the quantum Hall regime in Josephson junctions based on twisted bilayer graphene. I will discuss the underlying mechanisms and their relation to unconventional topology of these materials.

Plenary Talk PLV V Wed 8:30 H1

Ultrafast magnetism- terra incognita beyond the classical approximations — •Alexey Kimel — Radboud University, Nijmegen, The Netherlands

While the conventionally accepted Curie-Neumann's principle states that "the symmetries of the causes are to be found in the effects" [1], in ultrafast magnetism the principle fails and magnetization dynamics becomes counter-intuitive. We will demonstrate that ultrafast (sub-100 ps) heating with the help of ultrashort laser pulses causes magnetization reversal without any magnetic fields [2], laser-induced spin dynamics is strongly non-linear, where new channels of spin-lattice interaction open-up [3,4], the principle of superposition fails i.e. 1+1>2 [5] and the approximation of macrospin is no longer adequate [6].

[1] P. Curie, J. Phys. Theor. Appl., 393-415(1894).
[2] T.A. Ostler et al, Ultrafast heating as a sufficient stimulus for magnetization reversal in a ferrimagnet, Nature-Communications 3, 666 (2012).
[3] E. A. Mashkovich et al, THz light driven coupling of antiferromagnetic spins to lattice, Science 374, 1608-1611 (2021).
[4] T. W. J. Metzger et al, Magnon-phonon Fermi resonance in antiferromagnetic CoF2, Nature Communications 15, 5472 (2024).
[5] T. G. H. Blank et al, Empowering control of antiferromagnetic spins by THz spin coherence, Phys. Rev. Lett. 131, 096701 (2023).
[6] F. Formisano et al, Coherent THz spin dynamics in antiferromagnets beyond the approximation of the Neel vector, APL Mater. 12, 011105 (2024).

Plenary Talk PLV VI Wed 14:00 H1

Topological spin-textures – from domain walls to Hopfions: Current innovations and future challenges — •Stefan Blügel — Peter Grünberg Institute, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Topological spin- and magnetization textures, generally associated with Skyrmions, is a very exciting, timely and multidisciplinary field, where mathematicians, theoretical and computational physicists meet with experts on film and multilayer growth, on high-resolution magnetization and electronic structure characterization, transport and dynamics, and on device concepts and devices in order to integrate these particles into the field of spintronics. It is very fascinating to observe that simple spin models, which can be determined for real materials by density functional theory calculations, lead to micromagnetic equations whose solutions are localized topological textures in an homogeneous solid, which can now be studied by experimental methods, e.g. by means of quantitative off-axis electron holography or x-ray ptychography. Drawing a line between the first solitary wave discovered by John Scott Russel and Heisenberg's question of how countable particles can appear in continuous fields, I will give an elementary overview of the field, introduce the core objects and the primary interactions, discuss their nonlinear behavior which can be useful for neuromorphic spintronics, discuss their electric detection and magnetic hopfions, a new type of solitonic structure in three dimensions shaped as bounded knots, and their recent discovery stabilized by a skyrmion filament.

Work is supported by the ERC Grant 856538 - 3D MAGiC.

Plenary Talk PLV VII Wed 14:00 H2

Variance sum rule for dissipative systems — •Felix Ritort — Small Biosystems Lab, Condensed Matter Physics Department, University of Barcelona, C/ Marti i Franques, 1, 08028 Barcelona (Spain)

Nonequilibrium pervades nature, from the expanding universe to climate dynamics, living cells, and molecular machines. Key to nonequilibrium states is the entropy production rate σ at which energy is dissipated to the environment. Despite its importance, σ remains challenging to measure, especially in nanoscale systems with limited access to microscopic variables. I present a recently introduced variance sum rule for displacement and force variances that permits measuring σ by constraining energetics through modeling [1,2]. We apply it to measure the first heat map of human red blood cells in experiments with laser optical tweezers and ultrafast life-imaging microscopy. The variance sum rule sets a new resource for energy inference in nonequilibrium systems [3], from measuring entropy production in active and living matter to identifying hidden sources of energy and dissipation.

[1] Di Terlizzi, I., Gironella, M., Herráez-Aguilar, D., Betz, T., Monroy, F., Baiesi, M., & Ritort, F. (2024). Variance sum rule for entropy production. Science, 383(6686), 971-976. [2] Di Terlizzi, I., Baiesi, M., & Ritort, F. (2024). Vari-

ance sum rule: proofs and solvable models. New Journal of Physics, 26, 063013. [3] Roldán, É. (2024). Thermodynamic probes of life. Science, 383(6686), 952-953.

Plenary Talk PLV VIII Thu 8:30 H1

Learning how biomolecules move and undergo chemical reactions — •Frauke Gräter — Max Planck Institute for Polymer Research, Mainz, Germany

Life is biochemistry in action. While molecular simulations of systems as complex as whole cells are now within reach, predicting chemical reactivity on relevant time and length scales remains a challenge. I will present our recent work towards bringing action * here: chemistry * to classical atomistic simulations and molecular design through machine learning.

We substitute costly quantum mechanical calculations with a graph neural network-based emulator which predicts reaction rates without explicitly modelling the reaction. To deal with the chemistries arising from the such reactions, we have developed a framework to parametrize a classical force field. GRAPPA leverages graph attention, is highly accurate, and can be easily fine-tuned. Our ML-based simulations can predict cascades of chemical reactions amidst the 'jiggling and wiggling' of biomolecules at an efficiency close to classical simulations.

Finally, I will demonstrate how we harness a flow-matching model based on geometric algebra and trained on Molecular Dynamics simulations to design novel proteins with tailored flexibilities. Our method generates conformational ensembles of unseen proteins without the need to run costly Molecular Dynamics simulations, and paves the way for generating novel proteins with biochemical functions that rely on molecular motions.

Plenary Talk PLV IX Thu 14:00 H1

Tunable Ultrafast Dynamics of Antiferromagnetic Vortices in Nanoscale Dots — •Jelena Klinovaja[1], Ji Zho[1], Even Thingstad[1], Se Kwon Kim[2], and Daniel Loss[1] — [1]Department of Physics University of Basel Klingelbergstrasse 82 4056 Basel, Switzerland — [2]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea

Topological vortex textures in magnetic disks have garnered great attention due to their interesting physics and diverse applications. However, up to now, the vortex state has mainly been studied in microsize ferromagnetic disks, which have oscillation frequencies confined to the GHz range. We propose an experimentally feasible ultrasmall and ultrafast vortex state in an antiferromagnetic nanodot surrounded by a heavy metal, which is further harnessed to construct a highly tunable vortex network. We theoretically demonstrate that, interestingly, the interfacial Dzyaloshinskii-Moriya interaction (iDMI) induced by the heavy metal at the boundary of the dot acts as an effective chemical potential for the vortices in the interior. Mimicking the creation of a superfluid vortex by rotation, we show that a magnetic vortex state can be stabilized by this iDMI. Subjecting the system to an electric current can trigger vortex oscillations via spin-transfer torque, which reside in the THz regime and can be further modulated by external magnetic fields. Coherent coupling between vortices in different nanodisks can be achieved via an antiferromagnetic link. Remarkably, this interaction depends on the vortex polarity and topological charge and is also exceptionally tunable through the vortex resonance frequency.

Plenary Talk PLV X Thu 14:00 H2

Process-directed formation of nonequilibrium structures in copolymer materials — •Marcus Müller — Georg-August-Universität, Göttingen, Germany

Macromolecular systems often become trapped in metastable structures rather than reaching true equilibrium, offering opportunities to fabricate structures with unique properties. Process-directed structure formation refers to reproducibly trapping the kinetics of structure transformation into a desired (meta)stable target structure after a quench of the thermodynamic state, such as solvent evaporation or light-stimulated chemical conversions. This strategy leverages several unique advantages of copolymer systems, including a comprehensive knowledge of equilibrium properties and a clear separation of timescales between the quench of thermodynamic variables, the system's spontaneous relaxation toward the nearest metastable structure, and its thermally activated escape toward equilibrium. Both highly coarse-grained particle-based and continuum models will be discussed, highlighting challenges for quantitatively predicting copolymer material processing at the molecular scale.

Plenary Talk PLV XI Fri 8:30 H1

Exploring correlated phases and topology in van der Waals platforms — •Roser Valenti — Institute of Theoretical Physics, Goethe University Frankfurt

In recent years a plethora of new correlated states have been observed by stacking, twisting and straining two dimensional van der Waals materials of different kind. Some prominent examples are twisted bilayer graphene, bilayer heterostructures of graphene with the spin-orbit assisted Mott insulator α-RuCl3 -a candidate for Kitaev spin physics-, or bilayer heterostructures of the Mott insulator 1T-TaS2 with the metal 1H-TaS2. Unique to these bilayer structures is the possible emergence of phases not foreseable from the single layers alone, such as heavy fermions, Kondo insulators, quantum spin liquids, correlated metals, or topological superconductors.

In this talk I will discuss the microscopic modelling of such heterostructures by a combination of first-principles calculations, effective-model considerations, many-body techniques and statistical/ machine learning methods and will present exemplary cases on the emerging correlated electronic and magnetic properties[1-5] and will compare with experimental results.

[1] Rai et al. PRX 14, 031045 (2024)
[2] Crippa et al. Nature Communications 15, 1357 (2024)
[3] Akram et al. Nano Letters 24, 890 (2024)
[4] Hu et al. PRL 131, 166501 (2023)
[5] Yang et al. Nature Materials 22, 50 (2023)

Prize Talks

Prize Talk PRV I Mon 13:15 H2

Correlated phases in the vicinity of tunable van Hove singularities in Bernal bilayer graphene — •Anna Seiler — ETH Zürich — University of Göttingen — Laureate of the Gustav-Hertz-Prize 2025

The band structure of naturally occurring Bernal bilayer graphene features four linearly dispersed Dirac cones [1] but undergoes significant changes under the application of large electric displacement fields across the two layers. In this regime, tunable van Hove singularities give rise to complex correlated states. Our experiments reveal signatures consistent with various interaction-driven phases, including fractional metals of the Stoner type [2, 3]. More strikingly, we identify competing nontrivial insulating phases at both hole [2] and electron doping [3]. These phases exhibit intriguing temperature dependence and nonlinear I-V characteristics at zero magnetic field, consistent with sliding Wigner crystals of both trivial and nontrivial topology [2-4].

[1] A.M. Seiler, N. Jacobsen, M. Statz, N. Fernandez, F. Falorsi, K. Watanabe, T. Taniguchi, Z. Dong, L.S. Levitov, R.T. Weitz, Nat. Commun. 13, 4187 (2024)
[2] A.M. Seiler, F.R. Geisenhof, F. Winterer, K. Watanabe, T. Taniguchi, T. Xu, F. Zhang, R.T. Weitz, Nature 608, 298-302 (2022)
[3] A.M. Seiler, M. Statz, I. Weimer, N. Jacobsen, K. Watanabe, T. Taniguchi, Z. Dong, L.S. Levitov, R.T. Weitz, Phys. Rev. Lett. 133, 066301 (2024)
[4] A.M. Seiler, M. Statz, C. Eckel, I. Weimer, J. Pöhls, K. Watanabe, T. Taniguchi, F. Zhang, R. T. Weitz, arXiv:2408.16628 (2024)

Prize Talk PRV II Tue 13:15 H2

Single-molecule electron spin resonance by means of atomic force microscopy — •Lisanne Sellies — University of Regensburg, Regensburg, Germany — IBM Research Europe - Zurich, Rüschlikon, Switzerland — Laureate of the Gustav-Hertz-Prize 2025

Recently, we combined the high energy resolution of electron spin resonance (ESR) with the spatial resolution offered by atomic force microscopy (AFM) [1]. This ESR-AFM technique relies on driving electron spin transitions between the non-equilibrium triplet state levels of a single molecule. Since these triplet states typically have different lifetimes, driving such transitions modifies the overall triplet lifetime [1,2], which can be detected by an electronic pump-probe scheme [3].

In this talk, an introduction to ESR-AFM will be given. It will be shown that the ESR-AFM spectra feature a sub-nanoelectronvolt energy resolution. Thereby, molecules only differing in their isotopic configuration can be distinguished. Moreover, due to the minimally invasive nature of the ESR-AFM technique, the electron spins of pentacene can be coherently manipulated over tens of microseconds [4]. The high energy resolution and long spin coherence represent a leap forward for local studies of future artificial quantum systems and fundamental local quantum-sensing experiments.

[1] L. Sellies et al., Nature, 624, 64 (2023)
[2] J. Peng et al., Science, 373, 452 (2021)
[3] J. Köhler et al., Nature, 363, 242 (1993)
[4] J. Wrachtrup et al., Nature, 363, 244 (1993)

Prize Talk PRV III Wed 13:15 H2

Complex liquids under confinement — •Regine von Klitzing[1,2], Michael Ludwig[1], Thomas Tilger[1], and Larissa Braun[1] — [1]Institute for Condensed Matter Physics, Hochschulstrasse 8, 64289 TU Darmstadt — [2]Laureate of the Gentner-Kastler-Prize 2025

Complex liquids are widely used in many applications, from industrial painting processes to personal care products. Despite their numerous applications, they are still actively discussed in basic research, e.g. their structural behaviour under confinement. In the present study, colloidal dispersions (e.g. nanoparticle suspensions, micellar solutions) are confined between two surfaces in a Colloidal Probe Atomic Force Microscope (CP-AFM) or in a Thin Film Pressure Balance (TFPB). When approaching the surface, the depletion of the dispersion from the thin film leads to oscillations of the interaction force between the confining surfaces. The structure of the confined colloidal dispersions is compared with their bulk structure, which is analysed by small-angle neutron or X-ray scattering (SANS, SAXS). The results show that the softness and the charge of the particles have a strong influence on the scaling law for the particle distance and the correlation length of the particle distribution, which is not yet fully understood. Another open question is when a charged object can be considered as an ion contributing to the electrostatic screening between two confining surfaces and when it behaves like a charged particle, where the jellium approach could provide a suitable model to describe the experimental data.

Prize Talk PRV IV Wed 13:15 H4

Nanowire-based THz polarimetry — •Michael Johnston — Department of Physics, University of Oxford, Oxford, UK. — Laureate of the Max-Born-Prize 2025

Semiconductor nanowires show extreme polarization selectivity for both visible and terahertz photons. We are utilising an in-depth knowledge of ultrafast charge-carrier dynamics in nanowires to develop unique devices for THz polarimetry. Our photoconductive THz sensors based on a hash-nanowire architecture are compact and recover the full polarisation state of THz pulses. These nanowire-based devices are showing promise in areas including semiconductor characterisation and the development of metamaterials for THz polarisation manipulation.

Prize Talk PRV V Thu 13:15 H2

Altermagnetism and spin symmetries — •Libor Šmejkal — Max Planck Institute for the Physics of Complex Systems — Laureate of the Walter-Schottky-Prize 2025

Since the 1930s, magnetism had been divided into two main branches: ferromagnetism and antiferromagnetism. Recently, we have identified a new branch, altermagnetism, characterized by a d-, g-, or i-wave spin order [1]. Our discovery emerged from our systematic spin symmetry classification [1], analogous to the well-established classifications in the fields of superconductors, superfluids, or the Standard Model.

In this talk, we will outline our decade-long journey to uncover altermagnets, including the prediction of the anomalous Hall effect and unconventional electronic structure in compensated collinear magnets [2,3]. We will present our systematic classification that revealed beside the even-partial wave altermagnets also odd-partial wave unconventional magnets [4]. Additionally, we will highlight experimental observation of altermagnetism using photoemission spectroscopy [5] and nanoscale X-ray microscopy [6]. Finally, we will explore emerging research directions [7], more than 300 material candidates, and potential applications of altermagnets across and beyond solid-state physics [8], e.g. in ultrafast and low power nanoelectronics.

[1] PRX 12, 031042 (2022)
[2] Science Adv. 6, 23 (2020)
[3] PNAS 118 42 (2021)
[4] arXiv:2309.01607v3
[5] Nature 626, 517(2024)
[6] Nature 636, 348 (2024)
[7] arXiv:2411.19928
[8] https://www.science.org/content/article/breakthrough-2024, https://www.economist.com/science-and-technology/2024/01/24/scientists-have-found-a-new-kind-of-magnetic-material

Prize Talk PRV VI Thu 13:15 H4

Confining strongly correlated quasiparticles in 2D semiconductors — •Wouter Jolie — II. Physikalisches Institut, Universität zu Köln, Germany — Laureate of the Gaede-Prize 2025

Electrons are prone to strong correlations when confined into one-dimensional (1D) or 0D cavities. Many exotic ground states can emerge, depending on the type of interactions at play. Examples are Peierls transitions, Tomonaga-Luttinger liquids or Anderson impurities.

An ideal experimental testbed for the observation of correlated electronic behaviour are metallic mirror twin boundaries (MTBs) in the two-dimensional semiconductor MoS_2. These MTBs have well-defined structural and electronic properties, are only weakly coupled to the environment and accessible to spatially resolved spectroscopic techniques such as scanning tunnelling microscopy.

In my talk I will show that the confined quasiparticles within finite MoS_2 MTBs transform into spin and charge excitations as described by the Tomonaga-Luttinger liquid theory of strongly interacting 1D electrons. In addition, a Kondo resonance emerges when the highest occupied state is filled by a single electron, in quantitative agreement with the Anderson impurity model. Lastly, I will outline possible ways to create and manipulate new types of correlated states in this system.

Ceremonial, Lunch, Evening Talks and Discussions

Discussion PSV I Mon 13:15 H1

Karriere auf Zeit: Perspektiven auf befristete Arbeitsverträge in der Wissenschaft — •Carolin Wagner[1], •Axel Dürkop[2], •Raja Hoffmann[3,4], Pauleo Nimtz[4], David Smolinski[4], Susanne Liese[5] und Alexander Schlaich[5] — [1]Mitglied der Bundestags, Ausschuss für Bildung, Forschung und Technikfolgenabschätzung — [2]Universität Regenburg, Konvent der wissenschaftlichen und künstlerischen Mitarbeiterinnen und Mitarbeiter — [3]Universität Jena — [4]jDPG — [5]AGyouLeaP

Befristete Arbeitsverträge prägen den Alltag vieler Wissenschaftlerinnen und Wissenschaftler. Die Diskussionsrunde beleuchtet die Herausforderungen und Chancen dieser Beschäftigungsform aus der Perspektive von Expert:innen aus Wissenschaft und Politik. Wie lassen sich Planungssicherheit, Innovation und wissenschaftliche Freiheit vereinbaren? Gemeinsam suchen wir nach Wegen für faire und zukunftsfähige Karrierewege in der Wissenschaft.

AGyouLeaP und jDPG freuen sich auf eine spannende Diskussion mit Dr. Carolin Wagner, Prof. Dr. Axel Dürkop und Raja Hoffmann.

Lunch Talk PSV II Tue 13:15 H1

Research Funding by the DFG - Funding of Coordinated Programmes — •Christian Hahn[1], Mario Bomers[1], Joanna Kowalska[1], Michael Mössle[1], and Uwe Bovensiepen[2] — [1]German Research Foundation (DFG), Bonn — [2]Fakultät für Physik, Universität Duisburg-Essen and CENIDE, Duisburg

The German Research Foundation (DFG) is the central research funding organization in Germany. It is self-governed by the scientific community, supports research projects and funds cooperation between researchers. The DFG offers a broad range of funding opportunities from individual grants to larger coordinated programmes. This talk will focus on the DFG funding lines for coordinated projects, such as Collaborative Research Centres, Priority Programmes or Research Units. These programmes promote cooperation and structural innovation by fostering national and international collaboration in areas of current relevance. Also, we will give some first-hand insights into the review and decision process for the coordinated programmes from the perspective of the DFG head office and a current review board member.

Lunch Talk PSV III Tue 13:15 H4

Menschheitsaufgabe Klimawandel und die DPG: Gründung der AG Klima — •Gregor Schaumann — JMU Würzburg

Der menschengemachte Klimawandel mit allen humanitären Folgen ist ein physikalischer Fakt. Wie gehen wir als einzelne Wissenschaftler:in, beziehungsweise im Verband wie der DPG mit dem Befund um? Worin besteht die Verantwortung der Wissenschaft in dem Kontext? Seit einem Jahr gründet sich innerhalb der DPG die AG Klima, die das Thema als Querschnittthema in der DPG begreift. Im Vortrag werden das Selbstverständnis und die Aktivitäten der AG Klima vorgestellt. Im Anschluss gibt es in der Klima-Lounge die Möglichkeit zum Austausch und Einbringen Ihres Standpunkts.

PSV IV: Ceremonial Session with Award Ceremony

Time: Tuesday 16:00–18:00 Location: H1

Ceremonial Talk PSV IV H1

How to build a biological cell from scratch — •Petra Schwille — MPI of Biochemistry, Martinsried

Researchers at the interface of biology with the quantitative sciences, like physics and chemistry, have in the past years been pursuing a new approach towards a fundamental understanding of living systems, termed "bottom-up synthetic biology". The underlying idea is that only a radical simplification and abstraction of a biological cell will allow us to decipher the distinctive features of life, because even the simplest life forms on earth have accumulated a huge degree of redundancy, in order to remain viable in a hostile and competitive environment. Thus, in order to arrive at a self-sustaining minimal reaction system with the ability to replicate and evolve - a minimal living system - we likely need to build it from scratch. I will show how the bottom-up assembly of a minimal functional machinery accomplishes the spontaneous division of a vesicle-based artificial cell. Important functions that we have successfully reconstituted in a minimal model system include autonomous assembly, positioning, and contraction of a minimal division ring.

Discussion PSV V Wed 13:15 H1

Career Paths: Academia or Industry? — •Adelind Elshani[1], •Jan Wilhelm[2], •Valentin Kahl[3], Hans-Georg Grothues[4], Pauleo Nimtz[5], and Susanne Liese[6] — [1]RWTH Aachen — [2]University of Regensburg — [3]ibidi GmbH, Munich — [4]Arbeitskreis Industrie und Wirtschaft — [5]jDPG — [6]AGyouLeaP

After completing your undergraduate studies, your PhD, or, at the latest, your first postdoc, you may ask yourself the question: Do I want to stay at a research institution or work in industry? In this panel discussion, we would like to talk about this question with experts from different areas of science and industry representing different varieties of career paths. We are looking forward to a diverse panel discussion with Adelind Elshani RWTH Aachen, Dr. Jan Wilhelm, University of Regensburg, and Dr. Valentin Kahl, ibidi GmbH, Munich.

Lunch Talk PSV VI Wed 13:15 H3

Book Launch – Physik: Erkenntnisse und Perspektiven (in German) — Joachim Ullrich[1], Ulrich Bleyer[1], •Sarah Köster[2], Claus Lämmerzahl[3], Dieter Meschede[4] und •Lutz Schröter[1] — [1]Deutsche Physikalische Gesellschaft e. V., Bad Honnef — [2]Universität Göttingen, Institut für Röntgenphysik, Göttingen — [3]Universität Bremen, Weltraumwissenschaft ZARM, Bremen — [4]Universität Bonn, Institut für Angewandte Physik, Bonn

Join us for the book launch of the new DPG publication. You will have the opportunity to pick up a free copy – while stocks last!

The title "Physik: Erkenntnisse und Perspektiven" (Physics: Insights and Perspectives) refers to a publication, which was produced on a voluntary basis by almost 200 authors. It provides a detailed exploration of the fundamentals of physics, current research and future developments. The book offers readers an engaging and inspiring insight into the world of physics! The publication is also available at www.physik-erkenntnisse-perspektiven.de – along with exclusive video interviews. Printed copies can also be ordered by covering the shipping costs.

Evening Talk PSV VII Wed 19:00 H1

Leben in einer wärmer werdenden Welt: Wie der Klimawandel unser Leben beeinflusst — •Thomas Jung — Alfred Wegener Institut, Bremerhaven, Deutschand

In seinem Vortrag erklärt Professor Thomas Jung vom Alfred-Wegener-Institut, wie der Klimawandel unser Leben auf lokaler Ebene beeinflusst. Mit Hilfe von Beobachtungsdaten und modernen Klimamodellen zeigt er, wie sich eine wärmere Welt auf unser Wetter auswirkt, von häufigeren Extremwetterereignissen bis hin zu Veränderungen in den Jahreszeiten. Gleichzeitig veranschaulicht er, wie das heutige Wetter unter den Bedingungen eines vorindustriellen Klimas ausgesehen hätte. Professor Jung präsentiert dabei neue Ergebnisse aus der Klimaforschung, die durch hochauflösende Klimasimulationen und sogenannte Storyline-Verfahren gewonnen wurden. Diese innovativen Methoden ermöglichen es, den Klimawandel und dessen Auswirkungen greifbar zu machen. Dabei möchte er nicht nur die Herausforderungen des Klimawandels aufzeigen, sondern auch Perspektiven für positive Veränderungen entwickeln, die uns alle zum Handeln inspirieren können.

Lunch Talk PSV VIII Thu 13:15 H1

Let's talk about science communication! — •Nicolas Wöhrl and Peter Kohl — University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

Trust in science is essential – not as blind acceptance, but as informed trust based on an understanding of how the scientific method works. At a time when social issues are increasingly politicized and overshadowed by desinformation, the ability to critically assess data, distinguish between fact and fiction and develop evidence-based arguments makes researchers indispensable voices. Trust in science is not solely built on reliable data and conclusions; it also hinges on the transparency of the scientific process itself. The public should be familiar with how science works and how knowledge is generated to be able to make societal decisions that are based on facts.. Trust in science is not only gained through excellent research, but also by getting to know the actual people that stand behind the results. This is a communication challenge that, in principle, all researchers

can take on. They can convey, how the scientific method makes an evidence-based world view possible.

Some topics, addressed in this talk: Why do we need communicating scientists alongside press offices and science journalism? How can science communication be done despite all other tasks in research and teaching? What role can it play in a scientific career? Do I have talent for outreach and how do I find out which formats are best for me?

Lunch Talk PSV IX Thu 13:15 H3

From PhD to Head of Product Management at a Biotech Company — •Judith Stolwijk — ibidi GmbH

ibidi is a leading supplier for functional cell-based assays and advanced products for cellular microscopy. ibidi is located in Gräfelfing, Germany, close to Munich. In 2001, ibidi was founded by three physics PhD students and their group leader as a spin-off from the Technische Universität München (TUM) and the Center for Nanoscience (CeNS) at the University of Munich (LMU). Today, a close-knit team of physicists, biologists, and engineers work together to develop ground-breaking products.

Tutorials

TUT 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:
https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:
https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial TUT 1.1 Sun 16:00 H2

Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial TUT 1.2 Sun 16:40 H2

Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial TUT 1.3 Sun 17:30 H2

Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

TUT 2: Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)

NOMAD (nomad-lab.eu) [1] is an open-source, community-driven data infrastructure, that supports automated (meta)data extraction from a wide range of simulations, including ab initio and advanced many-body calculations as well as molecular dynamics simulations. NOMAD allows users to store both standardized and custom complex simulation workflows, which not only streamlines data provenance and analysis but also facilitates the curation of AI-ready datasets. This tutorial will focus on recently developed workflow functionalities and utilities within the NOMAD infrastructure. These advances enable high-throughput interfacing with the NOMAD repository, opening improved discovery pipelines by leveraging the benefits of NOMAD's comprehensive and FAIR-compliant data management system [2].

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

Time: Sunday 16:00–18:00 Location: H3

Tutorial TUT 2.1 Sun 16:00 H3

FAIR-data management with the NOMAD infrastructure: Core functionalities — •Joseph F. Rudzinski — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this first part of the tutorial series, an overview of the NOMAD infrastructure will be provided. Attendees will learn how NOMAD processes raw data and stores it within a generalized data structure, and the corresponding GUI features that allow users to comfortably browse data. An example scenario will also be set up for use throughout the remainder of the tutorial series: *A researcher with a variety of data obtained within a project workflow would like to upload this data to NOMAD in order to link it to their manuscript while exposing the details of their (meta)data and retaining the scientifically relevant connections between the individual project tasks.*

Tutorial TUT 2.2 Sun 16:30 H3

Using NOMAD's API for project management — •Nathan Daelman — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, you will learn how to interface with NOMAD programmatically using a Python module built to simplify the API (application programming interface). Functionalities for uploading data, editing metadata of uploads, creating datasets with multiple uploads, and publishing data will be covered. Attendees will use these functionalities to manage a portion of the data from the example project workflow, in particular, the subset of data that is automatically recognized and processed by one of NOMAD's existing parsers. *(For attendees without any Python experience, an alternative route to upload via the GUI will also be demonstrated!)*

Tutorial TUT 2.3 Sun 17:00 H3

Creating custom entries in NOMAD using yaml schema and ELN integration — •Andrea Albino — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, attendees will learn how to create custom entries to store data that is not already supported by one of NOMAD's parsers. The basics of writing a schema, using NOMAD's ELN (electronic lab notebook) integration, and how to create simple plots of your data to visualize in the GUI will be covered. Attendees will then use this knowledge to manage the remainder of the data from the example project workflow, which is not automatically recognized by NOMAD.

Tutorial TUT 2.4 Sun 17:30 H3

Creating custom workflow entries in NOMAD to link multiple uploads — •Bernadette Mohr — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this last part of the tutorial series, attendees will complete the example project workflow storage by creating a custom workflow entry in NOMAD that connects all the uploaded tasks. The basics of the schema for defining custom workflows will be covered, followed by a demonstration of the straightforward creation of the required workflow file using the same workflow utility Python module as in the first part of the tutorial series. Finally, attendees will navigate NOMAD's interactive workflow graph visualizations to investigate the uploaded data, and learn how to obtain a DOI for their workflow.

TUT 3: Tutorial: Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism (joint session MA/TUT)

Nanostructured magnetic materials have found several applications in everyday objects, such as data storage devices, sensors, and biomedical devices. When one brings these materials to the third dimension, a variety of new physics, and opportunities for applications appear. However, until recently, the vast majority of experimental investigations have primarily been focused on 2D planar geometries, as 3D systems provide a set of experimental challenges that still needs to be overcome. This tutorial seeks to provide a comprehensive overview for both experts and non-experts in the field of 3D imaging to gain a deeper understanding of the recent advances and experimental challenges connected to the investigation of 3D magnetic systems.

Organized by Claire Donnelly (MPI-CPFS, Dresden, Germany) and Simone Finizio (Paul Scherrer Institut, Villigen, Switzerland).

Time: Sunday 16:00–18:15 Location: H4

Tutorial TUT 3.1 Sun 16:00 H4

3D Magnetic Imaging: Utilizing Synchrotron X-Ray Coherence for Nanometric Resolution in Thick Samples — •Marisel Di Pietro Martinez — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2)

In recent years, there has been a growing interest from the magnetism community in expanding to three-dimensional magnetic systems - from exploring new geometries to revealing complex magnetic textures arising in micrometer-thick samples. A key aspect of this exploration is the ability to visualize the magnetization vector field at the nanoscale throughout the entire sample, made possible by the development of 3D magnetic imaging. This technique can achieve nanometric spatial resolution in micrometer-thick samples by leveraging the penetration depth and coherence of synchrotron X-rays. Furthermore, the coherence of the X-ray beam provides magnetic contrast not only in the absorption of the transmitted wave, but also in the phase. This phase contrast enables the investigation of micron-sizes magnets, even with soft X-rays, while minimizing the sample damage. In this tutorial, I will introduce how to exploit these advantages using coherence-based techniques, such as Fourier transform holography and ptychography, to perform 3D magnetic imaging. Visualizing the magnetization vector field with nanometer spatial resolution in micrometer thick samples opens the door to studying magnetic textures in higher dimensions, offering insights into fundamental physical phenomena as well as promising new applications in information storage and processing.

Tutorial TUT 3.2 Sun 16:45 H4

Nanoscale Mapping of Magnetic Textures in 3D Using Vector Field Electron Tomography — •Axel Lubk[1,2] and Daniel Wolf[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany

Vector field Electron Tomography (VFET) combines Electron Holography and Electron Tomography in the Transmission Electron Microscope (TEM) to reconstruct magnetic induction vector fields in 3D down to several nanometer resolution. In this tutorial we discuss the foundations of the technique, the practical workflow including pitfalls, and application to topical examples in nanomagnetism including domain walls in nanowires and skyrmion strings.

Tutorial TUT 3.3 Sun 17:30 H4

3D magnetic imaging: an experimental window to study 3D magnetization at the nanoscale — •Aurelio Hierro-Rodriguez — Department of Physics, University of Oviedo,33007, Oviedo, Spain — CINN (CSIC-University of Oviedo) , 33940, El Entrego, Spain

The synergetic confluence of technological and scientific developments in nanofabrication and characterization techniques is paving the way towards the advance in Three-Dimensional Nanomagnetism, fuelled by the richness of phenomena and technological potential of the exploitation of the magnetization vector field in their natural dimensionality: three dimensions. In this lecture, a broad picture of the importance of the topic, in the framework of the novel physics that can be explored and exploited will be given, with a brief description of the methods that allow to fabricate almost any 3D magnetic geometry with nanometer resolution. The core of the lecture will deal with the advanced magnetic imaging techniques, which are opening a window towards the characterization of the full three-dimensional magnetization vector. Specifically, X-ray based magnetic vector tomography will be described and exemplified, showing the capabilities of the technique to volume resolve the magnetization vector field in arbitrary systems with nanometer resolution. These developments in vector magnetic imaging are making possible a change in the actual paradigm on how magnetization is characterized and studied at the nanoscale, by bringing a direct experimental probe to realize experimental micromagnetism.

TUT 4: Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)

This tutorial is designed for students, early-career researchers, and anyone interested in the foundational principles and practical methods for simulating magnetic materials. The journey begins with an introduction to the fundamentals of spin lattice Hamiltonians and their various forms, including a detailed discussion of their derivation (Lecture 1). Next, we explore state-of-the-art techniques for extracting magnetic exchange interactions from first-principles calculations through an engaging overview (Lecture 2). The final session (Lecture 3) delves into atomistic spin-dynamics simulations using the SPIRIT code, a versatile tool compatible with both smartphones and laptops. Throughout, we will emphasize the theoretical framework underpinning these approaches. The participants will have the freedom to explore a large range of phenomena, such as domain walls, skyrmions, and their dynamics under applied currents or torques.

Time: Sunday 16:00–18:15 Location: H10

Tutorial TUT 4.1 Sun 16:00 H10

Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange — •Hiroshi Katsumoto — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52428 Jülich, Germany

Magnetization textures, such as domain walls, skyrmions, or hopfions, are very active areas of condensed matter physics. These magnetic textures are usually explained based on the Heisenberg and the relativistic Dzyaloshinskii-Moriya interaction (DMI). Comparisons with experiments have shown that, in many cases, these interactions are insufficient, and a whole range (sometimes called a zoo) of higher-order symmetric and antisymmetric interactions have been proposed. In this tutorial, based on four elemental ingredients: Coulomb interaction, indistinguishability of electrons, spin, and spin-orbit interaction (SOI), I present a framework for systematically constructing exact spin-lattice models containing all spin Hamiltonians, including higher-order terms dependent on spin quantum numbers and lattice size. Examples of spin Hamiltonians for spin-1/2 and spin-1 systems up to four lattice sites are discussed. The tutorial also explores higher-order relativistic exchange interactions derived from SOI. I consider perturbations up to the 2^{nd} order of SOI and organize (anti)symmetric interactions. Finally, the classicalization of quantum spin relevant to magnetism in solids is discussed, culminating in a spin-lattice model that provides a theoretical framework for extracting material-dependent exchange interactions via numerical calculations and enables the modeling of magnetic textures. – DFG supports the work through SPP-2137 Skyrmionics.

Tutorial TUT 4.2 Sun 16:45 H10

Computing magnetic exchange interactions using DFT — •Manuel dos Santos Dias — Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom

Magnetic materials are an unending source of fascinating physical behaviour which have fundamental appeal but also important technological applications. In order to understand, quantify and predict the properties of magnetic materials, we need information about the magnetic exchange interactions (introduced in the preceding tutorial), which control how the different magnetic atoms interact with each other and respond to external stimuli. This tutorial will give an overview on first-principles approaches to the calculation of magnetic exchange interactions using density functional theory (DFT). First I will outline how the properties of magnetic materials can be computed with and what capabilities are offered by different DFT codes. Next I will discuss how to map DFT calculations to spin models and when such a mapping is expected to work, followed by a discussion of the two main approaches to compute magnetic exchange interactions: the infinitesimal rotation method and the spin cluster expansion. Lastly, I will explain how to obtain simple information from the computed magnetic exchange interactions, such as the magnetic ground state and the spin wave spectrum, and how to connect to atomistic spin dynamics (for instance using the Spirit code covered in the next tutorial), Monte Carlo and micromagnetic simulations.

Tutorial TUT 4.3 Sun 17:30 H10

Hands-on atomistic spin-dynamics simulations with Spirit — •Thorben Pürling[1,2] and Moritz Sallermann[1,2,3] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, D-52425 Jülich — [2]Physics Department, RWTH-Aachen University, D-52062 Aachen — [3]University of Iceland

Atomistic spin-dynamics is a powerful, fascinating and educational simulation approach to studying the stability and dynamics of mesoscopic spin-textures such as skyrmions on the basis of atomistic spin-models. It can be used as digital twin to experiments.In this tutorial, participants will be introduced to the atomistic spin model and learn interactively how to perform atomistic spin simulations using the Spirit code [1]. We will cover common computational methods employed in atomistic spin simulations, emphasizing their practical application through the Spirit software framework [2]. The majority of the session will be dedicated to engaging exercises, where participants will work through example problems using Jupyter notebooks that interface directly with Spirit. Participants are encouraged to come with basic knowledge of Python and bring their charged laptops to fully engage in the tutorial. We provide a website [3] to keep you updated such that you arrive at the tutorial prepared for a hands-on experience.
We acknowledge funding from the ERC grant 856538 (project "3D MAGIC").

[1] Gideon P. Müller *et al.*, 10.5281/zenodo.7746551 (2024)
[2] https://spirit-code.github.io
[3] https://spirit-code.github.io/dpg-regensburg2025

TUT 5: Tutorial: Automated Worksflows (joint session MM/TUT)

Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: H15

Tutorial TUT 5.1 Sun 16:00 H15

Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations — •Jörg Neugebauer[1], Tilmann Hickel[2], and Ralf Drautz[3] — [1]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [2]BAM, Berlin, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application.

In this hands-on tutorial, we provide an interactive, practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The tutorial gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, all steps of the workflow for the construction of ab initio phase diagrams will be performed interactively by all participants, e.g. the generation of DFT datasets, the training and validation of machine learning potentials as well as the construction of the phase diagram.

Symposium AI in (Bio-)Physics (SYAI)

jointly organised by
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Physics of Socio-economic Systems Division (SOE)

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Artificial intelligence is revolutionizing scientific research, including the study of biophysical systems. The symposium will explore how AI and machine learning can enhance biophysics research, with applications ranging from predictive modeling of biomolecular interactions and high-throughput data analysis to the development of machine-learned force fields and artificial scientific discovery. The goal of this symposium is to create a dynamic forum for scientific exchange in this rapidly developing field, providing novices with a valuable head start while helping experts stay at the forefront of cutting-edge developments. The conceptual nature of AI-powered research approaches will make the discussed topics highly relevant to a broad audience.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

SYAI 1.1–1.5	Thu	9:30–12:15	H1	**AI in (Bio-)Physics**

Sessions

– Invited Talks –

SYAI 1: AI in (Bio-)Physics

Time: Thursday 9:30–12:15 Location: H1

Invited Talk SYAI 1.1 Thu 9:30 H1

Predicting interaction partners and generating new protein sequences using protein language models — •Anne-Florence Bitbol — École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Protein sequences are shaped by functional optimization on the one hand and by evolutionary history, i.e. phylogeny, on the other hand. A multiple sequence alignment of homologous proteins contains sequences which evolved from the same ancestral sequence and have similar structure and function. In such an alignment, statistical patterns in amino-acid usage at different sites encode structural and functional constraints.

Protein language models trained on multiple sequence alignments capture coevolution between sites and structural contacts, but also phylogenetic relationships. I will discuss a method we recently proposed that leverages these models to predict which proteins interact among the paralogs of two protein families, and improves the prediction of the structure of some protein complexes. Next, I will show that these models can be used to generate new protein sequences from given protein families.

While multiple sequence alignments are very useful, their construction is imperfect. To address these limitations, we developed ProtMamba, a homology-aware but alignment-free protein language model based on the Mamba architecture, which efficiently uses long contexts. I will show that ProtMamba has promising generative properties, and is able to predict fitness.

Invited Talk SYAI 1.2 Thu 10:00 H1

Realizing Schrödinger's dream with AI-enabled molecular dynamics — •Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg

The convergence between accurate quantum-mechanical (QM) models (and codes) with efficient machine learning (ML) methods seem to promise a paradigm shift in molecular simulations. Many challenging applications are now being tackled by increasingly powerful QM/ML methodologies. These include modeling covalent materials, molecules, molecular crystals, surfaces, and even whole proteins in explicit water (https://www.science.org/doi/abs/10.1126/sciadv.adn4397). In this talk, I attempt to provide a reality check on these recent advances.

In particular, I will introduce the recently developed SO3LR force field (https://doi.org/10.26434/chemrxiv-2024-bdfr0), trained on a diverse set of 4 million neutral and charged molecular complexes computed at the PBE0+MBD level of quantum mechanics, ensuring a comprehensive coverage of covalent and non-covalent interactions. SO3LR is characterized by computational and data efficiency, scalability to 200 thousand atoms on a single GPU, and reasonable to high accuracy across the chemical space of organic (bio)molecules. SO3LR is applied to study units of four major biomolecule types, polypeptide folding, and nanosecond dynamics of larger systems such as a protein, a glycoprotein, and a lipid bilayer, all in explicit solvent. Finally, I discuss the future challenges toward truly general molecular simulations by combining ML force fields with traditional atomistic models.

Invited Talk SYAI 1.3 Thu 10:30 H1

Emergent behavior of artificial intelligence — •Steffen Rulands — Arnold-Sommerfeld Center for Theoretical Physics, LMU München, Theresienstr. 37, 80333 München

Can artificially intelligent systems show emergent behavior that does not originate from the data they are trained on? This question is relevant for understanding the potential dangers and possibilities of powerful AI systems. In this talk, I will address this question from two different perspectives drawing on ideas from theoretical biophysics. First, I will show that neural networks exhibit an instability that gives rise to the emergent formation of structures independent of the training data. I will show how these structures aid the interpretation of data. In the second part of my talk, I will then draw on the biophysics of subcellular compartments and insect societies to demonstrate ways in which emergent behavior of artificially intelligent systems can facilitate and jeopardize deep learning.

15 min. break

Invited Talk SYAI 1.4 Thu 11:15 H1

AI in medical research - navigating complexity with AI — •Daniel Truhn — University Hospital Aachen, Germany

Modern artificial intelligence (AI) systems, including Large Language Models (LLMs) and advanced multimodal vision systems, are transforming clinical practice and medical research. This talk outlines how these technologies navigate complex medical challenges and enhance clinician efficiency. By showcasing practical applications, I demonstrate how AI empowers healthcare professionals to make better and faster decisions, ultimately improving patient outcomes.

Invited Talk SYAI 1.5 Thu 11:45 H1

Computational Modelling of Morphogenesis — •Dagmar Iber — Department of Biosystems Science and Engineering, ETH Zürich, Switzerland

Epithelia are fundamental building blocks of life, playing pivotal roles in morphogenesis and are at the origin of most cancers. This talk will explore epithelial organization across scales, from individual cell geometry to tissue-level architecture. I will introduce theoretical work that sheds light on long-standing, unexplained phenomena in epithelial cell organization, enabling the development of advanced 2D and 3D simulation tools. These tools allow for data-driven simulations of epithelial dynamics, advancing our understanding of both development and disease. Additionally, I will examine how chemical gradients drive precise epithelial patterning during development and demonstrate how their interplay with geometric and mechanical constraints shapes epithelial morphogenesis. Case studies include neural tube formation, lung branching morphogenesis, nephrogenesis, and bladder cancer progression. By integrating experimental insights with computational approaches, this work offers a comprehensive view of the mechanisms driving epithelial morphogenesis in health and disease.

Symposium Physics of Embryonic Development Across Scales: From DNA to Organisms (SYED)

jointly organised by
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Physics of Socio-economic Systems Division (SOE)

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The development of a single fertilized cell into a fully functional embryo is a prime example of non-equilibrium self-organization. While biological research on development has focussed on molecular aspects, recent progress has brought into the spotlight the underlying physical phenomena across scales in space and time. This includes polymer physics of DNA organization, dynamical systems and information theory of gene regulation, signaling and pattern formation, and the active mechanics of cells and tissues. Development therefore presents tantalizing challenges at the interface between physics and biology, experiment and theory. Addressing these challenges requires an integrative approach that bridges scales and disciplines. This symposium will bring together researchers from diverse backgrounds and provide an overview of the exciting recent advances in experiment and theory and highlight future challenges.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher
SYED 1.2	Mon	10:00–10:30	H1	**A tissue rigidity phase transition shapes morphogen gradients** — Camilla Autorino, Diana Khoromskaia, Bernat Corominas-Murtra, Zena Hadjivasiliou, •Nicoletta Petridou
SYED 1.3	Mon	10:30–11:00	H1	**Building quantitative dynamical landscapes of developmental cell fate decisions** — •David Rand
SYED 1.4	Mon	11:15–11:45	H1	**Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate** — •Anne Grapin-Botton, Byung Ho Lee, Masaki Sano, Daniel Riveline, Kana Fuji, Tetsuya Hiraiwa
SYED 1.5	Mon	11:45–12:15	H1	**Chromosomes as active communication and memory machines** — •Leonid A. Mirny

Sessions

SYED 1.1–1.5	Mon	9:30–12:15	H1	**Physics of Embryonic Development Across Scales: From DNA to Organisms**

Sessions

– Invited Talks –

SYED 1: Physics of Embryonic Development Across Scales: From DNA to Organisms

Time: Monday 9:30–12:15 Location: H1

Invited Talk SYED 1.1 Mon 9:30 H1

Emergent crystalline order in a developing epithelium — Kartik Chhajed[1], Natalie Dye[2], Marko Popović[1], and •Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzerstrasse 38, 01187 Dresden, Germany — [2]Cluster of Excellence Physics of Life, TU Dresden, Arnoldstrasse 18, 01307 Dresden, Germany

A fundamental question in Biology is to understand how patterns and shapes emerge from the collective interplay of large numbers of cells. Cells forming two-dimensional epithelial tissues behave as active materials that can undergo remodeling and spontaneous shape changes. Focussing on the fly wing as a model system, we will discuss the physics underlying the emergence of crystalline order in the wing epithelium during the pupal phase of morphogenesis. Using a vertex model of epithelial tissue, we demonstrate that when cell size heterogeneity exceeds a critical value, cellular packing remains disordered, whereas reducing heterogeneity below this value induces a phase transition to crystalline packing. Combining these results with analysis of experimental data reveals that cell size heterogeneity controls crystallization in the developing fly wing. Shear flows facilitate this process but are not the main driver of the disorder-to-order transition. Our work reveals how order can emerge during morphogenesis by the dynamic remodeling of tissues.

Invited Talk SYED 1.2 Mon 10:00 H1

A tissue rigidity phase transition shapes morphogen gradients — Camilla Autorino[1], Diana Khoromskaia[2], Bernat Corominas-Murtra[3], Zena Hadjivasiliou[2], and •Nicoletta Petridou[1] — [1]EMBL Heidelberg, Germany — [2]Francis Crick Institute, UK — [3]University of Graz, Austria

Transitions between solid-like and fluid-like tissue material states are essential for morphogenesis. However, if phase transitions instruct cell function is still unknown. Here, we show that tissue rigidification impacts cell signalling by regulating the length-scales and time-scales of morphogen gradients. By combining rigidity percolation theory, reaction-diffusion modelling, quantitative imaging, genetics and optogenetics in zebrafish germ layer formation we uncover that a tissue rigidity phase transition defines the dynamics of fate specification by restricting Nodal morphogen transport and facilitating its signalling dynamics. This is a self-generated mechanism where Nodal, besides triggering cell fate specification, increases cell adhesion via regulating planar cell polarity genes. Once adhesion strength reaches a critical point it triggers a rigidity transition which sharply minimises tissue porosity and induces the formation of tricellular contacts. The resulted tissue reorganisation negatively feeds back to Nodal signalling by sealing the interstitial paths of Nodal diffusion and restricting it close to the source, and by speeding up its degradation. This leads to prompt expression of its inhibitor resulting in robust pattern formation. Overall, we reveal how phase transitions shape morphogen gradients and uncover macroscopic mechanisms of positional information.

Invited Talk SYED 1.3 Mon 10:30 H1

Building quantitative dynamical landscapes of developmental cell fate decisions — •David Rand — University of Warwick, Coventry CV4 7AL, UK

I will discuss the dynamics of decision-making in the early embryo. As cells proliferate and assemble into tissues, their molecular identity changes in discrete step-like transitions to produce diverging sequences of distinct cell states that culminate in the differentiation of specific functional cell types. Hence, cellular development can be viewed as sets of branching cell lineages generating increasing diversity and comprising increasingly specialised cell types. I will outline an approach to understanding this that relies on geometry and dynamics, and I will illustrate this with recent work on the early development of the nervous system. New methods for the analysis of single-cell temporal data combined with ideas from dynamical systems can be used to deduce the topology of the branching network, the dynamical nature of the branching transitions and a quantitative model of the underlying dynamics that reproduces the data.

15 min. break

Invited Talk SYED 1.4 Mon 11:15 H1

Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate — •Anne Grapin-Botton[1], Byung Ho Lee[1], Masaki Sano[2,5], Daniel Riveline[3], Kana Fuji[2], and Tetsuya Hiraiwa[2,4] — [1]Max Planck Institute of Molecular Cell Biology and Genetics Dresden — [2]The University of Tokyo — [3]IGBMC, Strasbourg — [4]Academia Sinica, Taipei — [5]Shanghai Jiao Tong University

Many organs in multicellular organisms comprise epithelia which enclose fluid-filled cavities referred to as lumens. Their formation is regulated by a wide range of processes, including polarization, secretion, exocytosis and actomyosin contractility. While these mechanisms have shed light on lumen growth, what controls lumen morphology remains enigmatic. Here we use organoids to explore how lumens acquire either a spherical shape or a branched topology. We develop a multicellular phase field model with the following basic components: conditions for the timing and volume of cell division, lumen nucleation rules, and lumenal pressure. Combining computational simulations with experimental measurements we reveal that lumen morphology arises from the balance between the cell cycle duration and lumen pressure, with more complex lumen at low pressure and fast proliferation rates. Moreover, the perturbation of proliferation and lumen pressure in silico and in vitro is sufficient to alter and reverse the morphological trajectories of the lumens. We further show that low pressure depends on epithelial permeability enabling complex lumen shapes.

Invited Talk SYED 1.5 Mon 11:45 H1

Chromosomes as active communication and memory machines — •Leonid A. Mirny — Institute for Medical Engineering and Science, and Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA

Chromosomes are long polymers of genomic DNA decorated by myriads of proteins. We are interested in understanding how cells fold them to read, write, and process genetic and epigenetic information. Can the way chromosomes are folded carry information itself?

Recent work from my group and others has shown that chromosomes are active polymers. First, we found that chromosomes are folded by the active (ATP-dependent) process of loop extrusion, where molecular motors form progressively larger loops. The collective action of these nanometer-sized motors shapes micron-sized chromosomes. This active mechanism also enables long-range communication between the *regulatory genome* and protein-coding genes.

Second, we found that chromosome folding can help store *epigenetic memory* patterns of chemical marks along the genome. Such marks are lost and spread by enzymes, yet when marks influence genome folding, the pattern of marks can be preserved for hundreds of cell divisions. We further identified a parallel between this mechanism of epigenetic memory and associative memory in a neural network, suggesting that this system may perform more complex information processing tasks.

Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

jointly organised by
the Surface Science Division (O),
the Low Temperature Physics Division (TT),
the Magnetism Division (MA),
the Crystalline Solids and their Microstructure Division (KFM),
the Semiconductor Division (HL), and
the Metal and Material Physics Division (MM)

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The next generation of quantum technologies will utilize microscopic properties without classical counterparts, often encoded in the quantum-mechanical wave function phase. These properties unify phenomena like noncollinear magnetism, multiferroicity, and superconductivity. Noncollinear magnets create emergent electromagnetic fields driving novel transport effects for spintronics, while superconductors enable dissipationless supercurrents and working qubits for quantum computers. Combining magnetic and superconducting materials can produce quantum entities like Majorana states, relevant to topological quantum computing. In this context, exciting developments based on ab-initio methods will be discussed at the symposium, providing an ideal platform for fostering collaboration among experts, students, and early-career researchers.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

SYES 1.1–1.5	Fri	9:30–12:15	H1	**Electronic Structure Theory for Quantum Technology**

Sessions

– Invited Talks –

SYES 1: Electronic Structure Theory for Quantum Technology

Time: Friday 9:30–12:15 Location: H1

Invited Talk SYES 1.1 Fri 9:30 H1

Ab-initio Design of superconductors — •Lilia Boeri — Physics Department, Sapienza University, Rome, Italy

Over the last ten years, ab-initio methods for superconductivity and crystal structure prediction have seen a substantial advancement, opening the concrete possibility of designing new conventional superconductors completely in silico. The most spectacular demonstration of the power of this approach is the prediction of high-temperature conventional superconductivity in compressed sulfur hydride, which started the so-called hydride rush towards room-temperature superconductivity.[1] However spectacular these discoveries might be, bridging the gap with applications requires devising new strategies to realize high-Tc at more accessible pressures [2], and understanding the origin of superconductivity in seemingly simple materials, like Hg and NbTi. Finally, I will addressed the challenges that the community needs to address after recent reputation breaches due to false claims of room-temperature superconductivity [3].

[1] J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, Physics Reports 856, 1-78 (2020).

[2] R. Lucrezi, S. di Cataldo, W. von der Linden, L. Boeri and Christoph Heil, NPJ Computational Materials, 8, 119 (2022).

[3] P. Ferreira , L. J. Conway, A. Cucciari, S. Di Cataldo, F. Giannessi, E. Kogler, L. T. F. Eleno, C. J. Pickard, C. Heil and L. Boeri, Nature Comm. 14, 5367 (2023)

Invited Talk SYES 1.2 Fri 10:00 H1

Topological superconductivity from first principles — Bendegúz Nyári[1,2], András Lászlóffy[3], Levente Rózsa[3,2], Gábor Csire[4], Balázs Újfalussy[3], and •László Szunyogh[2,1] — [1]HUN-REN BME Condensed Matter Research Group, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria

Magnetic chains manufactured on superconductors are possible candidates for fault tolerant quantum computing architectures. Due to the interplay of magnetism and superconductivity these systems are suitable to host topological zero-energy end states, the so-called Majorana Zero Modes (MZM). In this talk we present a first-principles approach suitable to study atomic chains by employing an embedding technique within the Multiple Scattering Theory, combined with the solution of the Bogoliubov–de Gennes equations. In case of Fe chains on an Au monolayer on Nb(110) we show that the formation of MZMs is supported in a broad range of spin-spiral states. Through computer experiments we also demonstrate the emergence of topological fragmentation and simulate the shifting of MZMs within the nanowire. Our computational method allows for calculating the one-dimensional band structure of infinite chains which provides a clear picture to analyze the topological properties of Shiba bands. The band structure is calculated and compared with the quasiparticle interference spectrum for Mn chains on Nb(110) and Ta(110).

Invited Talk SYES 1.3 Fri 10:30 H1

First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe — •Myrta Grüning[1,2], Abyay Ghosh[1], and Piotr Chudzinski[1,3] — [1]Centre for Quantum Materials and Technologies, Queen's University Belfast, Belfast, Northern Ireland (UK) — [2]European Theoretical Spectroscopy Facility — [3]Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland

FeSe is the simplest quasi-two-dimensional iron chalcogenide superconductor, yet its phase diagram exhibits exotic phases like superconductivity, spin density wave, and nematicity, which are intensely studied in condensed matter physics. Understanding the interaction of orbital and spin degrees of freedom is key to explaining FeSe's diverse phases. Using density-functional theory within the generalized gradient approximation, we calculated the structural, electronic, and magnetic properties of FeSe in its tetragonal phase. First, we explored how the d-band bandwidths at the Fermi energy evolve with corrections and long-range magnetic orders. Introducing striped or staggered dimer antiferromagnetic order significantly reduced the bandwidth overestimation seen at the generalized gradient approximation level, aligning more closely with experimental data. Next, we examined the magnetic formation energy for ferromagnetic and antiferromagnetic orders, under pressures up to 6 GPa and derived bilinear and biquadratic spin-exchange energies. We uncovered non-trivial spin-exchange behavior dependent on magnetization and proposed a field-theory model linking this to strong two-dimensional spin-orbital fluctuations.

15 min. break

Invited Talk SYES 1.4 Fri 11:15 H1

Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects. — •Thomas Olsen — Department of Physics, Technical University of Denmark

We present a systematic classification of the magnetic ground states in hundreds of two-dimensional (2D) materials. Non-collinear order is shown to be abundant and may typically be represented by planar spin spiral ground states. We discuss a range of physical effects associated with non-collinear order and take specific materials as examples. The $Ni(Cl,Br,I)_2$ compounds exhibit type II multiferroic order where the spontaneous polarization is induced by spiral order and we discuss the subtleties associated with the calculation of the polarization from first principles. The breathing Kagomé compounds $Nb_3(Cl,Br,I)_8$ are pyroelectric and have spiral ground states with ordering vectors that couple strongly to out-of-plane external electric fields. Finally we discuss a set of 2D altermagnets and analyse the important role of spin-orbit coupling with respect to the band structure, magnons and non-collinearity.

Invited Talk SYES 1.5 Fri 11:45 H1

Spin-phonon and magnon-phonon interactions from first principles — •Marco Bernardi — Caltech

Electron-phonon interactions have become a major research focus in first-principles electronic structure calculations. This talk discusses our recent efforts to include the spin degree of freedom in this framework.

First, I will present precise predictions of spin-phonon interactions and electron spin relaxation using a new approach that unifies the description of spin-flip and precession mechanisms. Second, I will describe an approach to compute magnon-phonon interactions and the associated magnon relaxation times and mean-free paths, focusing on results for 2D ferromagnetic materials. Our calculations shed light on which phonon modes couple more strongly with free spins and magnons and limit their transport, providing valuable microscopic insight for applications in spintronics and spin-based quantum technologies.

To conclude, I will highlight new frontiers of this research, including data-driven compression of electron-phonon and spin-phonon interactions and extending these methods to the strong spin-phonon coupling regime. Advances in the Perturbo code enabling these calculations will also be discussed.

Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

jointly organised by
the Surface Science Division (O),
the Chemical and Polymer Physics Division (CPP),
the Thin Films Division (DS), and
the Magnetism Division (MA)

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This symposium will highlight best practice in FAIR data and the development of streamlined workflows for open data and machine learning techniques. To be jointly organised by DAPHNE4NFDI and FAIRmat, topics will cover optimizing data collection methodologies and workflows, implementing electronic lab notebooks for efficient data recording, and integrating on-the-fly analysis techniques to enhance experimental outcomes. Moreover, the seminar will showcase cutting-edge advancements in data analysis methodologies, with a particular focus on on-the-fly analysis and machine learning techniques tailored to synchrotron and neutron data. Participants will discuss the integration of machine learning algorithms for data processing, analysis, and interpretation, thereby unlocking new avenues for scientific discovery and innovation. Furthermore, the DPG symposium will address the challenges associated with the storage and management of big data generated by modern data collection techniques and in particular, for condensed matter at synchrotron and neutron facilities. The symposium will provide the international state-of-the-art of the different disciplines and technology and give a platform to discuss future challenges and develop common solutions.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Sessions

SYFD 1.1–1.5	Wed	9:30–12:15	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights**

Sessions

– Invited Talks –

SYFD 1: Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights

Time: Wednesday 9:30–12:15 Location: H1

Invited Talk SYFD 1.1 Wed 9:30 H1

Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight — •Astrid Schneidwind — JCNS at MLZ Garching, FZ Jülich, Germany

The scientific impact of experiments using neutron, synchrotron and free-electron X-ray sources is drastically increasing, not least related to recent experimental and technical developments, which increase the demand for experiments, too. In parallel, new opportunities attract new researchers with less experience. The request for advanced computing opportunities - from data collection to robotics and AI-assisted experiments to the re-use of data and reproducible data analysis - is increasing accordingly. Adopting FAIR practices [1] opens further space for efficient, extended usage of the highly valuable data. Within the DAHNE4NFDI [2] initiative such workflows along the whole data pipeline are exemplarily developed, provided within use cases and systematically connected to prior and subsequent laboratory work. Standards are agreed on European level, as well as data repositories and reference data bases. ML-compatible data formats link the data to theoretical and computational approaches - closing the loop for increasing the efficiency of the experiments and exciting new outcomes.

[1] Wilkinson et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci Data 3, 160018 (2016).

[2] https://doi.org/10.5281/zenodo.8040606.

Invited Talk SYFD 1.2 Wed 10:00 H1

Establishing Workflows of Experimental Solar Cell Data into NOMAD — Edgar Nandayapa[1], Paolo Graniero[1], Jose Marquez[2], Michael Götte[1], and •Eva Unger[1,3] — [1]Helmholtz-Zentrum Berlin für Materialen und Energie GmbH, HySPRINT Innovation Lab, Kekuléstraße 5, 12489 Berlin, Germany — [2]Humboldt University Berlin, FAIRmat Project, Zum Großen Windkanal 2, 12489 Berlin, Germany — [3]Humboldt University Berlin, Department of Chemistry and CSMB, Zum Großen Windkanal 2, 12489 Berlin, Germany

Materials for solar energy conversion are key enablers for the green energy transition. Perovskite Solar Cells (PSCs) are an excellent example of an emerging technology, where an intense and world-wide R&D activities has enabled a very fast improvement in the reported power conversion efficiencies. The monthly output of new reports in the peer-reviewed literature is in the hundreds to thousands and it is at this point neither effective nor possible to still make effcient use of the research results reported. Considering data reported in the peer-reviewed literature, this just represent the "tip of the iceberg" of research data that is actually being measured in labs around the world.

Out of desparation, our team started a fairly manual "data digging" initiative in 2019 to compile data from the then published data in the peer-reviewed literature into a single database based on a very rudimentary and single-metric representation of the actual research data resulting in the Perovskite Database (www.perovskitedatabase.com). In close collaboration with the FAIRmat project, we are now taking steps towards transferring the literature dataset into NOMAD and are creating NOMAD platforms to capture, store, analyse and share the actual experimental research data within and beyond our research community. The goal is to, both, initiate community driven data sharing platforms that can be used to directly share and disseminate experimental datasets to adhere to FAIR data principles, and make photovoltaic research data AI-ready to enable the utilization of modern ML-tools to facilitate a further acceleration of the technological exploitation of new materials.

Invited Talk SYFD 1.3 Wed 10:30 H1

Building up the EOSC Federation — •Ute Gunsenheimer — EOSC Association

The European Open Science Cloud (EOSC) envisions a unified system in Europe to enable researchers to store, share, process, and reuse FAIR data and services across disciplines and borders. Central to this vision is the EOSC Federation, a network of interconnected nodes, that will provide seamless access to scientific data and resources. With the public launch of the EOSC EU Node in October 2024, the development of the EOSC Federation has gained significant momentum. To realise its full potential, the EOSC Federation requires the enrolment of additional EOSC Nodes. The nodes will act as entry points to the Federation.

To enable the establishment of such a distributed system, many questions remain to be addressed, including defining minimum requirements for EOSC Nodes, establishing enrolment rules, ensuring effective governance, and developing financial mechanisms to support resource sharing. Answering these questions is critical to building a robust, distributed infrastructure that drives Open Science and innovation in Europe.

By the time of the conference, the first wave of EOSC Nodes will have been identified, representing a diverse range of thematic and national communities across Europe. At the same time, active work on the enrolment process will have been kicked-off.

This talk will explore the progress, challenges, and future steps in shaping the EOSC Federation.

15 min. break

Invited Talk SYFD 1.4 Wed 11:15 H1

Data-Driven Materials Science for Energy-Sustainable Applications — •Jacqueline Cole — Cavendish Laboratory, University of Cambridge, Cambridge, UK

Data-driven materials discovery is coming of age, given the rise of 'big data' and machine-learning (ML) methods. However, the most sophisticated ML methods need a lot of data to train them. Such data may be custom materials databases that comprise chemical names and their cognate properties for a given functional application; or data may comprise a large corpus of text to train a language model. This talk showcases our home-grown open-source software tools that have been developed to auto-generate custom materials databases for a given application. The presentation will also demonstrate how domain-specific language models can now be used as interactive engines for data-driven materials science. The talk illustrates the application of these data-science methods using case studies from the energy sector. The talk concludes with a forecast of how this 'paradigm shift' away from the use of static databases will likely evolve materials science.

Invited Talk SYFD 1.5 Wed 11:45 H1

Machine Learning and FAIR Data in X-ray Surface Science — •Stefan Kowarik — Phys. Chemistry, Univ. of Graz, Austria

Synchrotrons are among the world's largest producers of scientific data, yet many experiments fail to contribute adequately to databases. Publishing raw data without comprehensive metadata fails to align with the "Findable" and "Reusable" principles of FAIR data, which are essential to unlocking the full potential of these datasets.ML not only benefits from large FAIR datasets but also facilitates their creation. Our recent work highlights live ML-based analysis of X-ray reflectometry (XRR) for thin-film characterization, enabling adaptive experimentation with a fourfold increase in speed. Additionally, we demonstrate automated crystal structure solutions from grazing-incidence X-ray diffraction (GIXD) of thin films. These advancements lay the foundation for self-driving laboratories, where integrated ML algorithms can control thin-film deposition processes, enhancing precision and throughput.Importantly, live ML analysis generates metadata, such as unit cell parameters in textured thin films, improving data findability and reusability. While XRR requires standardized structural model formats*efforts championed by groups like ORSO*GIXD leverages established crystallographic formats for database integration.*In the future, these advancements could culminate in expansive, standardized databases for surface science, encompassing thin-film crystal structures, surface reconstructions, and thin film material properties, analogous to established bulk crystallographic databases.

Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

jointly organised by
the Semiconductor Physics Division (HL),
Crystalline Solids and their Microstructure Division (KFM), and
Surface Science Division (O)

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Electron-phonon interaction is crucial to predict and explain material behaviour under a variety of equilibrium and non-equilibrium conditions. Though recent developments in theoretical and computational methods have significantly advanced our capability, significant challenges still remain to be addressed. An accurate description of electron-phonon interactions in complex materials, including e.g., disordered perovskites, correlated oxides, superconductors, interfaces, and heterostructures, is often beyond the capability of existing methodologies. This symposium will bridge different communities working on electron-phonon interactions in solids and pinpoint common problems and open challenges in the field.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger

Sessions

SYIS 1.1–1.5	Tue	9:30–12:15	H1	**Progress and Challenges in Modelling Electron-Phonon Interaction in Solids**

Sessions

– Invited Talks –

SYIS 1: Progress and Challenges in Modelling Electron-Phonon Interaction in Solids

Time: Tuesday 9:30–12:15 Location: H1

Invited Talk SYIS 1.1 Tue 9:30 H1

Electron-phonon and exciton-phonon coupling in advanced materials — •Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Treating various excitations in materials on equal footing allows us not only to achieve excellent agreement with experiment, but, importantly, to gain a deeper understanding of complex processes and materials. Prominent examples are organic-inorganic hybrid systems whose building blocks are very different in nature. I will discuss the critical role of both the mutual dynamical screening of the constituents and electron-phonon coupling (EPC) [1] to obtain the correct ground state and excitation spectra. Many-body perturbation theory (MBPT) is the state-of-the-art methodology for such problems. In particular, the Bethe-Salpeter equation (BSE) is the method of choice for computing optical excitations. For polar materials, the dielectric screening of both the electronic and vibrational degrees of freedom must be considered to obtain correct exciton binding energies and spectral features [2]. Finally, I will show, how the BSE together with EPC matrix elements can be used to treat exciton-phonon coupling and thus geometry relaxation in the excited state [3], giving a handle to the description of photoluminescence and exciton dynamics.

[1] I. Gonzalez Oliva, B. Maurer, B. Alex, S. Tillack, M. Schebek, and C. Draxl, phys. stat. sol. (a) 221, 2300170 (2024).

[2] M. Schebeck, P. Pavone, C. Draxl, and F. Caruso, J. Phys.: Condens. Matter (2024); https://arxiv.org/abs/2409.15099

[3] M. Yang and C. Draxl, https://arxiv.org/abs/2212.13645

Invited Talk SYIS 1.2 Tue 10:00 H1

Exciton-phonon dynamics from first principles — •Enrico Perfetto — Physics Department University of Rome Tor Vergata

Exciton dynamics, encompassing ultrafast photogeneration, diffusion, and thermalization, plays a fundamental role in optoelectronic, photovoltaic, and photocatalytic processes. In this talk we discuss a novel many-body approach to describe exciton dynamics from first-principles. We show that the introduction of an auxiliary exciton species, termed 'irreducible exciton', is crucial to formulate a theory free from overscreening of the electron-phonon interaction. The resulting Excitonic Bloch Equations, while having the same computational cost as the well-known Excitonic Boltzmann Equations, enable a comprehensive description of the temporal evolution of coherent, irreducible, and incoherent excitons during and after the optical excitation.

Within this framework, we explore the real-time dynamics of exciton formation, elucidating the mechanism by which quasi-free electron-hole pairs, generated by above-gap photoexcitation, are dynamically converted into bound excitons.

Invited Talk SYIS 1.3 Tue 10:30 H1

Polarons and exciton polarons from first principles — •Feliciano Giustino — The University of Texas at Austin

Polarons are quasiparticles formed when a charge carrier interacts with lattice vibrations. In materials with strong electron-phonon couplings, this phenomenon results in self-trapped polarons. Similarly, excitons, which are composite quasiparticles formed by the binding of an electron and a hole, can polarize the surrounding crystal lattice through spatial fluctuations in their charge density. This polarization, in turn, can promote the spatial localization of the exciton, leading to the formation of exciton polarons or even self-trapped excitons in the presence of strong exciton-phonon couplings. First-principles calculations of these effects are challenging because they require large supercells potentially involving hundreds or thousands of atoms. In this talk, I will discuss recent methodological developments that combine density-functional perturbation theory and the Bethe-Salpeter approach to compute polarons and exciton polarons from first principles. The main advantage of the present approach is that it does not require supercells, and all necessary information is generated via calculations in the crystal unit cell. To illustrate these developments, I will report on two recent applications: (i) the discovery of topological polarons in halide perovskites, wherein the distortion of the atomic lattice describes a vector field with definite topological invariants; and (ii) the discovery of large polarons and exciton polarons in rutile and anatase titanium dioxide, which provide a natural explanation for why anatase exhibits diffusive carrier transport while rutile supports thermally-activated transport.

15 min. break

Invited Talk SYIS 1.4 Tue 11:15 H1

Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors — •Alexander Steinhoff[1], Matthias Florian[2], and Frank Jahnke[1] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, USA

Marrying the predictive power of ab initio calculations with many-body effects of ever increasing complexity remains a challenging task. In particular, for van der Waals materials, understanding carrier-phonon interaction from first principles is a field of growing interest. Here, we present a many-body theory for coupled free-carrier, exciton, phonon and photon dynamics based on carrier-carrier and carrier-phonon interaction matrix elements obtained from first principles via projection on Wannier orbitals. We demonstrate the impact of carrier-two-phonon scattering processes on optical spectra and coupled nonequilibrium carrier-phonon kinetics in monolayer $MoSe_2$. Our studies open a perspective to advance the material-realistic description of nonequilibrium physics in two- dimensional nanostructures to new many-body levels.

Invited Talk SYIS 1.5 Tue 11:45 H1

Phonon influence on (cooperative) photon emission from quantum dots — •Erik Gauger[1], Julian Wiercinski[1], and Moritz Cygorek[2] — [1]Institute of Photonics and Quantum Sciences, Heriot Watt University — [2]Technische Universität Dortmund

Semiconductor quantum dots (QDs) provide an established on-demand single-photon source platform. Integrating such sources into quantum networks comes with the requirement of producing fundamentally indistinguishable photons, and the ability to generate and preserve coherence between different emitters.

The leading source of decoherence of solid state emitters such as quantum dots is typically their coupling to longitudinal acoustic lattice vibrations, as can be observed under coherent control experiments such as Rabi oscillations as well as in their emission resonance spectrum.

In this presentation, I will give an overview of our theoretical work on modelling, understanding, and mitigating the interaction between solid-state emitters and their vibrational environment, and how this interaction manifests in measurable signatures such as photon statistics and spectral properties.

With a view towards scaling up to networks of coupled emitters, a particular focus of this presentation will be our recent progress in understanding the interplay between collective light-matter coupling and phonon decoherence, by utilising intuitive and interpretable master equation approaches as well as state-of-the-art numerical process tensor methods. I will also make connections to experimental data for up to five quantum dots displaying signatures of cooperative behaviour.

Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

jointly organised by
the Metal and Material Physics Division (MM),
the Magnetism Division (MA),
the Surface Science Division (O),
the Crystalline Solids and their Microstructure Division (KFM), and
the Semiconductor Division (HL)

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In a surprisingly short time, AI (artificial intelligence) has demonstrated its transformative potential in materials science by integrating machine learning algorithms and generative models to predict and optimize material properties. High-throughput computational frameworks powered by AI enable rapid screening of vast chemical spaces, significantly reducing the time and cost associated with traditional experimental approaches and providing new physical insights. By leveraging large data sets and sophisticated algorithms, researchers have successfully uncovered hidden patterns and relationships in material behavior, leading to the discovery of novel materials with superior mechanical, electrical, magnetic, or catalytic properties.
The interdivisional symposium highlights the latest advances and success stories in AI and data-driven materials design, focusing on both machine learning and generative approaches. Leading experts in the field present the latest methods in AI used to predict material properties, optimize manufacturing processes, and accelerate the discovery of new materials. Key topics include the development and application of machine learning models, highthroughput computational techniques, and the integration of AI with experimental and theoretical methods, as well as current challenges and future perspectives.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Sessions

SYMD 1.1–1.5	Mon	15:00–17:45	H1	**AI-driven Materials Design: Recent Developments, Challenges and Perspectives**

Sessions

– Invited Talks –

SYMD 1: AI-driven Materials Design: Recent Developments, Challenges and Perspectives

Time: Monday 15:00–17:45 Location: H1

Invited Talk SYMD 1.1 Mon 15:00 H1

Learning physically constrained microscopic interaction models of functional materials — •Boris Kozinsky — Harvard University, Cambridge MA, USA — Bosch Research, Watertown MA, uSA

Discovery and understanding of next-generation materials requires a challenging combination of the high accuracy of first-principles calculations with the ability to reach large size and time scales. We pursue a multi-tier development strategy in which machine learning algorithms are combined with exact physical symmetries and constraints to significantly accelerate computations of electronic structure and atomistic dynamics. First, current DFT approximations fall short of the required accuracy and efficiency for predictive calculations of defect properties, band gaps, stability and electrochemical potentials of materials for energy storage and conversion. To advance the capability of DFT we introduce nonlocal charge density descriptors that satisfy exact scaling constraints and learn exchange functionals called CIDER. These models are orders of magnitude faster in self-consistent calculations for solids than hybrid functionals but similar in accuracy. On a different level, we accelerate MD simulations by using machine learning to construct generalized potential and free energy functions with arbitrary nonlinear dependence on external fields and temperature. This framework enables learning and prediction of dielectric and vibrational response properties and coarse-grained free energies. We demonstrate these methods via first principles ML MD simulations of dynamics of phase transformations, heterogeneous reactions, ferroelectric transitions, nuclear quantum effects, and soft materials.

Invited Talk SYMD 1.2 Mon 15:30 H1

GRACE universal interatomic potential for materials discovery and design — •Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Universal interatomic potentials parameterize the interaction between all chemical elements in the periodic table simultaneously. In my talk I will introduce the Graph Atomic Cluster Expansion (GRACE). GRACE builds on a complete set of graph basis functions and generalizes equivariant message passing neural networks and other machine learning interatomic potentials. Next, I will discuss the parameterization of GRACE across the periodic table and compare the performance of universal GRACE to element-specific potentials.

The ability to simulate thousands or millions of atoms with complex chemistries for extended time scales opens completely new routes for materials discovery and design. I will demonstrate usage scenarios for widely different materials, chemistries and applications.

Finally, I will focus on limitations of current universal interatomic potentials and suggest steps to overcome these.

Invited Talk SYMD 1.3 Mon 16:00 H1

Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction — •Nong Artrith — Debye Institute for Nanomaterials Science, Utrecht University, NL

Machine learning (ML) has emerged as a powerful tool to accelerate the discovery of catalytic materials by integrating information from computation and experiment. While ML excels at pattern detection in large, uniform datasets, many catalyst studies rely on small, experimentally measured datasets. Our approach combines ML and first-principles calculations to extract insights from such small experimental datasets by training a complex ML model on a large computational library of transition-state energies and combining it with simple linear regression models fitted to experimental data. We use this approach to explore the catalytic activity of monolayer bimetallic catalysts for ethanol reforming, identifying key reactions and predicting promising catalyst compositions. For the explicit modeling of catalytic reactions, we performed ML-driven molecular dynamics and metadynamics simulations of the oxygen evolution reaction (OER) over oxide materials. Using a neural network potential, trained using transfer learning, we captured the dynamic mechanistic details of OER, elucidating the impact of nickel doping on the catalytic activity of $BaTiO_3$, a perovskite oxide synthesized from earth-abundant precursors. The combined insights from these case studies illustrate the versatility of ML in guiding the design of efficient and sustainable catalysts, ranging from ethanol reforming to water-splitting reactions.

15 min. break

Invited Talk SYMD 1.4 Mon 16:45 H1

Inverse Design of Materials — •Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Machine learning has been widely applied to obtain statistical understanding and rational design of advanced materials to map out the processing-(micro-)structure-property-performance relationships, mostly in the forward manner. In this work, focusing on the structure-property relationships, I am going to introduce the concept of inverse design and to showcase how it can be carried out based on Bayesian optimization and generative deep learning. To explore a well-defined and possibly vast design space efficiently, Bayesian optimization can be applied for reliable recommendations, either based on ranking schemas balancing exploration and exploitation or by using proper sampling strategies. This leads to a closed loop adaptive design strategy, which can be integrated with theoretical scale-bridging simulations and experimental synthesis and characterization, resulting in a domain expertise- and physics-informed active learning paradigm. Furthermore, to go beyond the known design space, generative deep learning (such as GAN, VAE, and diffusion models) can be applied. I will demonstrate such a strategy for the polycrystalline microstructure-property mapping, with the physical properties constrained based on an integrated ControlNet in stable diffusion models.

Invited Talk SYMD 1.5 Mon 17:15 H1

Data-Driven Materials Science — •Miguel Marques — Ruhr University Bochum, Germany

We summarize our recent attempts to discover, characterize, and understand inorganic compounds using novel machine learning approaches. We start by motivating why the search for new materials is nowadays one of the most pressing technological problems. Then we summarize our recent work in using crystal-graph attention neural networks for the prediction of materials properties. To train these networks, we developed a dataset of over 5 million density-functional calculations with consistent calculation parameters. Combining the data and the newly developed networks we have already scanned thousands of structural prototypes spanning a space of several billion materials and identified tens of thousands of theoretically stable compounds. We then discuss how these techniques can be used to discover new materials with tailored properties, using as an example the transition temperature of conventional superconductors. Finally, we speculate which role data-driven research will have in the future of materials science.

Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

jointly organised by
the Thin Films Division (DS),
the Magnetism Division (MA),
the Low Temperature Physics Division (TT), and
the Surface Science Division (O)

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Spin hyperpolarization in molecular systems describes the transient electronic or nuclear spin order that surpasses the Boltzmann distribution. There is an enormously increasing interest in the fundamental aspects of building-up, transport and relaxation of spin hyperpolarization. Strategies that have been tested for building-up spin hyperpolarization include the controlled realization of molecule-based interfaces, spin pumping, spin injection, intersystem crossing or the chiral induced spin selectivity in molecular solids, thin films or devices. On the other hand, significant efforts are being made on the experimental and theoretical side to understand the mechanisms of transport of spin hyperpolarization and the related relaxation processes. This interdisciplinary symposium brings together experts working on various experimental and theoretical aspects of thin films, magnetism, surface science as well as device physics, aiming to identify common mechanisms involved in different hyperpolarization strategies in order to push synergistic advances in this field.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Sessions

SYMS 1.1–1.5	Wed	15:00–17:45	H1	**Spins in Molecular Systems: Strategies and Effects of Hyperpolarization**

Sessions

– Invited Talks –

SYMS 1: Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Time: Wednesday 15:00–17:45 Location: H1

Invited Talk SYMS 1.1 Wed 15:00 H1

Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer — •Christoph Boehme — Department of Physics & Astronomy, University of Utah, Salt Lake City, UT 84112, USA

Spin-dependent charge carrier recombination currents in π-conjugated polymers can be governed by radical pair physics, reflecting the spin-permutation symmetry of electron-hole spin-pair states, rather than spin-polarization states. This effect can be used to detect magnetic resonance under conditions unsuitable for conventional spectroscopy, such as low spin polarization or thin-film systems containing small spin ensembles (Frankevich et al., Phys. Rev. B, 1992, 46, 9320; Roundy and Raikh, Phys. Rev. B, 2013, 88, 125206). Recent work has demonstrated this mechanism's utility for studying strong-drive, non-perturbative magnetic resonance, where magnetic radiation amplitudes comparable to the static Zeeman field create hybrid spin-light states. This results in non-linear behaviors like spin-collectivity (Waters et al., Nat. Phys., 2015, 11, 910-914), multi-photon transitions, and fractional g-factor effects (Jamali et al., Nat. Commun., 2021, 12, 465; Jamali et al., Nano Lett., 2017, 17, 4648-4653; Ashton et al., 2020). Experimental confirmations include monochromatic multi-photon transitions, angular dependence of resonance shifts, and hybrid light-matter states, promising advancements in high-fidelity sensing qubits with long coherence times [S. I. Atwood et al., Phys. Rev. B 110, 195304 (2024); S. I. Atwood et al., Phys. Rev. B 110, L060103 (2024)].

Invited Talk SYMS 1.2 Wed 15:30 H1

The puzzle of spin and charge transport in the chirality induced spin selectivity effect — •Bart van Wees — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

I will present an overview of the current understanding of the chirality induced spin selectivity effect [1], as measured as a magnetoresistance in electronic devices and scanning probe geometries. I will describe the principles of chirality induced coupling of spin and charge currents, and show that this indeed allows to observe the specific chirality in non-linear transport experiments [2,3]. However, experiments at low bias, in the linear transport regime, show that Onsager's reciprocity relations are not obeyed. This, together with the large magnetoresistances which are observed, (sometimes exceeding 90% or more) are not compatible with descriptions in terms of spin (polarized) transport. I will discuss alternative mechanisms, which are based on the modification of the electrostatic potential profile, which depend on the interplay between chirality and magnetisation. These lead to a magnetoresistance due to a modification of the charge transport, not the spin transport. I will point out that open questions remain for these alternative mechanisms, and propose experimental stategies to address these.

[1] Evers et al., Advanced Materials 34,13, 2106629 (2022)
[2] X.Yang et al., Nano Letters 20, 8,6148 (2020)
[3] X.Yang et al., Phys. Rev. B99, 024418 (2019
[4] S.H Tirion, and B.J. van Wees, ACS Nano 18/81, 6028 (2024)
[5] Y. Zhao et al., ArXiv2201.03623v3

Invited Talk SYMS 1.3 Wed 16:00 H1

Nano- and Microscale NMR spectroscopy with spin qubits in diamond — •Nabeel Aslam — Leipzig University

Expanding nuclear magnetic resonance (NMR) spectroscopy to the micro- and nanoscale holds significant potential to advance research across disciplines. Potential applications include the chemical analysis of mass-limited samples, single-cell metabolomics for disease diagnostics, and the detection and characterization of individual proteins, such as functional membrane proteins.

In this talk, I will introduce a novel approach to nano- and microscale NMR using nitrogen-vacancy (NV) centers in diamond. These quantum defects can be optically polarized and read out, enabling highly sensitive detection of nuclear spins with exceptional spatial resolution. This capability is further enhanced through hyperpolarization techniques. I will provide an overview of the state-of-the-art in the field, including advancements in detecting nuclear spins on surfaces, integrating NV-based NMR with microfluidic technologies for high-throughput applications, and employing diffusion NMR to study molecular transport at the nanoscale.

Furthermore, I will discuss how nuclear spins in diamond can serve as quantum memories, enhancing the performance and versatility of NV-based sensing. This highly sensitive and versatile method has the potential to uncover new insights into complex systems in chemistry, biology, and material science.

15 min. break

Invited Talk SYMS 1.4 Wed 16:45 H1

Spin effects in adsorbed organometallic complexes — •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

By adsorbing organometallic complexes onto surfaces, high densities can be achieved and the molecules can be probed individually with a scanning tunneling microscope. This approach has enabled experiments on molecular spin switches and their interactions in artificial arrays. New insights have been gained into spin-crossover molecules, electrostatic interactions and their effect on spin states, and the role of orbital magnetic moments. The talk will highlight some results from this field as well as some of the challenges.

Invited Talk SYMS 1.5 Wed 17:15 H1

Quantum Computing with Molecules — •Mario Ruben — KIT, IQMT, 76344 Leopolshafen-Eggenstein — CESQ, Université Strasbourg, France

Nuclear spin states in molecules act as quantum registers for quantum operations. We report on the implementation of metal complexes into nanometer-sized spintronic devices by a combination of bottom-up self-assembly and top-down lithography techniques. The controlled generation of magnetic molecular nanostructures will be shown and persistence of their magnetic properties under confinement Molecular Quantum Devices will be proven. The Hilbert space spanned by the nuclear spins will be engineered synthetically and addressed both electrically and optically, partially at the single molecule level. Finally, Grovers quantum search algorithm will be implemented on the nuclear spin register of a TbPc2 Qudit.

Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

jointly organised by
the Dynamics and Statistical Physics Division (DY),
the Low Temperature Physics Divison (TT),
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP), and
the Physics of Socio-economic Systems Division (SOE)

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Nonequilibrium classical and quantum systems coupled to thermal or (driven) non-equilibrium environments have recently been shown to exhibit rich collective phenomena and phase transitions without equilibrium counterparts. From the classical side, intriguing examples are flocking and phase separation in active matter, but also patterns and bifurcations in driven-diffusive systems and spontaneous parity-time symmetry breaking in systems involving nonreciprocal couplings. From the quantum side much interest has been devoted, e.g., to ordering and phase transitions in non-equilibrium steady states, the formation of time crystals, superradiance, as well as phase transitions or critical behavior in time. The symposium and the accompanying focus session is devoted to connections between the quantum and the classical realms, as they have been explored recently both in theory and experiment.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Sessions

SYQS 1.1–1.5	Thu	15:00–17:45	H1	**Nonequilibrium Collective Behavior in Open Classical and Quantum Systems**

Sessions

– Invited Talks –

SYQS 1: Nonequilibrium Collective Behavior in Open Classical and Quantum Systems

Time: Thursday 15:00–17:45 Location: H1

Invited Talk SYQS 1.1 Thu 15:00 H1

Active quantum flocks — Reyhaneh Khasseh[1,2], Sascha Wald[3], Roderich Moessner[2], Christoph Weber[1,2], and •Markus Heyl[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [3]Statistical Physics Group, Centre for Fluid and Complex Systems, Coventry University, Coventry, England

Flocks of animals represent a fascinating archetype of collective behavior in the macroscopic classical world, where the constituents, such as birds, concertedly perform motions and actions as if being one single entity. Here, we address the outstanding question of whether flocks can also form in the microscopic world at the quantum level. For that purpose, we introduce the concept of active quantum matter by formulating a class of models of active quantum particles on a one-dimensional lattice. We provide both analytical and large-scale numerical evidence that these systems can give rise to quantum flocks. A key finding is that these flocks, unlike classical ones, exhibit distinct quantum properties by developing strong quantum coherence over long distances. We propose that quantum flocks could be experimentally observed in Rydberg atom arrays. Our work paves the way towards realizing the intriguing collective behaviors of biological active particles in quantum matter systems. We expect that this opens up a path towards a yet totally unexplored class of nonequilibrium quantum many-body systems with unique properties.

Invited Talk SYQS 1.2 Thu 15:30 H1

Robust dynamics and function in stochastic topological systems — •Evelyn Tang — Rice University, Houston, TX

Living systems exhibit various robust dynamics and cycles during system regulation, growth, and motility. However, how robustness emerges from stochastic components remains unclear. Towards understanding this, I develop topological theories that support robust edge currents and localization, effectively reducing the system function to a lower-dimensional subspace. I will introduce stochastic networks in molecular reaction space that model long and stable time scales, such as the circadian rhythm. More generally, we prove that unlike their quantum counterparts, stochastic topological systems require driving or nonequilibrium for edge states and strong localization. I will close by discussing experimental platforms for the detection and use of edge currents for self-assembly and replication in living systems.

Invited Talk SYQS 1.3 Thu 16:00 H1

Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases — •Artur Widera — University of Kaiserslautern-Landau, Department of Physics and state-research center OPTIMAS, 67663 Kaiserslautern, Germany

Ultracold quantum gases provide a unique platform to experimentally study many-body dynamics under precisely controlled external potentials and driving forces. In this talk, I will present recent results on the dynamics of an ultracold gas of spin-polarized fermionic lithium atoms subjected to a time-dependent disorder potential. For static disorder, we observe signatures of the well-known Anderson localization. In contrast, time-varying disorder with finite correlation time is expected to disrupt localization. Specifically, for weak disorder, we find that time-dependent disorder induces a transition in the transport behavior of the gas from normal diffusion to superdiffusion and eventually ballistic motion as the correlation time of the disorder decreases. This enhanced diffusion is well described by a stochastic Fermi acceleration model, where randomly fluctuating force fields drive the system. Interestingly, for strong disorder, normal diffusion persists over a broad range of disorder correlation times despite the time-varying potential. We attribute this resilience to the continued presence of destructive interference as quantified by the localized fraction of atoms, which remains intact even under the influence of time-dependent disorder. These results point toward a nonequilibrium phase transition between localized and diffusive regimes in this driven system.

15 min. break

Invited Talk SYQS 1.4 Thu 16:45 H1

Topological classification of driven-dissipative nonlinear systems — •Oded Zilberberg[1], Greta Villa[1], Kilian Seibold[1], Vincent Dumont[2], Gianluca Rastelli[3], Mateusz Michałek[4], Alexander Eichler[2], and Javier del Pino[1] — [1]Department of Physics, University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany — [2]Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zürich, Switzerland — [3]Pitaevskii BEC Center, CNR-INO and Dipartimento di Fisica, Università di Trento, I-38123, Trento, Italy — [4]Dept. of Mathematics and Statistics, University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany

Topological classification of matter has become crucial for understanding the linear response of (meta-)materials, with associated quantized bulk phenomena and robust topological boundary effects. Moving to nonlinear systems, we develop an approach that harnesses the topology of structurally stable vector flows, and thus propose a new topological graph invariant to characterize out-of-equilibrium dynamical systems. We exemplify our approach on the ubiquitous model of a dissipative bosonic Kerr cavity, subject both to one- and two-photon drives. Using our classification, we can identify the topological origin of phase transitions in the system, as well as explain the robustness of a multicritical point in the phase diagram. We, furthermore, identify that the invariant distinguishes population inversion transitions in the system in similitude to a Z2 index. Our approach spans across the classical-to-quantum regimes, and extensions to coupled nonlinear cavities are postulated.

Invited Talk SYQS 1.5 Thu 17:15 H1

Learning dynamical behaviors in physical systems — •Vincenzo Vitelli — University of Chicago, Chicago, USA

Physical learning is an emerging paradigm in science and engineering whereby (meta)materials acquire desired macroscopic behaviors by exposure to examples. So far, it has been applied to static properties such as elastic moduli and self-assembled structures encoded in minima of an energy landscape. Here, we extend this paradigm to dynamic functionalities, such as motion and shape change, that are instead encoded in limit cycles or pathways of a dynamical system. We identify the two ingredients needed to learn time-dependent behaviors irrespective of experimental platforms: (i) learning rules with time delays and (ii) exposure to examples that break time-reversal symmetry during training. After providing a hands-on demonstration of these requirements using programmable LEGO toys, we elucidate how they emerge from physico-chemical processes involving the causal propagation of fields. Our trainable particles can self-assemble into structures that move or change shape on demand, either by retrieving the dynamic behavior previously seen during training. This phenomenology is captured by a non-reciprocal Hopfield spin model amenable to analytical treatment. The principles illustrated here provide a step towards von Neumann's dream of engineering synthetic living systems that adapt to the environment.

Symposium SKM Dissertation Prize 2025 (SYSD)

jointly organised by
all divisions of the Condensed Matter Section of the DPG

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The divisions belonging to the Condensed Matter Section (SKM) of the DPG annually award the SKM Dissertation Prize. The prize acknowledges outstanding research during the doctoral studies in the research areas of the SKM completed in 2023 or 2024, and its excellent oral presentation. Based on nominations, a jury consisting of the chair persons of all SKM divisions has selected five finalists to present their work in this symposium. The winner will be selected after the symposium and publicly announced Tuesday, March 18, 2025 in the afternoon during the ceremonial sessionn (Lecture hall H1 (Audimax) starting at 16:00).

Overview of Invited Talks and Sessions

(Lecture hall H2)

Invited Talks

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Sessions

– Invited Talks –

SYSD 1: SKM Dissertation Prize Symposium

Time: Monday 9:30–12:00 Location: H2

Invited Talk SYSD 1.1 Mon 9:30 H2

Nanoscale Chemical Analysis of Ferroic Materials and Phenomena — •Kasper Aas Hunnestad — Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, Norway

The discovery of new physical phenomena in materials is closely linked to the progress in characterization, and is propelled by the ability to observe and study physical processes occurring at the atomic level. In this talk, I will present how atom probe tomography (APT) can be incorporated into the toolkit of nanoscale research to study ferroelectric oxide materials. The aim is to demonstrate its feasibility and power to unravel correlations between the local chemical composition and emergent functional properties.

A range of systems with fundamental importance to ferroelectrics are investigated, including solute dopants in bulk, naturally occurring interfaces in ferroelectrics, such as grain boundaries and domain walls, and artificially grown interfaces in heterostructures. Using a correlative microscopy approach, a complex and diverse defect chemistry is revealed in 3D, which further clarify the origin of anomalous electronic properties. The work presented demonstrates the outstanding potential and general feasibility of applying APT to study ferroelectric oxide systems. Correlations between defect chemistry and ferroic phenomena can be experimentally probed with nanoscale spatial resolution, opening an avenue to obtain a deeper understanding of ferroic materials.

Invited Talk SYSD 1.2 Mon 10:00 H2

Advanced Excitation Schemes for Semiconductor Quantum Dots — •Yusuf Karli — Cavendish Laboratory, University of Cambridge, Cambridge, UK — Institut für Experimentalphysik, Universität Innsbruck, 6020, Innsbruck, Austria

Semiconductor quantum dots are nanometer-scale structures that confine electrons in three dimensions, creating discrete energy levels similar to those in atoms. This unique property makes them an excellent platform for generating high-quality single photons with high purity and indistinguishability. As such, they are critical for advancing quantum technologies, serving as essential building blocks for quantum communication, quantum computing, and photonic quantum networks.

In this talk, I address practical challenges associated with traditional excitation methods for semiconductor quantum dots by introducing innovative approaches. These include below-bandgap excitation (the SUPER scheme), a two-pulse technique (Stimulated TPE), and Adiabatic Rapid Passage (ARP). These methods enhance robustness, improve photon indistinguishability, and enable efficient population transfer, positioning semiconductor quantum dots as reliable and scalable sources for quantum photonic systems.

Invited Talk SYSD 1.3 Mon 10:30 H2

Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors — •Clemens Kuhlenkamp — Harvard University, Cambridge, USA

Due to their high level of control two-dimensional (2D) materials are emerging as fascinating platforms to explore correlated electronic phases of matter. In this talk, I will discuss opportunities to control, prepare, and probe exotic states in structures of transition metal dichalcogenides (TMDs), a class of 2D semiconductors. Remarkably, already a single TMD layer can reach an interaction-dominated regime upon doping electrons. By analyzing the optical response of the material, we directly reveal the formation and properties of an electronic Wigner crystal—a state where electrons break translational symmetry by arranging in a triangular lattice. Moving on to multi-layer TMDs, I will demonstrate how Moiré patterns—arising from misalignments between the layers—can realize highly tunable, frustrated Hubbard models in the presence of large magnetic fields. Our theoretical analysis predicts that such materials can exhibit exotic insulator-to-insulator transitions and give rise to exceptionally robust spin liquid phases in the Mott insulating limit. I will conclude with an outlook on future directions, particularly highlighting opportunities to realize unconventional superconductivity.

Invited Talk SYSD 1.4 Mon 11:00 H2

Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics — •Till Münker — Third Institute of Physics - Biophysics, University of Göttingen, 37077 Göttingen

Vital cellular functions rely on the interplay between the viscoelastic mechanical properties of the cytoplasm and the active force generated by the consumption of metabolic energy. However, quantifying these properties poses significant challenges due to the complexity of the physical quantities and the elaborate, low-throughput experimental methods required for their investigation. We propose two techniques to meet these challenges. Firstly, we introduce a mechanical fingerprint that reduces the complexity of intracellular active mechanical properties to six parameters. We demonstrate how the fingerprint captures changes in mechanics upon disrupting cytoskeletal components and enables identification of individual cells through their unique fingerprint. By introducing a phase space of resistance, activity, and fluidity, we observe how position in phase space correlates with expected cell function. Secondly, we introduce the Mean Back Relaxation (MBR) as a novel statistical tool to determine the breaking of detailed balance in confined systems. In living cells, we observe surprising relations between the MBR and intracellular activity. Strikingly, by deploying this relation, we determined the mechanical properties of MDCK cells by purely passive observations. Together, these techniques simplify the quantification of intracellular mechanics, reducing experimental complexity while enhancing throughput.

Invited Talk SYSD 1.5 Mon 11:30 H2

Coherent Dynamics of Atomic Spins on a Surface — •Lukas Veldman — TU Delft, Department of Quantum Nanoscience, Delft, The Netherlands — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, 70569 Stuttgart, Germany

Studying dynamical interactions between individual spins is vital for understanding exotic magnetic materials as well as for development of applications that require control over solid state spins like spintronics and quantum computation. Here, we introduce the possibility to inject a single spin flip with atomic precision into a magnetic nanostructure and trace the resulting coherent spin dynamics. We achieve this by combining electron spin resonance (ESR) and DC pump-probe techniques with scanning tunneling microscopy (STM). In our first proof-of-concept measurement, we apply this method to two coupled Ti atoms and resolve the resulting coherent flip-flop oscillations between their electron spins [1]. Next, we investigate larger structures up to 6 spins and study magnon dynamics in the few-atom limit [2]. Lastly, we resolve the magnetic dynamics between an electron and a nucleus within a single atom [3,4], further expanding the potential of this new measurement scheme to nuclear spins. These experiments add to the understanding of the microscopic mechanism behind magnetic interactions and open the door to detailed control of individual spins on surfaces for quantum coherent applications. [1] L.M. Veldman et al., Science 372 (2021) [2] L.M. Veldman et al., in preparation [3] L. Farinacci, L.M. Veldman et al., Nano Lett. 22 (2022) [4] L.M. Veldman et al., Nat. Commun. 15 (2024)

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Overview of Invited Talks and Sessions

(Lecture halls H44 and H46; Poster P3 and P4)

Invited Talks

BP 3.7	Mon	11:15–11:45	H44	**Killing to survive - how protein-lipid interactions drive programmed cell death** — •Kristyna Pluhackova
BP 4.1	Mon	9:30–10:00	H46	**Spatiotemporal organization of bacterial biofilm formation and functions** — •Knut Drescher
BP 7.1	Mon	15:00–15:30	H44	**Single-molecule dynamic structural biology with Graphene Energy Transfer** — •Philip Tinnefeld, Alan Szalai, Giovanni Ferrari, Lars Richter, Ingrid Tessmer, Andres Vera-Gomez, Izabela Kaminska
BP 8.6	Mon	16:15–16:45	H46	**In situ control of cells and multicellular structures at the microscale by two-photon lithography** — •Christine Selhuber-Unkel
BP 11.1	Tue	9:30–10:00	H44	**Network connectivity determines the mechanisms responsible for cytoskeletal elasticity** — •Martin Lenz
BP 15.1	Tue	11:45–12:15	H44	**Does Oncology Need Physics of Cancer?** — •Josef Käs
BP 18.1	Wed	9:30–10:00	H44	**Mechanical Imprints of Cell Competition** — •Benoit Ladoux
BP 19.8	Wed	11:30–12:00	H46	**Rolling vesicles: From confined rotational flows to surface-enabled motion** — •Laura R. Arriaga, Paula Magrinya, Pablo Palacios, Pablo Llombart, Rafael Delgado-Buscalioni, Alfredo Alexander-Katz, Juan L. Aragones
BP 20.6	Wed	16:30–17:00	H44	**Centrosome positioning in cell migration and immune response** — •Heiko Rieger
BP 22.1	Wed	15:00–15:30	H46	**From DNA Nanotechnology to biomedical insight: Towards single-molecule spatial omics** — •Ralf Jungmann
BP 25.1	Thu	9:30–10:00	H44	**Oncogenic signaling and stiffness sensing** — •Johanna Ivaska
BP 26.6	Thu	11:00–11:30	H46	**Theory for sequence selection via phase separation and oligomerization** — •Christoph Weber
BP 29.1	Thu	15:00–15:30	H44	**Community-driven software and data training for computational biology** — •Toby Hodges
BP 30.5	Thu	16:00–16:30	H46	**Topology in biological matter - are there double knots in proteins or maybe even more complicated knots? Prediction and in vitro verification.** — •Joanna I Sulkowska
BP 31.1	Fri	9:30–10:00	H44	**Wave propagation in systems of active filaments** — •Kirsty Y. Wan
BP 35.1	Fri	13:15–14:00	H2	**Active control of forces, movement and shape: from biological to non-living systems** — •Ulrich S. Schwarz

Invited Talks of the joint Symposium Physics of Embryonic Development Across Scales: From DNA to Organisms (SYED)

See SYED for the full program of the symposium.

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher
SYED 1.2	Mon	10:00–10:30	H1	**A tissue rigidity phase transition shapes morphogen gradients** — Camilla Autorino, Diana Khoromskaia, Bernat Corominas-Murtra, Zena Hadjivasiliou, •Nicoletta Petridou

SYED 1.3	Mon	10:30–11:00	H1	**Building quantitative dynamical landscapes of developmental cell fate decisions** — •David Rand
SYED 1.4	Mon	11:15–11:45	H1	**Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate** — •Anne Grapin-Botton, Byung Ho Lee, Masaki Sano, Daniel Riveline, Kana Fuji, Tetsuya Hiraiwa
SYED 1.5	Mon	11:45–12:15	H1	**Chromosomes as active communication and memory machines** — •Leonid A. Mirny

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Invited Talks of the joint Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

See SYQS for the full program of the symposium.

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — Reyhaneh Khasseh, Sascha Wald, Roderich Moessner, Christoph Weber, •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg, Greta Villa, Kilian Seibold, Vincent Dumont, Gianluca Rastelli, Mateusz Michałek, Alexander Eichler, Javier del Pino
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Sessions

BP 1.1–1.3	Sun	16:00–18:15	H2	**Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)**
BP 2.1–2.11	Mon	9:30–12:45	H37	**Active Matter I (joint session DY/BP/CPP)**
BP 3.1–3.12	Mon	9:30–13:00	H44	**Computational Biophysics I**
BP 4.1–4.6	Mon	9:30–11:15	H46	**Bacterial Biophysics**
BP 5.1–5.6	Mon	11:30–13:00	H46	**Membranes and Vesicles I**
BP 6.1–6.7	Mon	15:00–17:00	H37	**Active Matter II (joint session BP/CPP/DY)**
BP 7.1–7.6	Mon	15:00–17:00	H44	**Single Molecule Biophysics**
BP 8.1–8.6	Mon	15:00–16:45	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session BP/CPP)**
BP 9.1–9.4	Mon	17:00–18:00	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)**

BP 10.1–10.9	Tue	9:30–12:30	H43	**Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)**
BP 11.1–11.7	Tue	9:30–11:30	H44	**Cytoskeleton**
BP 12.1–12.6	Tue	9:30–11:15	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials III (joint session CPP/BP)**
BP 13.1–13.11	Tue	9:30–13:00	H47	**Active Matter III (joint session DY/BP/CPP)**
BP 14.1–14.25	Tue	10:00–12:30	P3	**Poster Session I**
BP 15.1–15.4	Tue	11:45–13:00	H44	**Cell Mechanics I**
BP 16.1–16.4	Tue	14:00–15:15	H43	**Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)**
BP 17.1–17.82	Tue	18:00–20:30	P4	**Poster Session II**
BP 18.1–18.12	Wed	9:30–13:00	H44	**Tissue Mechanics**
BP 19.1–19.12	Wed	9:30–13:00	H46	**Membranes and Vesicles II**
BP 20.1–20.10	Wed	15:00–18:00	H44	**Statistical Physics of Biological Systems I (joint session BP/DY)**
BP 21.1–21.9	Wed	15:00–17:30	H45	**Networks, From Topology to Dynamics (joint session SOE/BP/DY)**
BP 22.1–22.9	Wed	15:00–17:45	H46	**Bioimaging**
BP 23.1–23.1	Wed	18:00–20:00	P2	**Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)**
BP 24	Wed	18:15–19:15	H46	**Members' Assembly**
BP 25.1–25.12	Thu	9:30–13:00	H44	**Cell Mechanics II**
BP 26.1–26.9	Thu	9:30–12:15	H46	**Synthetic life-like systems and Origins of Life**
BP 27.1–27.7	Thu	15:00–17:30	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)**
BP 28.1–28.9	Thu	15:00–17:45	H37	**Microswimmers and Microfluidics (joint session DY/BP/CPP)**
BP 29.1–29.11	Thu	15:00–18:00	H44	**Focus Session: Innovations in Research Software Engineering (joint session BP/DY)**
BP 30.1–30.10	Thu	15:00–18:00	H46	**Protein Structure and Dynamics**
BP 31.1–31.12	Fri	9:30–13:00	H44	**Active Matter IV (joint session BP/CPP/DY)**
BP 32.1–32.13	Fri	9:30–13:00	H46	**Computational Biophysics II**
BP 33.1–33.7	Fri	10:30–12:45	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)**
BP 34.1–34.5	Fri	11:30–13:00	H43	**Statistical Physics in Biological Systems II (joint session DY/BP)**
BP 35.1–35.1	Fri	13:15–14:00	H2	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Biological Physics Division

Wednesday 18:15–19:15 H46

- Report of the speaker team
- Election of a new member of the speaker team
- Any other business

Sessions

– Invited Talks, Tutorials, Contributed Talks, and Posters –

BP 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:
https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:
https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial BP 1.1 Sun 16:00 H2

Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial BP 1.2 Sun 16:40 H2

Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial BP 1.3 Sun 17:30 H2

Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

BP 2: Active Matter I (joint session DY/BP/CPP)

Time: Monday 9:30–12:45 Location: H37

BP 2.1 Mon 9:30 H37

Odd dynamics and pattern formation in mixtures of magnetic spinners and passive colloids — •Dennis Schorn[1], Stijn van der Ham[2], Hanumantha Rao Vutukuri[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

Starfish embryos aggregate into chiral crystals exhibiting odd elasticity (Tan *et al.* Nature **607**, 287 (2022)). Similar structures have been recently observed in externally driven magnetic colloids. In this talk, I present experiments and simulations of binary mixtures of magnetic spinners and passive colloids. We develop a model to predict the phase diagram of the system, which comprises four distinct phases that can be systematically reproduced in experiments. In particular, our simulations and experiments show a phase where the passive particles form a gel-like network featuring significant holes filled with self-organized rotating chiral clusters made of spinners. This phase can be reversed by changing the system's composition and magnetic field strength, featuring a system spanning spinner phase with embedded counter-rotating chiral clusters made of passive colloids. Our system may open the route towards a new type of viscoelastic active chiral matter involving nonreciprocal interactions between both species.

BP 2.2 Mon 9:45 H37

Symmetry breaking in active non-reciprocal systems — •Kim L. Kreienkamp and Sabine H. L. Klapp — TU Berlin, Germany

Non-reciprocity significantly impacts the dynamical behavior in mixtures. One of its particularly striking consequences is the spontaneous emergence of time-dependent phases that break parity-time symmetry [1-3]. Here, we study a paradigmatic model of a non-reciprocal polar active mixture with completely symmetric repulsion [4,5]. Using a combination of field theory and particle-based simulations, we identify two qualitatively distinct regimes of non-reciprocity-induced dynamics. In the regime of weak intra-species alignment, non-reciprocity leads to asymmetric clustering in which only one of the two species forms clusters. Notably, the asymmetric density dynamics is driven alone by non-reciprocal orientational couplings [4,5]. In contrast, in the strongly coupled regime, the corresponding field theory exhibits exceptional points that have been associated with the emergence of chiral phases where the polarization direction rotates over time [2]. Our simulations confirm that spontaneous chirality arises at the particle level. In particular, we observe chimera-like states with co-existing locally synchronized and disordered regions. At the coupling strengths associated with exceptional points, the spontaneous chirality peaks.

[1] Z. You et al., PNAS 117, 19767 (2020).
[2] M. Fruchart et al., Nature 592, 363 (2021).

[3] K. L. Kreienkamp and S. H. L. Klapp, NJP 24, 123009 (2022).
[4] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRE (2024).
[5] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRL (2024).

BP 2.3 Mon 10:00 H37

Emergent phases in a discrete flocking model with non-reciprocal interaction — •Swarnajit Chatterjee, Matthieu Mangeat, and Heiko Rieger — Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Non-reciprocal interactions arise in systems that seemingly violate Newton's third law "actio=reactio". They are ubiquitous in active and living systems that break detailed balance at the microscale, from social forces to antagonistic interspecies interactions in bacteria. Non-reciprocity affects non-equilibrium phase transitions and pattern formation in active matter and represents a rapidly growing research focus in the field. In this work, we have undertaken a comprehensive study of the non-reciprocal two-species active Ising model (NRTSAIM), a non-reciprocal discrete-symmetry flocking model. Our study uncovers a distinctive *run-and-chase* dynamical state that emerges under significant non-reciprocal frustration. In this state, A-particles chase B-particles to align with them, while B-particles avoid A-particles, resulting in B-particle accumulation at the opposite end of the advancing A-band. This run-and-chase state represents a non-reciprocal discrete-symmetry analog of the chiral phase seen in the non-reciprocal Vicsek model. Additionally, we find that self-propulsion destroys the oscillatory state obtained for the non-motile case, and all the NRTSAIM steady-states are metastable due to spontaneous droplet excitation and exhibit motility-induced interface pinning. A hydrodynamic theory supports our simulations and confirms the reported phase diagrams.

BP 2.4 Mon 10:15 H37

Emergent phases in a discrete flocking model with reciprocal interaction — •Matthieu Mangeat[1], Swarnajit Chatterjee[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We have undertaken a comprehensive study of the two-species active Ising model (TSAIM), a discrete-symmetry counterpart of the continuous-symmetry two-species Vicsek model, motivated by recent interest in the impact of complex and heterogeneous interactions on active matter systems. In the TSAIM, two species of self-propelled particles undergo biased diffusion in two dimensions, interacting via local intraspecies alignment and reciprocal interspecies anti-alignment, along with the possibility of species interconversion. We observe a liquid-gas phase transition, exhibiting macrophase-separated bands, and the emergence of a high-density parallel flocking state, a feature not seen in previous flocking models. With species interconversion (species-flip dynamics), the TSAIM corresponds to an active extension of the Ashkin-Teller model and exhibits a broader range of steady-state phases, including microphase-separated bands that further enrich the coexistence region. We also find that the system is metastable due to droplet excitation and exhibits spontaneous motility-induced interface pinning, preventing the system from reaching long-range order at sufficiently low noise. A hydrodynamic theory complements our computer simulations of the microscopic model and confirms the reported phase diagrams.

BP 2.5 Mon 10:30 H37

Emergent collective behavior from cohesion and alignment — •Jeanine Shea and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany.

Collective behavior is all around us, from flocks of birds to schools of fish. These systems are immensely complex. To explore their basic characteristics, we introduce a minimal model for cohesive and aligning self-propelled particles in which group cohesion is established through additive, non-reciprocal torques [1]. These torques cause constituents to effectively turn towards one another, while an additional alignment torque competes in the same spatial range. By changing the strength and range of these torque interactions, we uncover six states which we distinguish via their static and dynamic properties. These states range from disperse particles to closely packed worm-like formations. A number of the states generated by this model exhibit collective dynamics which are reminiscent of those seen in nature.

[1] Knežević, M., Welker, T. and Stark, H. Collective motion of active particles exhibiting non-reciprocal orientational interactions. Sci Rep 12, 19437 (2022).

Invited Talk BP 2.6 Mon 10:45 H37

Collective behavior of photoactive macroscopic particles — •Iker Zuriguel — University of Navarra, Pamplona, Spain

Active matter refers to systems of interacting, self-propelled agents that convert energy into mechanical motion, representing a nice example of out-of-equilibrium systems. In this work, a novel type of active particles is introduced. These are active granular (i.e. they interact solely through physical contacts) and photoactive, meaning that they self-propel using energy from light. Therefore, by means of a programmable LED panel, we are able to change the illumination pattern and, consequently, the particle activity in space and time, allowing a precise exploration of a variety of scenarios related to collective behavior. This possibility has been exploited in microscopic systems but is genuinely new in macroscopic ones.

First, we will present the clustering behavior of these agents under homogeneous illumination. By varying the illumination intensities and changing the population size, we observed a power-law-like distribution for both the cluster sizes and durations. We identified a transition from unstable to stable clusters, as indicated by the divergence of average cluster durations. Higher particle activities and smaller populations led to the creation of small unstable clusters, while lower particle activities and larger populations result in big, stable clusters that persist over time. This transition is explained with the help of a simple model capturing the most important processes involved in cluster dynamics. In the last part of the talk, the collective behavior under inhomogeneous illumination patterns will be introduced.

15 min. break

BP 2.7 Mon 11:30 H37

Swarming model with minority interaction exhibits temporal and spatial scale-free correlations — •Simon Syga[1], Chandraniva Guha Ray[2,3,4], Josué Manik Nava Sedeño[5], Fernando Peruani[6,7], and Andreas Deutsch[1] — [1]Technische Universität Dresden — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Center for Systems Biology Dresden — [5]Universidad Nacional Autónoma de México — [6]Université Côte d'Azur, Nice — [7]CY Cergy Paris Université

Collective motion is a widespread phenomenon in social organisms, from bird flocks and fish schools to human crowds and cell groups. Swarms of birds and fish are particularly fascinating for their coordinated behavior and rapid escape maneuvers during predator attacks. Critical motion is hypothesized as an optimal trade-off between cohesive group behavior and responsiveness to well-informed individuals. However, traditional models only show criticality at the phase transition between ordered and unordered motion. Here, we extend the Vicsek model with a minority interaction, where individuals primarily follow neighbors but can switch to follow a defector moving against a well-aligned group. This triggers cascades of defections, leading to rich dynamics, including large-scale fluctuations, scale-free velocity distributions, and a scale-free return time distribution of the order parameter. Our model underscores the biological importance of minority interactions in swarming and their role in critical behavior.

BP 2.8 Mon 11:45 H37

'Predator-prey' driven swarmalator systems — •Ginger E. Lau, Mario U. Gaimann, and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Swarmalators are an active matter system of oscillators which exhibit swarming and collective motion in physical space, as well as synchronization behavior in an additional phase variable space, originally introduced by O'Keeffe *et al.* (*Nat. Commun.* 8(1), 1504, 2017). Such systems with bidirectional couplings in space and phase can be observed in nature, such as in the chorusing behavior of Japanese tree frogs characterized by Aihara *et al.* (*Sci. Rep.* 4(1), 3891, 2014). The interplay between attraction, repulsion, and phase synchronization provides several distinct regimes of self-organizational behavior. Akin to biological swarm systems responding to predator interactions, swarmalators can respond collectively to external perturbations by a repulsive driver. In previous work, driving was realized with a mobile 'pacemaker' by Xu *et al.* (*Chaos* 34(11), 113103, 2024). The present study introduces a new 'predator-prey' driven swarmalator model showing rich adaptive behavior. This could have a wide variety of potential future applications, from biological physics to swarm robotics to nature-inspired learning algorithms and methods of inference.

BP 2.9 Mon 12:00 H37

Inertial active matter governed by Coulomb friction — •Alexander Antonov[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]University of Rome La Sapenzia, Rome, Italy

Coulomb, or dry friction, is a common phenomenon that can be encountered in various systems, such as granular matter or Brownian motors. The Coulomb friction force resists the motion and, unlike the friction in wet systems, is almost independent of the relative velocity. We show that this characteristic feature of Coulomb friction leads to emergence of dynamical states when subjected to active, or self-propelled motion [1]. At low activity levels, the dynamics resembles Brownian motion, while at greater activity, a dynamic Stop & Go regime emerges, marked by continuous switching between diffusion and accelerated motion. At even higher activity levels, a super-mobile regime arises, characterized by fully accelerated motion and an anomalous scaling of the diffusion coefficient with activity. Near the transition between the Stop & Go and super-mobile regimes, we reveal a novel activity-induced phase separation in collective behavior [2]. Our theoretical findings have been also demonstrated in experiments, where

vibrobots on a horizontal surface are activated by vertical oscillations generated using an electromagnetic shaker.

[1] A.P. Antonov, L. Caprini, A. Ldov, C. Scholz, and H. Löwen, Phys. Rev. Lett. 133, 198301 (2024)

[2] A.P. Antonov et al., in preparation.

BP 2.10 Mon 12:15 H37

Active nematic turbulence with substrate friction — •Peter A. E. Hampshire[1,2] and Ricard Alert[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, Dresden, Germany

Active nematics with high activity exhibit turbulent-like flows, characterized by vortices, spatio-temporal chaos and power laws in the energy spectra [1-3]. Continuum models have been successfully used to predict the scaling of the energy spectra with the wavevector. Most theoretical work has focused on free-standing, active nematic films. However, in several experimental realisations, such as bacterial colonies and epithelial monolayers, the active nematic is in contact with a solid substrate. We generalised a 2D, incompressible active nematic model to include substrate friction, and studied its impact on the transition to turbulence and the energy spectra of the turbulent-like flows. We find a variety of dynamic states including flow in lanes, stable vortices and both isotropic and anisotropic turbulence. At high activity and moderate friction, we found a power-law scaling in the kinetic energy spectrum $E(q) \sim q^3$, where q is the wavevector, at low wavevectors. The exponent of 3 can be justified with a power-counting argument. Overall, we have developed a model for active nematic turbulence on a substrate that can be compared to biological systems. [1] L. Giomi, *Phys. Rev. X* **5**, 031003 (2015). [2] R. Alert, J.-F. Joanny, J. Casademunt, *Nat. Phys.* **16**, 682-688 (2020). [3] B. Martínez-Prat*, R. Alert*, et al., *Phys. Rev. X* **11**, 031065 (2021).

BP 2.11 Mon 12:30 H37

Self-sustained patchy turbulence in shear-thinning active fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg

Bacterial suspensions and other active fluids are known to develop highly dynamical vortex states, denoted as active or mesoscale turbulence. We reveal the pronounced effect of non-Newtonian rheology of the carrier fluid on these turbulent states, concentrating on shear thinning. As a consequence, a self-sustained heterogeneous state of coexisting turbulent and quiescent areas develops, which results in anomalous velocity statistics. The heterogeneous state emerges in a hysteretic transition under varying activity. We provide an extensive numerical analysis and find indirect evidence for a directed percolation transition. Our results are important, for instance, when addressing active objects in biological media with complex rheological properties.

BP 3: Computational Biophysics I

Time: Monday 9:30–13:00 Location: H44

BP 3.1 Mon 9:30 H44

RNA plasticity emerges as an evolutionary response to fluctuating environments — •Paula García-Galindo[1] and Sebastian E. Ahnert[1,2] — [1]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS United Kingdom — [2]The Alan Turing Institute, 96 Euston Road, London NW1 2DB, UK

Phenotypic plasticity, the ability of a single genotype to produce multiple distinct phenotypes, can be studied effectively using RNA. RNA is a dynamic macromolecule that probabilistically shifts its structure due to thermal fluctuations at the molecular scale. To model the evolution of RNA plasticity, we use the RNA sequence-to-structure non-deterministic mapping, a computationally tractable genotype-phenotype (GP) map where probabilistic phenotypes are derived from the Boltzmann distribution of structures for each RNA sequence. Through evolutionary simulations with periodic environmental switching on the GP map, we observe that RNA phenotypes adapt to these fluctuations by evolving toward optimal plasticity. These optimal phenotypes are defined by nearly equal Boltzmann probabilities for distinct structures, each representing the most advantageous configuration for alternating environments. Our findings demonstrate that phenotypic plasticity, a widespread biological phenomenon, is a fundamental evolutionary adaptation to fluctuating environments.

BP 3.2 Mon 9:45 H44

Symmetry of loop extrusion by dimeric SMC complexes is DNA-tension-dependent — Biswajit Pradhan[1], •Adrian John Pinto[2], Peter Virnau[2], and Eugene Kim[1] — [1]Max Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany — [2]Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

Structural maintenance of chromosome (SMC) complexes are involved in genome organization and regulation via DNA loop extrusion. During extrusion SMC proteins reel DNA from one or both sides and a loop forms and increases. At low DNA tension (< 0.1pN), Smc5/6 and Wadjet extrude DNA from both sides of the loop. At higher tension, however, they transition to a behavior akin to one-sided extruders, yet still capable of extruding from one or the other side thereby switching the direction of extrusion [1]. In order to model this process in simulations, we propose a coarse-grained model for DNA loop extrusion using a Kratky-Porod chain as a basis for DNA and a handcuff for SMC proteins. By matching stalling forces, we are able to simulate loop extrusion on experimental time and length scales. We find that the observed switching from two- to one-sided behavior does not require a change in motor activity, but can be explained as a complex interplay of extrusion, stalling and thermal fluctuations.

[1] Pradhan, B., Pinto, A., Kanno, T., et al. (2024). Symmetry of loop extrusion by dimeric SMC complexes is DNA-tension-dependent. bioRxiv. https://doi.org/10.1101/2024.09.12.612694

BP 3.3 Mon 10:00 H44

NucleoSeeker - Precision filtering of RNA databases to curate high-quality datasets — •Utkarsh Upadhyay[1], Fabrizio Pucci[2], Julian Herold[3], and Alexander Schug[1,4] — [1]Jülich Supercomputing Centre, Germany — [2]Universite Libre de Bruxelles, Belgium — [3]Karlsruhe Institute for Technology, Germany — [4]University of Duisburg- Essen, Germany

The structural prediction of biomolecules via computational methods complements the often involved wet-lab experiments. Unlike protein structure prediction, RNA structure prediction remains a significant challenge in bioinformatics, primarily due to the scarcity of RNA structure data and its varying quality. Many methods have used this limited data to train deep learning models but redundancy, data leakage and bad data quality hampers their performance. In this work, we present NucleoSeeker, a tool designed to curate high-quality, tailored datasets from the Protein Data Bank (PDB) database. It is a unified framework that combines multiple tools and streamlines an otherwise complicated process of data curation. It offers multiple filters at structure, sequence and annotation levels, giving researchers full control over data curation. Further, we present several use cases. In particular, we demonstrate how NucleoSeeker allows the creation of a non-redundant RNA structure dataset to assess AlphaFold3's performance for RNA structure prediction. This demonstrates NucleoSeeker's effectiveness in curating valuable non-redundant tailored datasets to both train novel and judge existing methods. NucleoSeeker is very easy to use, highly flexible and can significantly increase the quality of RNA structure datasets.

BP 3.4 Mon 10:15 H44

Uncovering the Non-Canonical RNA Binding site on the Immune Sensor OAS2 by combining AI, MD simulations and experiments. — •Adrian F. Schnell[1], Veronika Merold[2], Indra Bekere[2], Carina C. de Oliveira Mann[2], and Nadine Schwierz[1] — [1]Institute of Physics, University of Augsburg — [2]Department of Bioscience, Technical University of Munich

Molecular dynamics (MD) simulations and machine learning provide powerful tools to predict protein-RNA interactions, but their predictions require experimental verification. In this talk, we showcase an advancement in understanding the immune sensor 2'-5'-oligoadenylate synthetase 2 (OAS2) by combining AlphaFold 3, MD simulations, cryo-electron microscopy (cryo-EM), and cellular assays. Although the structure of the OAS2 has been resolved through cryo-EM, the precise mechanisms underlying its activation and the RNA binding site remained elusive.

To fill this gap, we combined all-atom MD simulations based on cryo-EM structures and AlphaFold 3 predictions to identify non-canonical RNA binding interfaces on the catalytically deficient OAS2 domain. By integrating mutagenesis studies and contact data from MD simulations, we uncovered critical structural details of RNA binding and OAS2 activation. Importantly, our findings reveal how OAS2 domains discriminate RNA length, providing new insights into its function and regulatory mechanisms. These results enhance our understanding of OAS2's antiviral immune role and offer a foundation for developing antiviral strategies targeting the OAS-RNase L pathway.

BP 3.5 Mon 10:30 H44

Computational bridging between sequence design and network-level behaviour of programmable DNA-nanomotifs — •Aaron Gadzekpo[1] and Lennart Hilbert[1,2] — [1]Karlsruhe Institute of Technology, Institute of Biological and Chemical Systems — [2]Karlsruhe Institute of Technology, Zoological Institute

DNA can serve as a programmable material, by using the DNA sequence to control the 3D-structure of building blocks at the nanometre-scale. In our work, we construct X-shaped particles, or "nanomotifs", from four single-stranded DNA-oligomers, each 46 nucleotides in length. The X-motifs' four arms selectively and transiently hybridize, linking into large, dynamic networks guided by DNA sequence complementarity. We present our scale-bridging computational methods to predict how DNA-oligomer sequences translate into physical properties of X-motifs and the emergent behaviour of networks. In particular, we leverage machine learning to transition from base-pair resolution simulations of single X-motifs and linked pairs to coarse-grained molecular dynamics simulations of networks at increased time and length scales. These simulations are used to explore how nanomotif design at nucleotide level influences emergent behaviour, including liquid-liquid phase separation and condensation on target DNA strands with complementary binding motifs. We connect our observation to corresponding experiments, showcasing model-aided design of DNA-based materials.

BP 3.6 Mon 10:45 H44

Ionizable cationic lipids and helper lipids synergistically contribute to RNA packing and protection in lipid-based nanomaterials — •David Noel Zimmer[1,2], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Physics Department Johannes Gutenberg University Mainz — [2]Faculty of Physics and Astronomy Ruhr University Bochum

Lipid-based nanomaterials are used as a common delivery vehicle for RNA therapeutics. They typically include a formulation containing ionizable cationic lipids, cholesterol, phospholipids, and a small molar fraction of PEGylated lipids. The ionizable cationic lipids are considered a crucial element of the formulation for the way they mediate interactions with the anionic RNA as a function of pH. Here[1], we show, by means of molecular dynamics simulation of lipid formulations containing two different ionizable cationic lipids (DLinDMA and DLinDAP), that the direct interactions of those lipids with RNA, taken alone, may not be sufficient to determine the level of protection and packaging of mRNA. Our simulations help and highlight how the collective behavior of the lipids in the formulation, which determines the ability to envelop the RNA, and the level of hydration of the lipid-RNA interface may also play a significant role. This allows the drawing of a hypothesis about the experimentally observed differences in the transfection efficiency of the two ionizable cationic lipids.

[1] Zimmer, D. N., Schmid, F., & Settanni, G. (2024). J. Phys. Chem. B 2024, 128, 41, 10165-10177.

15 min. break

Invited Talk BP 3.7 Mon 11:15 H44

Killing to survive - how protein-lipid interactions drive programmed cell death — •Kristyna Pluhackova — University of Stuttgart, Stuttgart, Germany

Programmed cell death is an essential process of eukaryotic life, enabling e.g., embryonic development, regeneration, or fighting pathogens. Depending on the needs of an organism, diverse molecular mechanisms of cell death exist, determining among others the speed of cell death, its extent and the impact on surrounding cells. Not surprisingly, dysregulation of cell death culminates in diverse diseases, the most prominent of all being cancer.

Here, I reveal molecular details of protein-lipid interactions in programmed cell death by multiscaling molecular dynamics simulations. First, I unveil how lipids unplug medium-sized membrane pores formed by a pyroptotic agent gasdermin and reveal astonishing adaptability of the pore shape. Next, I demonstrate how the gasdermin species and the lipid composition determine the process of gasdermin pore formation. At last, I resolve the mechanism through which ninjurin-1 disrupts membranes during plasma membrane rupture, the terminal event of many cell-death processes.

BP 3.8 Mon 11:45 H44

Integrative Modeling of Cellular Dynamics: Applications to Viruses and Neurotransmission — •Mohsen Sadeghi — Freie Universität Berlin, Berlin, Germany

A comprehensive understanding of cellular processes requires a quantitative analysis of biomembrane dynamics in interaction with protein populations, within a model that integrates kinetics and protein structural information. This is crucial for deciphering and potentially manipulating complex biological pathways. In this work, we introduce a dynamic framework for modeling membranes and proteins [1-5], showcasing its large-scale applications. These include the first computational model of the human cytomegalovirus [6] and the simulation of synaptic vesicle docking. We highlight how large-scale mesoscopic simulations provide unprecedented insights into complex cellular dynamics, capturing spatiotemporal scales that are directly relevant to cell biology.

[1] Sadeghi and Noé, Nat. Commun. (2020) 11:2951.
[2] Sadeghi, Weikl and Noé, J. Chem. Phys. (2018) 148:044901.
[3] Sadeghi and Noé, J. Chem. Phys. (2021) 155:114108.
[4] Sadeghi and Noé, J. Phys. Chem. Lett. (2021) 12:10497-10504.
[5] Sadeghi, Soft Matter (2022) 18:3917-3927.
[6] Bogdanow, et al. Nat. Microbiol. (2023) 8:1732.

BP 3.9 Mon 12:00 H44

Hepatitis C Virus Infection Alters NK Cell Receptor Expression: A High-Dimensional Analysis — •Andrea Schneider — Heirich-Heine Universität Düsseldorf

Hepatitis C virus (HCV) infection influences the expression of receptors on natural killer (NK) cells, a crucial component of the innate immune system. Using fluorescent markers for flow cytometry measurements, receptor expression can be analyzed to identify differences between healthy individuals, recovered patients, and those with chronic infections. Due to the possibility of using many markers simultaneously in one measurement, algorithms for dimension reduction are necessary for the evaluation of flow cytometry data. These findings could provide a potential starting point for novel therapeutic approaches. A key focus of the talk is the application of t-SNE, a dimensionality reduction algorithm that visualizes high-dimensional data in two-dimensional scatterplots while preserving high-dimensional clustering. The analysis offers valuable insights into the cellular differences among the three patient groups and opens new perspectives for immunological research.

BP 3.10 Mon 12:15 H44

Activity enhanced shear-thinning of flexible linear polar polymers — •Arindam Panda[1], Roland G. Winkler[2], and Sunil P Singh[1] — [1]Indian Institute Of Science Education and Research, Bhopal, Madhya Pradesh, India — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

The rheological behavior of tangentially propelled flexible polymers in linear shear flow is investigated through computer simulations and compared with analytical predictions. Our study reveals a significant interplay between nonequilibrium active forces and shear-induced effects on the polymer's structural and dynamical properties. Polar activity enhances the shear-induced stretching along the flow direction while inducing compression in the transverse direction. This coupling leads to a pronounced shear-thinning response, where the viscosity decreases with increasing shear rate. In the high activity and shear limit, the polymer's behavior becomes largely independent of the active forces, with the shear flow predominantly driving the system's response. At asymptotically high shear rates, the system transitions to a regime where the polymer exhibits characteristics akin to passive polymers, with shear forces entirely overshadowing the influence of activity.

BP 3.11 Mon 12:30 H44

Patchy Particle Model for Biomolecular Condensates — •Devika Magan[1,2,3], Alena Taskina[1,4], Simon Dannenberg[1], and Stefan Klumpp[1,4] — [1]Institute for the Dynamics of Complex Systems, University of Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Indian Institute of Science Education and Research Mohali, India — [3]Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany — [4]Max Planck School Matter to Life

Biomolecular condensates are formed via liquid-liquid phase separation (LLPS) of proteins and nucleic acids, driven by interactions between low-affinity binding sites. Computational studies of biomolecular condensates often use coarse-grained patchy particle models, representing proteins with a repulsive core and directional attractive patches. However, these simulations are typically limited by slow dynamics and struggle to capture the full range of material properties of fluid-like condensates. We present an enhanced patchy particle model to study the formation and dynamics of biomolecular condensates. By incorporating flexible patches and weak isotropic attractions between cores, our model preserves key equilibrium characteristics, including phase behavior and local structure, while significantly accelerating system dynamics. These modifications enable the simulation of larger, more complex systems previously inaccessible due to prohibitive relaxation times and provide a versatile tool for studying condensate dynamics.

BP 3.12 Mon 12:45 H44

Co-translational (polysome-protein) condensation — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research , 01069, Dresden, Germany

Biomolecular condensates are ubiquitous in cells and play crucial roles in cellular regulation. These condensates typically form via liquid-liquid phase separation, where protein-protein interactions are crucial. However, how condensates interact with protein translation machinery is poorly studied. During translation, multiple ribosomes are simultaneously translating each mRNA forming a poly-ribosome structure (polysome), which resembles beads packed on a string. On one end of the mRNA, the ribosomes have only extruded the start of the nascent protein, and on the other end the ribosomes have a nearly finished pro-

tein. Nascent proteins from translating polysomes can interact with the finished proteins that make up the condensate (co-translational condensation). Using coarse-grained simulations, we show that the architecture of encoded proteins determines whether the polysome is adsorbed to the condensate surface or remains in the cytoplasm. Furthermore, we employ a reaction-diffusion model to analyze the time scales relevant to this process. Additionally, we model the potential cellular advantages of this phenomenon, including enhanced cellular response times, reduced noise in protein concentration, and facilitation of post-translational modifications. This work establishes a theoretical framework for co-translational condensation and highlights new functions for condensates in cells and offers promising directions for experimental validation.

BP 4: Bacterial Biophysics

Time: Monday 9:30–11:15 Location: H46

Invited Talk BP 4.1 Mon 9:30 H46

Spatiotemporal organization of bacterial biofilm formation and functions — •Knut Drescher — Biozentrum, University of Basel, Basel, Switzerland

In nature, bacteria often live in three-dimensional communities termed biofilms, in which cells are attached to each other through an extracellular matrix. In this presentation, I will first introduce microscopy, image processing, and spatiotemporal transcriptome measurement techniques that enable us to monitor all individual cells in living biofilms. Based on these techniques, I will then show how we can identify the cell-cell interaction processes that determine the architecture development of biofilm microcolonies, across different species. I will then proceed to discuss how individual cells in biofilms coordinate their activities so that the biofilm community develops emergent functions, such as the predation of human immune cells, as well as the protection from viral predators. This talk will therefore shed light on the spatiotemporal development of bacterial communities, and the mechanisms underlying emergent functions of these communities.

BP 4.2 Mon 10:00 H46

Modelling the growth of biofilms on soft substrates — •Anthony Pietz[1], Uwe Thiele[1], and Karin John[2] — [1]Universität Münster, Münster, Germany — [2]Université Grenoble Alpes

Bacteria invade surfaces by forming dense colonies encased in a polymer matrix. Successful settlement of founder bacteria, early microcolony development and later macroscopic spreading of these biofilms on surfaces rely on complex physical mechanisms. Data show that on soft hydrogels, substrate rigidity is an important determinant for biofilm initiation and spreading. Using a thermodynamically consistent thin-film approach for suspensions on soft elastic substrates we investigate in silico the role of substrate rigidity in the osmotic spreading of biofilms. We show that on soft substrates spreading is considerably slowed down and may even be arrested depending on the biomass production rate. We find, that the slowing down of biofilm spreading on soft surfaces is caused by a reduced osmotic influx of solvent into the biofilm results from the coupling between substrate deformation and interfacial forces.

BP 4.3 Mon 10:15 H46

Dynamics of bacterial growth and colony development in heterogeneous mechanical landscapes — •Chenyu Jin[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, 162 A, Avenue de la Faïencerie, L-1511, Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg, Avenue de l'Université, L-4365, Esch-sur-Alzette, Luxembourg

Bacteria inhabit diverse confinements, experiencing different mechanical cues including surface stiffness and adhesion, friction and wettability [1]. Recent studies have revealed how local crowding and phenotypic noise impact bacterial growth and structural changes like the monolayer-to-multilayer transitions (MTMT)[2,3]. Yet how colonies proliferate in heterogeneous physical landscapes remain largely unknown [4]. Here we combine quantitative imaging and numerical modeling to compare the dynamics of colony growth within soft hydrogels with those in liquid media for different bacterial species. We find that the growth rate typically decreases across species, at both the colony and individual scales, while the critical area at the MTMT increases by an order of magnitude in the confined environment. An accompanying bioenergetic model offers mechanistic insights into the colony development in heterogeneous mechanical settings.

[1] NAM Araújo, LMC Janssen, et al., *Soft Matter* 19, 1695-1704 (2023). [2] R Wittmann, …, A Sengupta, *Commun. Phys.* 6, 331 (2023). [3] J Dhar, …, A Sengupta, *Nat. Phys.* 18, 945 (2022). [4] C Jin, A Sengupta, *Biophys. Rev.* 16, 2024

BP 4.4 Mon 10:30 H46

Capillary interactions organize bacterial colonies — •Ricard Alert[1,2,3], Matthew E. Black[4], Chenyi Fei[4,5], Ned S. Wingreen[4], and Joshua W. Shaevitz[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Center for Systems Biology Dresden — [3]Cluster of Excellence Physics of Life, TU Dresden — [4]Princeton University — [5]Massachusetts Institute of Technology

Many bacteria inhabit hydrated environments like soil, textiles and agar hydrogels in the lab. In these environments, cells are surrounded by a water meniscus, and they experience capillary forces. I will show that capillary forces organize bacterial colonies, enabling cells to aggregate into densely packed nematic layers while still allowing them to slide past one another. Our collaborators developed an experimental apparatus that allows us to control bacterial collective behaviors by varying the strength and range of capillary forces. Our results suggest that capillary forces may be a ubiquitous physical ingredient in shaping microbial communities in partially hydrated environments.

BP 4.5 Mon 10:45 H46

CISS Effect in Bacterial Extracellular Electron Transfer — •Nir Sukenik[1], Mohamad El Naggar[1], Yossi Paltiel[2], Ron Naaman[3], and Lech Tomasz Baczewski[4] — [1]University of Southern California, Lis Angeles, CA, USA — [2]Hebrew University of Jerusalem, Jerusalem, Israel — [3]Weizmann Institute of Technology, Rehovot, Israel — [4]Polish Academy of Sciences, Warsaw, Poland

Electron transfer through chiral molecules is characterized by a coupling between the electron velocity and its spin through the Chirality Induced Spin Selectivity (CISS) effect. Since most biomolecules are homochiral, it was recently hypothesized that CISS underlies the highly efficient electron transfer observed in biological systems by reducing the probability of electron backscattering. A remarkable example of efficient long-distance electron transport in biology is the extracellular respiration of metal-reducing bacteria, where a pathway composed of multiheme cytochromes facilitates extracellular electron transfer (EET) from the cellular interior to external electrodes. Using conductive probe atomic force microscopy measurements of protein monolayers adsorbed onto ferromagnetic substrates, we show that electron transport is spin selective in two of the multiheme cytochromes, the membrane-associated decaheme MtrA and the tetraheme periplasmic STC. To assess the in vivo physiological impact of CISS, we also present evidence that the respiration of a different EET capable bacterium, depends on the magnetization direction of the underlying ferromagnetic electrode. Taken collectively, our results demonstrate the important role of spin in a biological mechanism essential to life.

BP 4.6 Mon 11:00 H46

Slower prior growth in E. coli confers a competitive advantage under carbon starvation — •Zara Gough[1], Hamid Seyed Allaei[1], Severin Schink[2], Elena Biselli[1], Sophie Brameyer[3], and Ulrich Gerland[1] — [1]Physics of Complex Biosystems, Physics Department, Technical University of Munich, 85748 Garching, Germany — [2]Department of Systems Biology, Harvard Medical School, 200 Longwood Ave, Boston, MA 02115, USA — [3]Microbiology, Faculty of Biology, Ludwig Maximilians University Munich, Martinsried, Germany

Bacteria spend much of their life cycle under nutrient limitation, competing for resources to survive. Recent research has quantitatively characterized the carbon starvation kinetics of E. coli in monoculture using two experimentally measurable parameters: the maintenance rate and the recycling yield. Building on this framework, we show that these same parameters can predict fitness changes when cultures with distinct prior growth rates are subjected to starvation in co-culture. We introduce an additional model that explores the interaction between intracellular energy reserves and extracellular medium energy during co-culture starvation, and accounts for different uptake rates resulting from prior growth rate. Using a bottom-up approach to modelling that is derived directly from bacterial physiology, our work extends the quantitative understanding of population dynamics in E. coli.

BP 5: Membranes and Vesicles I

Time: Monday 11:30–13:00 Location: H46

BP 5.1 Mon 11:30 H46

In-Plane Correlations in Fluid Lipid Monolayers - Experiments and Molecular Dynamics Simulations — •Kay-Robert Dormann[1], Joshua Reed[1], Matej Kanduč[2], Benno Liebchen[1], and Emanuel Schneck[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Department of Theoretical Physics, Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Biological membranes predominantly consist of fluid lipid phases featuring lateral mobility and a considerable disorder of their hydrocarbon chains. Langmuir monolayers of lipids at the air/water interface are versatile model systems for fundamental physicochemical and biophysical membrane investigations. Recent experimental studies utilizing grazing-incidence x-ray diffraction (GIXD) have probed the chain correlation peak in fluid phospholipid monolayers as a function of the lipids' lateral packing. However, interpretation of the peak characteristics with over-simplified models based, for example, on rod-like chains yields only limited insights.

Here, we perform molecular dynamics (MD) simulations of phospholipids in the same monolayer configuration and predict the diffraction patterns originating from the chain correlations for a rigorous comparison with the experimental ones. The MD simulations reproduce the peak characteristics and their dependence on lateral packing well. Moreover, the experimentally validated simulation trajectories contain comprehensive information on the underlying chain correlations.

BP 5.2 Mon 11:45 H46

Modelling Wave Propagation on Monolayers — •Philipp Zolthoff and Jan Kierfeld — TU Dortmund, Dortmund, Germany

Recent experimental advances have enabled precise studies of pressure wave propagation through monolayers at the air-water interface, triggered by embedded azobenzenes and light-induced trans-to-cis isomerization. This talk presents theoretical results, which show that fractional nonlinear wave equations of Lucassen type can describe wave propagation on monolayers quantitatively. The nonlinear differential wave equation includes fractional time derivatives, incorporates measured Langmuir isotherms and a dynamic second viscosity that depends on the local state of the monolayer.

BP 5.3 Mon 12:00 H46

Artificial Membranes Through Physical Vapor Deposition (PVD): Exploring the Lipid Rafts Model — •Nancy Gómez-Vierling[1], D.A. Saavedra[1], M.A. Cisternas[2], M. Soto-Arriaza[3], C. Shen[4], P. Huber[4], and U.G. Volkmann[1] — [1]Instituto de Física, Pontificia Univ. Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Univ. de Valparaíso, Santiago, Chile — [3]Facultad de Medicina y Ciencia, Univ. San Sebastian, Santiago, Chile — [4]DESY, Hamburg, Germany

Essential to life, cell membranes are currently modelled as functional microdomains known as lipid rafts. These cholesterol- and sphingolipid-enriched domains are fundamental for organizing and categorizing key cellular processes. This research explores the assembly of artificial membranes inspired by the lipid raft model using PVD. This solvent-free technique previously demonstrated in DPPC membranes, is now applied to mixtures of sphingomyelin, cholesterol, and DOPC to investigate the self-assembly of microdomains under controlled conditions. Optimizing parameters such as temperature, deposition time, and thickness enables the successful formation of thin films on silicon substrates. Preliminary FTIR and GISAXS analyses confirm molecular integrity after cholesterol and DOPC evaporation, while ongoing studies examine the desorption and thermal stability of these SLBs. This work advances our understanding of membrane physics and establishes a versatile platform for creating model membranes with potential applications in biotechnology and materials science. Acknowledgements: ANID Fellowships (DS, NGV); Puente UC 2024-25.

BP 5.4 Mon 12:15 H46

Structural and mechanical properties of lipid monolayers at the water-air interface — •Hyunyou Kim[1], Ivo Buttinoni[1], Laura Alvarez Frances[2], and Pantelis Mpourazanis[3] — [1]Institute of Experimental Physics of Condensed Matter, Heinrich-Heine University, Universitätsstr.1, 40225 Düsseldorf, Germany — [2]University of Bordeaux, CNRS, CRPP, UMR 5031, 33600 Pessac, France — [3]Fraunhofer IOSB, Gutleuthausstraße 1, 76275 Ettlingen, Germany

Lipid monolayers play a crucial role at air-water interfaces of body, such as in alveoli, where they regulate surface tension. When surface pressure increases, the interface transitions from liquid-expanded (LE) to liquid-condensed (LC) phases.

As experimental model, Dipalmitoylphosphatidylcholine (DPPC) and Cholesterol (Chol) are used. Langmuir-Blodgett trough monitors lipid monolayers during compression, while fluorescence microscopy visualizes the domains. Rheology is measured at various frequencies using an interfacial shear rheometer coupled with trough.

During compression, pure DPPC monolayers transition from LE to LC, with a plateau at surface pressure Π = 5-6 mN/m and collapse at Π = 60-65 mN/m. The domain shape changes from round to fractal. Adding Chol lowers the collapse pressure (Π = 45-50 mN/m) and eliminates the plateau when Chol exceeds 8.6 mol %. Rheology shows that Chol decreases surface viscosity and makes the monolayers more elastic at higher frequencies.

BP 5.5 Mon 12:30 H46

Study of Giant Unilamelar Vesicles' Fluidity in Microgravity Conditions — •Georgios Stogiannidis[1], Paulina Blair[1,3], Laura Alvarez[2], Thomas Voigtmann[1,3], and Ivo Buttinoni[1] — [1]Heinrich-Heine University, Düsseldorf, Germany — [2]Université de Bordeaux, Bordeaux, France — [3]Deutsche Zentrum für Luft- und Raumfahrt, Köln, Germany

In this study, we examine the effect of microgravity on the membrane fluidity of giant unilamellar vesicles (GUVs) made of DOPC and Cholesterol. GUVs are prepared using electroformation technique, during which a thin film of lipids is deposited on a conductive glass substrate while the application of AC electric field accelerates the swelling of the lipid film. We first study the fluidity of the vesicles over a range of DOPC/Cholesterol ratios using Fluorescence Recovery After Photobleaching (FRAP): a disk shaped area of the vesicle is bleached using a laser for a short amount of time and the fluidity is computed from the time of fluorescence-recovery time. The same fluidity also is investigated by means of fluorescence polarization anisotropy (FPA) technique, where the intensity of the sample's fluorescence emission is measured along two orthogonal polarization axes. The latter method can be implemented under microgravity conditions. We report a significant fluidity changes in microgravity conditions, where the vesicles display approximately 20% higher membrane fluidity compared to those measured on the ground. Our findings provide valuable insights on the cells' behavior in zero-gravity conditions and more specifically about the absorption of pharmaceuticals in the human body.

BP 5.6 Mon 12:45 H46

Translocation of vesicles through membrane-covered pores — •Nishant Baruah[1], Gerhard Gompper[1], Anil Kumar Dasanna[2], and Thorsten Auth[1] — [1]Theoretical Physics of Living Matter, Institute of Biological Information Processing and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Physical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Sector 81, Knowledge City, Mohali 140306, India

Apicomplexan parasites like Plasmodium, which transmits malaria, invade their host cells by translocating through a tight junction at the host plasma membrane. This process involves significant physical challenges, including the need for the parasite to deform its own membrane while squeezing through the tight junction and contending with the host membrane tension [1]. Here, we study as a model system the translocation of vesicles through membrane-covered pores driven by a contact interaction [2]. The calculations are performed using triangulated membranes and energy minimization. We predict stable translocation states for various vesicle- and host-membrane elastic properties and vesicle-to-pore size ratios. A finite-host membrane tension strongly suppresses pore translocation, which may explain protection against severe malaria in the Dantu blood group [3].

[1] S. Dasgupta et al, Biophys. J. 107, 43 (2014).
[2] N. Baruah et al. (https://doi.org/10.1101/2024.05.20.594296).
[3] S. N. Kariuki et al, Nature 585, 579 (2020).

BP 6: Active Matter II (joint session BP/CPP/DY)

Time: Monday 15:00–17:00 Location: H37

BP 6.1 Mon 15:00 H37

Emerging cellular dynamics from turbulent flows steered by active filaments — Mehrana Nejad[1,4], Julia Yeomans[2], and •Sumesh Thampi[2,3] — [1]Department of Physics, Harvard University, Cambridge, MA 02138 — [2]The Rudolf Peierls Centre for Theoretical Physics, Parks Road, Oxford OX1 3PU, UK — [3]Department of Chemical Engineering, Indian Institute of Technology, Madras, Chennai, India 600036 — [4]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Describing the mechanics of cell collectives and tissues within the framework of active matter, without resorting to the details of biology is an exciting area. We develop a continuum theory to describe the dynamics of cellular collectives, discerning the cellular force-generating active filaments from cells shape. The theory shows that active flows and straining part of the active turbulence can elongate isotropic cells, which form nematic domains. This is important as cell morphology is not only an indicator of diseases but it can affect the nucleus morphology, gene expression and other biochemical processes inside the cells. Our theory highlights the importance of distinguishing the roles of active filaments from cell shape and explains outstanding experimental observations such as the origin of cell-filament alignment patches. Further, we reconcile how the contractile forces generated by the cytoskeletal network makes the cells to exhibit flow behaviours similar to that of extensile active systems. Revealing the crucial role of activity and rheology to describe the dynamics of cellular layers, our study is in consonance with a number of experimental observations.

BP 6.2 Mon 15:15 H37

Defects in active solids: self-propulsion without flow — •Fridtjof Brauns[1], Myles O'Leary[2], Arthur Hernandez[3], Mark Bowick[1], and Cristina Marchetti[4] — [1]Kavli Institute for Theoretical Physics, Santa Barbara, USA — [2]Princeton University, Princeton, USA — [3]Leiden University, Leiden, the Netherlands — [4]University of California Santa Barbara, Santa Barbara, California 93106, USA

Topological defects are a key feature of orientational order and act as organizing centers of orientation fields. Self-propulsion of +1/2 defects has been extensively studied in active nematic fluids, where the defects are advected with the fluid through the flow field they generate. Here, we propose a minimal model for defect self-propulsion in a nematic active solid: a linear elastic medium with an embedded nematic texture that generates active stress and in turn is coupled to elastic strain. We show that such coupling gives rise to self-propelled +1/2 defects that move relative to the elastic medium by local remodeling of the nematic texture. This mechanism is fundamentally different from the fluid case. We show that this mechanism can lead to unbinding of defect pairs and stabilize +1 defects. Our findings might help explain how orientational order, e.g. of muscle fibers, is reconfigured during morphogenesis in solid-like tissues. For instance, motility and merging of +1/2 defects play a crucial role in setting up the body axis during Hydra regeneration.

BP 6.3 Mon 15:30 H37

Isovolumetric dividing active matter — Samantha R. Lish[1], Lukas Hupe[1], Ramin Golestanian[1,2], and •Philip Bittihn[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We introduce and theoretically investigate a minimal particle-based model for a new class of active matter where particles exhibit directional, volume-conserving division in confinement while interacting sterically, mimicking cells in early embryogenesis. We find that complex motion, synchronized within division cycles, displays strong collective effects and becomes self-similar in the long-time limit. Introducing the method of normalized retraced trajectories, we show that the transgenerational motion caused by cell division can be mapped to a time-inhomogenous random walk with an exponentially decreasing length scale. Analytical predictions for this stochastic process allow us to extract effective parameters, indicating unusual effects of crowding and absence of jamming. Robustness of our findings against desynchronized divisions, cell size dispersity, and variations in confinement hints at universal behavior. Our results establish an understanding of the complex dynamics exhibited by isovolumetric division over long timescales, paving the way for new bioengineering strategies and perspectives on living matter.

BP 6.4 Mon 15:45 H37

Tracking plankton-to-biofilm transition in phototrophic bacteria — •Anupam Sengupta — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — Institute for Advanced Studies, University of Luxembourg, Luxembourg

Phototrophic bacteria commonly inhabit natural aquatic and marine ecosystems, exhibiting both motile and sessile lifestyles [1]. Yet, how and when they switch between the two states has remained unknown. Using quantitative imaging, AFM and mathematical modeling, we track the conditions and phenotypic changes across multiple generations in Chromatium okenii, a motile phototrophic purple sulfur bacterium [2]. Enhanced cell-surface adhesion together with changes in the cell shape and cellular mass distribution facilitate the motile-to-sessile shift. Our results, supported by cell mechanics model, establish a synergistic link between motility, mass distribution and surface attachment in promoting biofilm lifestyle. [1] T. Sommer et al., Geophys. Res. Lett. 44, 2017. [2] F. Di Nezio,.., & A. Sengupta, Plos one 19, e0310265, 2024.

15 min. break

BP 6.5 Mon 16:15 H37

How localized active noises influence the conformations and dynamics of semiflexible filaments — •Shashank Ravichandir[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Universität Augsburg, 86159 Augsburg, Germany

The structure and dynamics of active polymers have been recently studied in some detail. In these works all the monomers are considered to be active. However, in most biological systems non-equilibrium fluctuations manifest as activity only at isolated locations within the polymer. There have been only few studies of such polymers, in which the active monomers occur periodically along the polymer contour. We consider arbitrary active-passive copolymers and isolate the effects of the number and locations of active monomers on the conformational and dynamical properties of polymers. We use Langevin dynamics simulations to calculate the end-to-end distance, radius of gyration, and mean-squared displacement of such semiflexible filaments and classify the various states of these polymers based on their conformational properties. We also present preliminary results of polymers in which the location of active monomer moves dynamically along the chain contour. This is an idealized model of biopolymers such as DNA, during DNA transcription, and microtubules, which are driven by kinetic motors that traverse along its length.

BP 6.6 Mon 16:30 H37

Sequence-specific folding of partially active polymers — •Shibananda Das — Department of Physics, Indian Institute of Science, Bengaluru, India

Biological polymers like actin filaments and microtubules exhibit important physical properties due to their out-of-equilibrium behavior induced by ATP or GTP. In contrast, synthetic polymers rely on energy from their surrounding environment, often using local chemical, electrical, or thermal gradients to remain far from equilibrium. Theoretically, active polymers serve as minimal models for these systems, enabling systematic study of the competition between thermodynamic and active forces while they undergo conformational changes.

Using a combined analytical and numerical approach, we investigate an active polymeric chain composed of multiple self-avoiding units, representing good solvent condition in the absence of active forces. For partially active polymers without orientational constraints, we find that distribution of the active units in distinct sequences along the backbone can induce a significant collapse into folded, globular structures. Detailed analysis shows that this activity-dependent collapse is driven by a reduction in swim pressure of the monomers, linking the distribution of active forces along the polymer contour to its folded conformations.

BP 6.7 Mon 16:45 H37

Effect of interactions on the chemotactic response of active-passive chains — •Hossein Vahid[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of Augsburg, Augsburg, Germany

Living organisms, from single cells to populations, exhibit complex behaviors driven by the need to navigate toward favorable environments. These behaviors are often shaped by interactions within clusters or mixed populations, where collective dynamics play a crucial role in the characteristic properties of multicellular systems.

Chemotactic bacteria, found in diverse environments such as the gastrointestinal tract, plant surfaces, and aquatic ecosystems, demonstrate the significance of chemotaxis at the population level. While extensive research has focused on the properties of active polymers in spatially homogeneous activity fields, their behaviors in inhomogeneous fields remain less explored.

This study investigates the behavior of self-propelled polymers in activity gradients, emphasizing the effects of inter- and intra-chain interactions, such as steric and excluded volume effects, on chemotactic responses. These interactions give rise to distinct phases or collective behaviors that influence the stability and persistence of chemotaxis. Additionally, polymer density emerges as a critical factor impacting diffusion and the overall efficiency of chemotaxis. This work aims to study the dynamics of the active polymer populations in non-uniform environments systematically.

BP 7: Single Molecule Biophysics

Time: Monday 15:00–17:00 Location: H44

Invited Talk BP 7.1 Mon 15:00 H44

Single-molecule dynamic structural biology with Graphene Energy Transfer — •Philip Tinnefeld[1], Alan Szalai[1], Giovanni Ferrari[1], Lars Richter[1], Ingrid Tessmer[2], Andres Vera-Gomez[1], and Izabela Kaminska[1] — [1]Chemistry Department and Center for NanoScience, Ludwig-Maximilians-Universität München — [2]Rudolf Virchow Center, University of Würzburg, Würzburg

Obtaining structural information from single molecules is commonly associated with Fluorescence Resonance Energy Transfer that typically yields one distance between a fluorescent donor and an acceptor. Energy transfer to graphene with graphene-on-glass coverslips can extend the dynamic range to more than 30 nm. Based on the discovery that DNA can be placed vertically on graphene, we developed GETvNA (graphene energy transfer with vertical nucleic acids) that enables Angstrom precise visualization of DNA conformations and protein-DNA complexes. We envision that the alignment of DNA will additionally make it amenable to combined energy transfer and superresolution interrogation for dynamic structural biology.

BP 7.2 Mon 15:30 H44

Doubling the resolution of fluorescence-lifetime single-molecule localization microscopy with image scanning microscopy — •Niels Radmacher[1], Oleksii Nevskyi[1], José Ignacio Gallea[1], Jan Christoph Thiele[2], Ingo Gregor[1], Silvio O. Rizzoli[3,4], and Jörg Enderlein[1,4] — [1]Third Institute of Physics, Georg August University, Göttingen, Germany — [2]Department of Chemistry, University of Oxford, Oxford, UK — [3]Department of Neuro- and Sensory Physiology, University Medical Center Göttingen, Göttingen, Germany — [4]Cluster of Excellence - Multiscale Bioimaging: from Molecular Machines to Networks of Excitable Cells (MBExC),Göttingen, Germany

In this study, we integrate a single-photon detector array into a confocal laser scanning microscope, enabling the combination of fluorescence-lifetime single-molecule localization microscopy with image scanning microscopy. This unique combination delivers a twofold improvement in lateral localization accuracy for single-molecule localization microscopy (SMLM) and maintains its simplicity. Moreover, the addition of lifetime information from our confocal laser scanning microscope eliminates chromatic aberration, particularly crucial for achieving few-nanometre resolution in SMLM. Our approach is named fluorescence-lifetime image scanning microscopy iSMLM. And is demonstrated through dSTORM and DNA PAINT experiments on fluorescently labelled cells, showcasing both resolution enhancement and fluorescence-lifetime multiplexing capabilities.

BP 7.3 Mon 15:45 H44

Two-color single-molecule coincidence detection for the analysis of biological processes and high-affinity bi-molecular binding — •Benno Schedler[1], Olessya Yuknovets[1], Alida Meyer[1], Lennart Lindner[1], and Jörg Fitter[1,2] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), Aachen, Germany — [2]FZ Jülich, ER-C-3, Jülich, Germany

Life on the molecular scale is based on a versatile interplay of biomolecules, a feature that is relevant for the formation of macromolecular complexes. Fluorescence based two-color coincidence detection is widely used to characterize molecular binding and was recently improved by a brightness-gated version which gives more accurate results [1]. We developed and established protocols which make use of coincidence detection to quantify binding fractions between interaction partners labeled with fluorescence dyes of different colors. Since the applied technique is intrinsically related to single molecule detection, the concentration of diffusing molecules for confocal detection is typically in the low pico-molar regime. This makes the approach a powerful tool for determining bi-molecular binding affinities, in terms of KD-values, in this regime. By measuring the affinity at different temperatures, we were able to determine thermodynamic parameters of the binding interaction. The results show that the ultra-tight binding is dominated by entropic contributions [2].

References:

[1] Höfig et al. Communication Biology 2019 2, 459

[2] Schedler et.al. Int. J. Mol.Sci 2023 24, 16379

15 min. break

BP 7.4 Mon 16:15 H44

Maximizing Flavor: Leveraging Nano-biophysical Methods in Food Perception and Formulation Research — •Melanie Koehler — Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Lise Meitner-Straße 34, 85354 Freising, Germany — TUM Junior Fellow at the Chair of Nutritional Systems Biology, Technical University of Munich, Lise-Meitner-Straße 34, 85354 Freising, Germany

The food industry faces the challenge of creating healthier products with less salt, sugar, fat, and calories while maintaining flavor and consumer satisfaction. Flavor perception, influenced by taste, smell, texture, and individual factors, requires a deeper understanding to drive innovation. This research highlights the use of nano-biophysical techniques, particularly bio atomic force microscopy (AFM), to explore taste and texture at the molecular level. AFM provides nanoscale insights into food components' interactions with sensory receptors (taste- and mechanoreceptors), and their role in flavor release. For instance, AFM revealed the binding of a bitter peptide (VAPFPEVF) to its receptor (TAS2R16) without triggering downstream signaling. It also sheds light on oral texture perception, which remains underexplored at the biomolecular level [1]. By combining AFM with biochemical assays, molecular simulations, and human sensory evaluations, this research bridges objective measurements and subjective flavor experiences. These findings offer new approaches to designing healthier, sensory-appealing foods, addressing critical health and nutrition challenges. [1] Koehler, M, et al. Nature Food (2024): 1-7.

BP 7.5 Mon 16:30 H44

Label-Free Photothermal Infrared Correlation Spectroscopy — •Arthur Markus Anton and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Correlation spectroscopy is an indispensable method in modern life science. It allows for retrieving analyte properties in solution like it's concentration or diffusion coefficient, and thus enables to calculate the hydrodynamic radius of proteins or the viscosity of membranes, for instance. Common techniques are based on fluorescence or scattering, such as fluorescence correlation spectroscopy or dynamic light scattering respectively, and therefore need fluorescent labeling of analytes or lack of molecular specificity.

In this contribution we present a novel spectroscopic correlation technique on the basis of pumping with IR light but probing by means of visible light. The absorption of IR light is highly specific and allows us for *label-free* addressing of specific vibrational modes within the analyte molecules via the particular pump wavelength. Upon absorption, energy is dissipated and transferred into heat which alters the refractive index of the medium surrounding the absorbing species. This *transient* refractive index change is then probed by means of visible light providing a similar probe focal volume as conventional correlation spectroscopy techniques. Consequently, on the basis of IR pumping and visible probing we calculate the analyte's concentration and diffusion coefficient.

BP 7.6 Mon 16:45 H44

Single-protein optical holography — •Jan Christoph Thiele[1,2], Emanuel Pfitzner[1,2], and Philipp Kukura[1,2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]Department of Chemistry, University of Oxford, UK

Light scattering by nanoscale objects is a fundamental physical property defined by their scattering cross-section and thus polarizability. Over the past decade, a number of studies have demonstrated single-molecule sensitivity by imaging the interference between scattering from the object of interest and a reference field. This approach has enabled mass measurement of single biomolecules in solution owing to the linear scaling of image contrast with molecular polarizability. Nevertheless, all implementations so far are based on a common-path interferometer and cannot separate and independently tune the reference and scattered light fields, thereby prohibiting access to the rich toolbox available to holographic imaging. Here we demonstrate comparable sensitivity using a non-common-path geometry based on a dark-field scattering microscope, similar to a Mach-Zehnder interferometer. We separate the scattering and reference light into four parallel, inherently phase-stable detection channels, delivering a five orders of magnitude boost in sensitivity in terms of scattering cross-section over state-of-the-art holographic methods. We demonstrate the detection, resolution and mass measurement of single proteins with mass below 100 kDa. Separate amplitude and phase measurements also yield direct information on sample identity and experimental determination of the polarizability of single biomolecules.

BP 8: Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session BP/CPP)

Time: Monday 15:00–16:45 Location: H46

BP 8.1 Mon 15:00 H46

Ferroelectric Microelectrodes for Hybrid Neuroelectronic Systems — •Maximilian T. Becker[1,2], Roland Thewes[3], and Günther Zeck[4] — [1]Department of Embedded Systems, Hahn-Schickard, Freiburg, Germany — [2]Faculty of Engineering, University of Freiburg, Freiburg, Germany — [3]Chair of Sensor and Actuator Systems, TU Berlin, Berlin, Germany — [4]Institute of Biomedical Electronics, TU Wien, Vienna, Austria

Direct electrical interfacing of semiconductor chips with individual neurons and neural networks forms the basis for a systematic assembly and investigation of hybrid neuroelectronic systems with future applications in information technology and biomedicine. The neuroelectronic interface is realized via microelectrodes to bidirectionally transmit electrical signals between neurons and the semiconductor chip. Here, we introduce the concept of ferroelectric microelectrodes and discuss the physics of ferroelectric interfaces in neuroelectronic applications. As an example, we present neural recordings from retinal ganglion cells (RGCs) interfaced with a ferroelectric complementary metal-oxide-semiconductor microelectrode array (CMOS-MEA) and discuss the results in detail.

BP 8.2 Mon 15:15 H46

Highly sensitive, specific and label-free detection of SARS-CoV-2, Influenza A and RSV proteins via surface plasmon resonance technique using the biofunctionalization with 1 nm thick carbon nanomembranes — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Rania Ennaciri[1], Martha Frey[1], Christof Neumann[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany

Accurate and rapid detection of respiratory viruses like SARS-CoV-2, Influenza A and RSV is crucial for improving global health outcomes. We present a novel surface plasmon resonance (SPR) platform using a biofunctionalized 1 nm-thick carbon nanomembrane (CNM) for enhanced viral protein detection. The azide-modified CNM (N3-CNM) enables covalent antibody binding, ensuring selective immobilization of target proteins. Our platform achieves equilibrium dissociation constants (KD) of 570 * 30 pM and 22 * 3 pM for SARS-CoV-2 nucleocapsid and spike proteins, with detection limits (LODs) of ~190 pM and ~10 pM, respectively. For Influenza A and RSV, KD values are 86 * 4 pM and 3 * 0.2 pM, with LODs of ~90 pM and ~2 pM. Multiplexed detection with no cross-reactivity supports rapid, accurate point-of-care diagnostics. Validation with nasopharyngeal swabs confirms a LOD of ~40 pM for SARS-CoV-2 spike protein, highlighting CNMs' promise in infectious disease diagnostics.

BP 8.3 Mon 15:30 H46

Superselective multivalent client recruitment in biomolecular condensates — •Xiuyang Xia and Erwin Frey — Ludwig-Maximilians-Universität München

Biomolecular condensates (BMCs) are membraneless organelles formed via liquid-liquid phase separation, playing a crucial role in organizing cellular functions by selectively concentrating specific molecules. In this talk, I will present a new theoretical framework that models multivalent client recruitment in valence-limited, multicomponent systems like BMCs. We uncover how enthalpic and entropic factors interplay under valence constraints to enable switch-like recruitment and precise compositional regulation.

This work advances our understanding of the principles governing BMC composition and highlights the broader significance of multivalency in biological systems, offering insights into cellular organization and potential therapeutic applications.

BP 8.4 Mon 15:45 H46

What is the structure of a biomolecular condensate? — •Charlotta Lorenz[1,2], Teagan Bate[1], Takumi Matsuzawa[1], Kaarthik Varma[1], Sully Bailey-Darland[1], George Wang[1], Dana Matthias[1], Harsha Koganti[2], Nicola Galvanetto[2], Matti Valdimarsson[2], Aleksander Rebane[3], Etienne Jambon-Puillet[4], Ben Schuler[2], and Eric R. Dufresne[1] — [1]Cornell University, Ithaca, NY, USA — [2]University of Zurich, Zurich, Switzerland — [3]New York University Abu Dhabi, Abu Dhabi, United Arab Emirates — [4]École Polytechnique Paris, Paris, France

Biomolecular condensates are important for a variety of cellular functions, such as biochemical regulation, structural organization, and RNA metabolism. While the properties and physiology of these condensates depend on their structure, this important aspect has received little experimental consideration. On the other hand, recent simulations of disordered proteins with interactions based on the sticker-and-spacer suggest fascinating structures in the bulk and surface of condensates. We aim to reveal the structure of biomolecular condensates using X-ray scattering. Here, we will present results for a simple model system and apply our approach to the structure of condensates made of disordered proteins. We particularly consider the change in condensate structure due to small molecules.

BP 8.5 Mon 16:00 H46

Encoding how shear stress during gelation boosts the stiffness of collagen networks — •Pavlik Lettinga[1,2], Lens Dedroog[2], Olivier Deschaume[2], Yovan de Coene[2], Carmen Bartic[2], Erin Koos[2], and Mehdi Bouzid[3] — [1]Forschungszentrum Jülich — [2]KU Leuven — [3]Université Grenoble Alpes

Collagen is one of the main building blocks of the mammalian extracellular matrix, due to its ability to form tough structures with a wide variety of non-linear mechanical properties allowing it to support multiple tissue types. However, the mechanical properties of collagen gels have been extensively studied under static conditions, whereas in nature gelation will mostly take place in the presence of flow. Here we show how the elastic modulus of collagen hydrogels can be increased up to an order of magnitude by applying a stress ramp at a well-defined moment during gelation. Where the first stress block induces most of the final strain and alignment, sequential increases in stress cause a dramatic increase of the modulus. This high modulus is preserved by keeping the high stress until the gel is fully matured. Coarse-grained simulations of a model gel system show that that the microscopic mechanism of inducing high stiffness is due to formation of extra cross bridges and could be very generic. Thus, we not only show that the true non-linear capabilities of biomaterials are tenfold higher than previously assessed, but also provide insight into in vivo structure formation of collagen and potentially other (bio-)polymers.

Invited Talk BP 8.6 Mon 16:15 H46

In situ control of cells and multicellular structures at the microscale by two-photon lithography — •Christine Selhuber-Unkel — Heidelberg University, IMSEAM, Heidelberg, Germany

In vivo, cells and multicellular assemblies often experience strong confinement by their surrounding tissue environment, particularly in cancer. Thus, replicating these confined environments in situ is essential for investigating their impact on cellular systems. Using two-photon lithography, we printed structures directly within and around multicellular assemblies. For example, we fabricated dome-shaped confinements with micrometer-scale openings to encapsulate cancer spheroids. This enabled us to study how confinement influences cancer cell migration and spheroid behavior. Our findings revealed that confinement slows cell migration and alters actin dynamics. In addition, in situ printed structures can also directly interfere with migrating cellular assemblies. Additionally, elastic structures can be created to mechanically stimulate cells, offering further control over cellular behavior. Therefore, two-photon lithography proves to be a powerful tool for manipulating the growth, migration, and morphology of live cells, making it particularly useful for exploring how changing physical microenvironment in situ affect cell responses.

BP 9: Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Monday 17:00–18:00 Location: H46

BP 9.1 Mon 17:00 H46

Polymer Assisted Condensation and Heterochromatin — •Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden (IPF), Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Many biomolecular condensates are formed through the co-condensation of proteins and polynucleotides. In most cases, the proteins that constitute the majority of the condensate exhibit a miscibility gap in aqueous solution at elevated concentrations in vitro. Recently, we published the theory of Polymer-Assisted Condensation (PAC), which predicts the formation of the condensate within the

polymer's volume of gyration, where interactions with the three-dimensional conformation of the polymer trigger the phase transition of the protein component [1]. A key feature of these liquid condensates is their robustness against changes in parameters, as well as the dominant role played by the condensation free energy of the protein component. The formation and properties of heterochromatin, a genetically silenced region of eukaryotic chromosomes, can be explained by PAC, which resolves several issues present in previously published theories. Recently, we developed a field-theoretic approach to PAC to better understand the adsorption and desorption scenarios of heterochromatin at the nuclear lamina.

[1] J.-U. Sommer, H. Merlitz, and H. Schießel, Macromolecules 55, 4841 (2022); L. Haugk, H. Merlitz, and J.-U. Sommer, Macromolecules 57, 9476 (2024)

BP 9.2 Mon 17:15 H46

How specific binding induces sol-gel transitions and liquid-liquid phase separation in RNA/protein solutions: Coarse-grained simulations versus Semenov-Rubinstein Theory — •Xinxiang Chen, Jude Ann Vishnu, Pol Besenius, Julian König, and Friederike Schmid — Johannes Gutenberg-University, Mainz, Germany

Liquid-liquid phase separation plays a central role in cellular organization, including RNA splicing. RNA-protein interactions are crucial to these processes. A key factor in controlling the phase behavior of RNA-protein systems is the sequence of binding and neutral domains. Using molecular dynamics simulations, we investigate phase transitions in RNA-protein solutions that are driven solely by specific binding interactions. The model omits nonspecific interactions including electrostatic interactions. We show that specific binding interactions induce a percolation transition with double reentrant behavior without phase separation, if the neutral linker size is long. Comparing our results with the two-component Rubinstein-Semenov theory, we find that the theory qualitatively reproduces the phase diagram of the percolation transition and the impact of the neutral domains. Phase separation is observed when reducing the neutral linker size in an asymmetric system, resulting in a closed-loop phase diagram. We also study the effect of modulating the sequence and find that blockiness of sticker sites introduces microstructure in the dense liquid phase. These insights enhance our understanding of how specific binding and domain arrangement regulates condensate formation in RNA-protein systems.

BP 9.3 Mon 17:30 H46

Model particles to study interaction of microplastic particles — •Kai Gossen, Andreas Fery, and Günter Auernhammer — IPF Dresden, Dresden, Germany

Microplastic in the environment is typically coated by natural organic matter forming an ecocorona. We present an approach to model ecocorona on particles with well-defined polymers, synthetic and derived from natural polymers. Polystyrene particles were coated with fluorescent polyelectrolyte multilayer systems, PS(Chitosan/Hyaluronic acid) and PS(Poly(dimethyldiallylammonium chloride) /Polystyrene sulfonate) by the layer-by-layer method. Systems with 2, 4 and 6 bilayers were synthesized. The second layers were fluorescently labelled with SNARF conjugated dextran.

It was found that zeta potentials of the PS(Chi/HS)2/4/6 systems assume values (-20 mV to -35 mV) that are similar to those of PS-ecocorona particles (-40 mV to -5 mV). The pH-dependent fluorescence of particle suspensions and individual particles were measured at pH values between pH 3 and pH 8. A well measurable pH dependence between pH 4.5 and 8 for the PS(Chi/HS) systems and the PS(PDADMAC/PSS) system could be measured. The system could serve to selectively study effects of surface properties of ecocorona coated particles such as surface stiffness or zeta potential.

BP 9.4 Mon 17:45 H46

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — •Souraj Mandal[1], Anna Fritschen[2], Alina Filatova[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany — [2]BioMedical Printing Technology, Department of Mechanical Engineering, Technical University of Darmstadt, 64289 Darmstadt, Germany — [3]Stem Cell and Developmental Biology, Technical University of Darmstadt, 64287 Darmstadt, Germany

Three-dimensional cellular models hold great promise for drug testing, but their success relies on maintaining a controlled supply of oxygen and nutrients. Artificial vascular networks aim to mimic blood vessel functions, yet ensuring robust endothelial cell (EC) attachment remains a significant challenge. In this study, we designed a mediator between artificial network surfaces and ECs using Poly(N-isopropylacrylamide) (PNIPAM) microgels (MGs) that remain mechanically stable in nutrient solutions. Charged MGs were synthesized and tested for adhesion on plasma-treated model surfaces. The microgel-coated substrates were exposed to cell static culture media and under defined flow. Atomic force microscopy (AFM) confirmed stable adhesion of MG particles before and after exposure. Initial experiments explored EC attachment on positively and negatively charged MG surfaces, followed by mechanical property characterization. The MG coatings were biofunctionalized with integrin-recognized ligands to enhance EC adhesion and proliferation further.

BP 10: Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 9:30–12:30 Location: H43

Invited Talk BP 10.1 Tue 9:30 H43

Robust signal amplification and information integration via self-tuned proximity to bifurcation points — •Isabella Graf — Developmental Biology Unit & Theory Transversal Theme, EMBL Heidelberg, Germany

Many living systems demonstrate exquisite sensitivity to small input signals. A tempting hypothesis is that these systems operate close to bifurcation or critical points, where the system's response exhibits a diverging susceptibility to the control parameter and small signals are amplified into a large collective response. A common concern, however, is that proximity to such points requires fine-tuning of parameters, which seems impossible for noisy biological systems. Based on several distinct sensory systems, we have investigated a feedback motif that robustly maintains these systems close to their respective bifurcation point. The key ingredient is that the collective response feeds back onto the control parameter. To illustrate this idea, I will mention several examples ranging from snake thermosensing to mammalian hearing and discuss the functional benefits associated with being near-critical.

BP 10.2 Tue 10:00 H43

Exceptional Points and Stability in Nonlinear Models of Population Dynamics having PT symmetry — •Alexander Felski — Max Planck Institute for the Science of Light, Erlangen, Germany

Nonlinearity and non-Hermiticity, for example due to environmental gain-loss processes, are a common occurrence throughout numerous areas of science. For the latter, parity-time-reflection (PT) symmetry has played an eminent role in understanding exceptional-point structures and phase transitions in these systems. Yet their interplay has remained by-and-large unexplored. We analyze models governed by the replicator equation of evolutionary game theory and related Lotka-Volterra systems of population dynamics. These foundational nonlinear models offer a broad platform for non-Hermitian theory beyond physics. In this context we study the emergence of exceptional points in two cases: (a) when the governing symmetry properties are tied to global properties of the models, and, in contrast, (b) when these symmetries emerge locally around stationary states–in which case the connection between the linear non-Hermitian

model and an underlying nonlinear system becomes tenuous. We outline further that when the relevant symmetries are related to global properties, the location of exceptional points in the linearization around coexistence equilibria coincides with abrupt global changes in the stability of the nonlinear dynamics. Exceptional points may thus offer a new local characteristic for the understanding of these systems.

BP 10.3 Tue 10:15 H43

Pattern selection and the route to turbulence in polar active fluids — Henning Reinken[1], Sebastian Heidenreich[2], •Markus Bär[2,3], and Sabine Klapp[3] — [1]OVGU Magdeburg, Germany — [2]Physikalisch-Technische Bundesanstalt, Germany — [3]TU Berlin, Germany

Active fluids, such as suspensions of microswimmers, are well known to self-organize into complex spatio-temporal flow patterns. An intriguing example is mesoscale turbulence, a state of dynamic vortex structures exhibiting a characteristic length scale. Here, we employ a minimal model for the effective microswimmer velocity field to explore how the turbulent state develops from regular, stationary vortex patterns when activity is increased. First, we demonstrate analytically that the system develops a stationary square vortex lattice in the absence of nonlinear advection. Subsequently, we perform an extended stability analysis and uncover a linear instability, above which the square vortex lattice becomes unstable. In numerical simulations, we confirm that this instability is predictive for the unset of turbulence. In addition, an extended region of hysteresis where turbulence and a stable vortex lattice coexist, is found Reference: H. Reinken, S. Heidenreich, M. Bär, S. Klapp, New J. Phys. 26 063026 (2024).

BP 10.4 Tue 10:30 H43

Likelihood-based inference for heterogeneous motile particle ensembles — •Jan Albrecht[1], Cristina M. Torres[1], Carsten Beta[1], Manfred Opper[2,3,4], and Robert Grossmann[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Faculty of Electrical Engineering and Computer Science, Technische Universität Berlin, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom — [4]Institute of Mathematics, University of Potsdam, 14476 Potsdam, Germany

The inherent complexity of biological agents often leads to motility behavior that appears to have random components. Robust stochastic inference methods are therefore required to understand and predict the motion patterns from time discrete trajectory data provided by experiments. In many cases second-order Langevin models are needed to adequately capture the motility. Additionally, population heterogeneity needs to be taken into account when analyzing data from multiple individual organisms. We present a maximum likelihood approach to infer stochastic models and, simultaneously, estimate the heterogeneity in a population of motile active particles from discretely sampled trajectories. To this end we propose a new method to approximate the likelihood for nonlinear second order Langevin models. We demonstrate that our approach outperforms alternative methods for heterogeneity estimation, especially for short trajectories, while also providing a measure of uncertainty for the estimates. We use the approach to investigate population heterogeneity in systems of ameboid cells.

BP 10.5 Tue 10:45 H43

Surviving the first "winter": Protocells with polymerization reactions protects against environmental fluctuations — •Xi Chen, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, Dresden, Germany

The origin of life has been a long standing question with various hypotheses describing the emergence of the first protocells. Phase separated condensates are promising candidates for protocells because they are compartments that enrich specific polymers and host nonequilibrium reactions that leads to growth and division. However, the ability of protocells to survive in an environment that has large fluctuations, such as temperature and composition, is poorly understood. We show with a mean-field model that condensates formed by polymers which undergo nonequilibrium polymerization/depolymerization reactions exhibit significant robustness to large environmental fluctuations.

This robustness occurs when the nonequilibrium polymerization reactions are faster inside condensate phases than outside. The first condensate does not form until environmental factors lead to strong enough reactions that polymers long enough to phase separate form. The effects of nonequilibrium polymerization is then fully realized because a condensate exists. From here, the condensate does not dissolve until the nonequilibrium reactions are diminished to significantly below when the condensate formed. Altogether, this forms a hysteretic loop with respect to the environmental factors that drive nonequilibrium reactions. We show this hysteretic loop prevents protocells from dying from environmental fluctuations.

BP 10.6 Tue 11:00 H43

How inter-particle interaction affects two species transport in nano-channels — •Wolfgang Bauer — Dept. of Internal Medicine I, UKW, Würzburg, Germany

Channel transport mechanisms of multiple species is essential for cell physiology and nanotechnology. Here, we present a model maintaining spatial correlations of two species, moving away from mean field approaches. The spatial occupations of the channel give the state space, where local flux and entropy production determine channel transport and its thermodynamic efficiency. Optimal transport coupling between species occurs in an attractive empty channel and strong repulsive forces between particles of the same species. This confines state space to a circular topology with concentration gradients of the two species acting as thermodynamic driving forces in series. For opposing gradients, the species with the stronger gradient produces positive entropy, while the other negative entropy. Attenuating the repulsive force within one species and maintaining that of the other adds a bypass path on the circular topology in state space. This enables a leak flow of the less repulsive species parallel to its gradient, generating local positive entropy on the bypass. For a certain range of opposing gradients, both species can produce positive overall entropy simultaneously. However, the rectifying potential of the concentration gradient of the species with bypass option is diminished, i.e. it cannot rectify flow of the other species above a threshold of the latter's opposing gradient. Vice versa the flow of the species with bypass option may always be rectified parallel to the concentration gradient of the other.

15 min. break

Invited Talk BP 10.7 Tue 11:30 H43

Beyond the connectionist view: (De-)synchronizing neural networks via cell-intrinsic dynamics — •Susanne Schreiber — Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany

Neural computation is thought to arise from the connectivity among neurons. Accordingly, we are often more than happy to ignore seemingly unimportant and potentially overwhelming biological detail, for example, related to the properties of the neurons themselves. In this talk, however, I will highlight how cell-intrinsic dynamics, namely the biophysics of action-potential generation, can have a decisive impact on network behaviour. Recent work of my lab shows that, among regularly firing neurons, the somewhat unattended homoclinic type (characterized by a spike onset via a saddle homoclinic orbit bifurcation) particularly stands out: First, spikes of this type foster specific network states - synchronisation in inhibitory and splayed-out/frustrated states in excitatory networks. Second, homoclinic spikes can be easily induced in by changes in a variety of physiological parameters (like temperature, extracellular potassium, or dendritic morphology). As a consequence, small changes in these parameters can suffice to induce drastic switches in network states. I will discuss functional consequences of homoclinic spikes for the design of pattern-generating motor circuits in Drosophila as well as for mammalian pathologies like febrile seizures. Our work predicts an interesting role for homoclinic action potentials as an integral part of brain dynamics in both health and disease.

BP 10.8 Tue 12:00 H43

Transient spatiotemporal chaos in cardiac excitable media — •Melvin Dix[1,2], Thomas Lilienkamp[1,3], Stefan Luther[1,4,5], and Ulrich Parlitz[1,2,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Faculty for Applied Mathematics, Physics, and General Science, Computational Physics for Life Science, Nuremberg Institute of Technology Georg Simon Ohm, Nürnberg, Germany — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany

Life-threatening cardiac arrythmia such as ventricular fibrillation have been linked to spatiotemporal chaotic dynamics governed by scroll or spiral waves. It has been observed in vivo and in vitro that these dynamics can be transient, e.g. abruptly stop. Using simulations with different numerical models we investigate the effects of factors such as heterogeneities, motivated by the complexity of the heart. We show that these perturbations can (significantly) prolong the duration of chaotic transients and may also lead to persistent chaos or stable periodic wave patterns [1].

[1] Melvin Dix et al. Physical Review E 110(4), 044207 (2024).

BP 10.9 Tue 12:15 H43

Nonlinear dynamics of heart and brain — •Irene Pellini[1,2], Simon Bauer[1], Johannes Zierenberg[1,3], Philip Bittihn[1,3], and Viola Priesemann[1,3] — [1]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany — [2]Max Planck School Matter to Life, Heidelberg, Germany — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The core function of the heart and brain arises from the coordinated interaction of their cells. Both organs rely on excitable units – cardiomyocytes and neurons – that propagate electrical signals when a specific threshold is exceeded. Despite

this similarity, the two organs exhibit opposed collective behavior due to marked differences in intercellular dynamics and network topology. In the heart, localized electrical connectivity through reciprocal gap junctions generates local synchronization and traveling waves, ensuring efficient pumping function with low entropy. In the brain, long-range connectivity via delayed, non-reciprocal chemical synapses promotes asynchronous dynamics with high entropy, supporting information processing.

Using coupled FitzHugh-Nagumo oscillators, we showcase that characteristic non-linear dynamics for the heart and brain can be related to the network structure, which places both systems on opposite sides of a synchronization phase transition. Crossing this phase transition would lead to pathological conditions, e.g., heart arrhythmia or brain seizures, quantifiable via entropy measures. Our joint view on heart and brain dynamics may foster new perspectives on the function and pathology of both organs.

BP 11: Cytoskeleton

Time: Tuesday 9:30–11:30 Location: H44

Invited Talk BP 11.1 Tue 9:30 H44

Network connectivity determines the mechanisms responsible for cytoskeletal elasticity — •Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France — PMMH, CNRS, ESPCI Paris, PSL University, Sorbonne Université, Université Paris-Cité, F-75005, Paris, France

Much of the cell's mechanics is dictated by the properties of its cytoskeleton, a dynamic collection of semiflexible filaments. Here we review both old and new results on the emergence of its large-scale elasticity from the filaments' individual mechanical properties. We emphasize the role of the network's connectivity in determining the underlying physical mechanism. At high connectivity or under high stress, the tensile strength of the filaments dominate. Moderately coordinated networks, on the other hand, are governed by the filaments' bending elasticity. Finally, we discuss the very low coordination of branched actin networks, and argue that it implies that interfilament contacts play a major role in its response. This makes the mechanics of these networks analogous to that of a ball of unspun sheep's wool under compression.

BP 11.2 Tue 10:00 H44

Buckling action of molecular motors damages microtubules beyond self-repair — •Shweta Nandakumar[1], Jonas Bosche[1], Morgan Gazzola[2], Mirko Wieczorek[1], Mona Grünewald[1], Manuel Thery[2], Reza Shaebani M[1], Ludger Santen[1], Stefan Diez[3], and Laura Schaedel[1] — [1]Center for Biophysics, Saarland University, Germany — [2]IPGG, Paris, France — [3]B-CUBE,TUD Dresden. Germany

Microtubules (MTs) are rigid, hollow biopolymers that constitute a key component of the cytoskeleton, essential for cellular processes such as mitosis, intracellular transport, and migration. Despite their large bending rigidity, MTs often adopt highly curved conformations, indicating that they are exposed to significant mechanical forces in cells. These forces typically arise from molecular motor proteins like kinesin.

In this study, we investigated microtubule damage and subsequent self-repair as a result of both bending as well as dynamic buckling using kinesin motor proteins in vitro. We reveal that motor-induced buckling imposes massive damage on MTs, occasionally leading to the renewal of majority of the MT lattice visualised by the incorporation of new tubulin subunits into the damaged regions. We find that at high motor densities, MT damage exceeds self-repair and leads to frequent MT breakage.

Our results highlight the impact of mechanical forces, which significantly speed up MT damage and self-repair, on MT integrity. Our findings provide a framework for understanding how cells maintain MT function under repeated mechanical stress.

BP 11.3 Tue 10:15 H44

Active self-organization of focal adhesions driving cell shape changes — •waleed ahmad mirza, matt govendir, alejandro torres-sánchez, and maria bernabeu — European Molecular Biology Laboratory, Barcelona

Focal adhesions (FAs) are dynamic protein complexes that mediate the interplay between the actin cytoskeleton and the extracellular matrix (ECM), enabling cells to sense and respond to mechanical and biochemical cues. These complexes drive essential processes such as cytoskeletal reorganization, cell shape modulation, and migration. To investigate these processes, we developed an active gel mathematical model that couples the dynamics of FAs, actin cytoskeleton, and cellular shape changes, capturing the three-way interplay between these components. Numerical solutions of the model successfully recapitulated experimental observations, demonstrating its ability to predict how cells adapt to mechanical and topographical cues. Specifically, the model reproduced key phenomena such as the influence of substrate stiffness on FA dynamics, with stiffer substrates promoting larger, more stable FAs, aligned stress fibers, and enhanced cell motility. It also captured how anisotropic ECM features, such as aligned collagen fibers or patterned topography, direct cytoskeletal organization and cell alignment. Additionally, the model demonstrated how curvature and shear flow provide critical mechanical cues that shape cellular morphology and behavior. This work provides a novel framework for understanding the mechanistic feedback loops underlying cell-ECM interactions and highlights the central role of FAs in regulating cellular behavior.

BP 11.4 Tue 10:30 H44

Interactions between single actin and vimentin filaments — •Pallavi Kumari and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton plays a crucial role in maintaining cellular structure, mechanics, and function. Recent advances suggest that the diverse tasks of the eukaryotic cytoskeleton depend on the interactions between its filamentous components - microtubules, actin filaments, and intermediate filaments. Despite a growing number of studies to better understand these interactions, it remains unclear whether actin and intermediate filaments interact directly without an auxiliary protein. Previous in vitro studies on reconstituted mixed filament networks have reported contradictory results. To clearly resolve this contradiction, it is essential to further simplify the system down to the single filament level. Here, we present a study on the direct interactions between actin filaments and vimentin intermediate filaments at the single filament level, examining the effects of different ions at varying concentrations on the interaction force. We employ quadruple optical tweezers combined with confocal microscopy and microfluidics to precisely control the conditions for the interaction of the two reconstituted protein filaments, visualize the interactions, and measure the forces involved. Our research provides direct indications of interactions between actin and vimentin filaments. Our findings will provide important insight that will help to unravel the interplay of cytoskeletal filaments at the network level.

BP 11.5 Tue 10:45 H44

Active Gel Theory for Cell Migration With Two Myosin Species — •Nils Winkler, Oliver M Drozdowski, Falko Ziebert, and Ulrich S Schwarz — Institut für theoretische Physik und Bioquant, 69120 Heidelberg

Motility of animal cells is essential for a wide range of biological phenomena, from the development of embryos to the spread of cancer. It is mainly driven by flow of the actin cytoskeleton, which in turn is generated by both actin polymerization and actomyosin contractility. Non-muscle myosin II is present in three different isoforms, but it is unclear what their respective roles are. Starting from phenomenological binding kinetics that include the competition of the myosin motors for binding sites through excluded volume interactions, we derive an active gel model for cell migration that includes a fast and a slow variant, corresponding to the non-muscle myosin II isoforms A and B, respectively. We find non-linear diffusion laws and predict species gradients that agree with experimental observations. Through numerical continuation and simulations, we identify a pull-and-push mechanism that can produce different system states, including steady migration as well as cell oscillations in length and velocity.

BP 11.6 Tue 11:00 H44

Keratin networks in epithelial cells under strain — •Ruben Haag, Ruth Meyer, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton is mainly made up of microtubules, actin and intermediate filaments (IFs). The composition of the IF-network is cell-type specific and influences the viscoelastic properties of cells. In epithelial cells, the keratin IF network connects to desmomes in the cell membrane, while in the cell center keratin IFs can bind to the nuclear lamina via plectin proteins. The keratin IF network thus forms a mechanical link from the nucleus to the cell membrane. In in-vitro experiments, it was previously observed that IFs, unlike actin filaments, resist being stretched to high strains. We now ask whether this force-extension behavior of IFs is also relevant in whole cells and, more specifically, if mechanical signals from outside the cell are transmitted to the nucleus via the keratin IF network. To answer this question, we stretch cells both uniaxially to linear strains of 80 % and equibiaxially to area strains of 87 %. During stretching, we image the nuclei, deconvolve the images to recover their 3D shape, segment the nuclei and track each nucleus during stretching. This procedure allows us to investigate their deformation at increasing strain. We compare wild type epithelial cells to keratin knockout cells to study the influence of the keratin IF network on the nuclei. We find that the deformation orthogonal to the stretching direction of the nuclei matches the deformation of the cell better in the keratin wild type cells. Our results suggest, that the keratin network helps to adapt the nucleus to mechanical perturbation.

BP 11.7 Tue 11:15 H44

Investigating the interaction between two single heart cells through TNTs using ROCS and Fluorescence microscopy — •Arash Felekary and Alexander Rohrbach — Lab for Bio and Nano Photonics, IMTEK, Freiburg, Germany

Cell-cell communication is vital for biological processes, particularly in the heart. Tunneling nanotubes (TNTs), dynamic and thin protrusions, facilitate cellular interactions by transferring organelles, including mitochondria. To investigate TNT composition and their roles in cardiac fibroblast (FB) communication, we employed Rotating Coherent Scattering (ROCS) microscopy, a label-free super-resolution technique, in addition to Fluorescence microscopy. ROCS enables up to 100 Hz recordings of lamellipodia dynamics along TNTs, and 3D imaging across different z-planes up to 6μm in depth, which is critical for visualizing TNTs. We observed a linear correlation between TNT density and lamellipodia motion velocity. Lamellipodia, driven by actin polymerization and branching via Arp2/3 activation, play a key role in FB migration and interaction. Collagen staining demonstrated that TNTs and lamellipodia interact with collagen fibers, a major component of the extracellular matrix (ECM). This interaction not only influences ECM remodeling, but also activates actin branching signals that enhance FB migration and protrusion dynamics. In this presentation, we investigate the coordinated roles of TNTs, lamellipodia, and collagen in regulating FB interaction and migration, offering new insights into heart tissue repair.

BP 12: Biomaterials, Biopolymers and Bioinspired Functional Materials III (joint session CPP/BP)

Time: Tuesday 9:30–11:15 Location: H46

Invited Talk BP 12.1 Tue 9:30 H46

Hybrid materials from colloidally stable nanocellulose and nanoparticles - scattering techniques are needed for characterization — •Eva Malmström[1], Åsa Jerlhagen[1], Benedikt Sochor[2], Korneliya Gordeyeva[1], and Stephan Roth[1,2] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Cellulose nanofibrils (CNFs) have rendered increasing interest during the last decades as their high stiffness, strength, and aspect ratio are attractive features to further explore on the pathway to a more sustainable society.

Controlled radical polymerization procedures allow for the synthesis of well-defined, nearly monodisperse, block-copolymers. The development of the polymerization-induced phase self-assembled (PISA) technique enables the production of well-defined nanoparticles (nanolatexes), with controlled size (typically with a diameter smaller than 200 nm), charge density, chemical functionality, and glass transition temperature.

The combination of CNFs and well defined nanolatexes allows for the design of novel materials with unique properties. Scattering techniques have proven very useful to characterize the corresponding materials, for instance, a method to assess cross-section orientation.

BP 12.2 Tue 10:00 H46

In situ GISAXS investigation of different protein-templated titania nanostructures — •Linus Fidelis Huber and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Nanostructured titania thin films have been studied for a large variety of applications. An environmentally benign and scalable synthesis route for this material class could be of interest to many state-of-the-art devices, from solar cells to battery materials. Protein-assisted sol-gel synthesis is a low-temperature, low-cost, and highly scalable technique, that can be used to achieve a nanostructured titania thin film. It has been shown that the bovine whey protein β-Lg forms differently shaped aggregates at different solution pH values. With simple changes to the solution chemistry, different domain sizes, porosities, and morphologies are possible. Therefore, it is a promising candidate to create tunable and mesoporous titania structures. In this work, we investigate the film formation with in situ small-angle/wide-angle grazing incidence X-ray scattering (GISAXS/GIWAXS) techniques. It is found that films printed at acidic pH form significantly different final bulk morphologies than films printed at neutral pH. The crystallite phase is strongly reduced in average domain size and domain-domain distance. Agglomerate size is increased for the acidic template. The in situ data is complemented by SEM, PL, UV-Vis and static GISAXS/GIWAXS measurements.

BP 12.3 Tue 10:15 H46

With digital luminescence towards minimalistic, biodegradable information storage — •Sebastian Schellhammer, Heidi Thomas, Tim Achenbach, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Materials showing persistent luminescence, characterized by extended excited state decay times in the millisecond range and beyond, have gained much attention. Recently, we have reported a photonic device architecture based on organic functional materials called programmable luminescent tag (PLT) that is well suited for sensing, labelling, and information exchange applications. Information can be erased and rewritten repeatedly by using the design principle of digital luminescence, i.e. the control of the local oxygen concentration in a polymer:emitter blend and accordingly the emission by room temperature phosphorescence (RTP). We present the design of PLTs made from industrially compostable, ready-to-use materials (bioPLTs). As natural emitters, quinoline alkaloids show sufficient RTP when being embedded in a polymer matrix. Polylactic acid is used as matrix material and flexible substrate. RTP can be controlled adding oxygen blocking layers made from Exceval. Although organic semiconductors provide the potential of biodegradable technologies, prototypes do only rarely exist. With this work, a promising technology for compostable information storage and sensing systems is introduced.

BP 12.4 Tue 10:30 H46

Enhancing drug release at interfaces with photoresponsive surfactant-polyelectrolyte mixtures — •Ipsita Pani, Michael Hardt, and Björn Braunschweig — Institute of Physical Chemistry, Center for Soft Nanoscience (SoN), University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Using micellar nanocarriers of a photoresponsive arylazopyrazole (AAP) surfactant, we have recently demonstrated the drug release at air-water interface.[1] In this work, we use a biopolymer poly-L-lysine (PLL) to form surfactant-polyelectrolyte mixtures to enhance the drug release of a chemotherapeutic drug doxorubicin. We observe a strong binding between the negatively charged AAP and the positively charged PLL at equimolar ratio. The information from UV-visible spectroscopy, light scattering studies, surface tensiometry and SFG spectroscopy has been utilized to identify the concentration of PLL at which the light-induced drug release is enhanced at the interface. We found that at higher PLL:AAP ratio, the complexes have low net charge and colloidal stability and the release of Dox from the bulk solution to the air-water interface is not observed. However, at lower PLL:AAP ratio, when the system is colloidally stable with a net negative charge, the drug release to the air-water interface is significantly enhanced. Further, the kinetics of drug release to the interface is faster in presence of PLL-AAP mixtures in comparison to pure AAP micelles. Reference : [1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

BP 12.5 Tue 10:45 H46

Proteins as foam stabilizers: From single foam lamellas to macroscopic foams — •Kevin Gräff, Sebastian Stock, Luca Mirau, Matthias Kühnhammer, Olaf Soltwedel, and Regine von Klitzing — Terchnische Universität Darmstadt, Darmstadt, Germany

Foams consist of foam lamellas, which separate single air bubbles from each other. Investigation of lamellas is crucial to understand foam properties. In order to untangle electrostatic, steric and network stabilization effects, we compare two globular proteins (β-lactoglobulin and Lupine Protein Isolate) and a disordered, flexible protein (whole casein) at different pH values. The Thin Film Pressure Balance (TFPB) device based on image intensity measurements generates spatially resolved disjoining pressure isotherms. We introduce feature tracking for the measurement of interfacial mobility and stiffness of lamellas as a novel method. Around the isoelectric point, Newton Black Films (NBFs) form, which are stable for the globular proteins while they are unstable for the disordered flexible one. This difference in film stability is explained by different characteristics of network structures in the lamellas from the respective protein solutions. Small-Angle Neutron Scattering (SANS) evaluation with a new model for foams proves the presence of NBFs within macroscopic foams. For a complete picture we compare the TFPB findings with X-ray reflectometry as well as with Brewster Angle Microscopy on single interfaces.

[1] Gräff, K. et al, (2022), Untangling effects of proteins as stabilizers for foam films, Front. Soft. Matter 2:1035377.

BP 12.6 Tue 11:00 H46

What makes a polysaccharide biomaterial a good candidate for tissue engineering applications? — •Emma Bobu Cimpoi[1], Codrut Costinas[1], Emilia Licarete[2], Tamás Gyulavári[3], Klara Magyari[4], and Monica Baia[4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Centre for Systems Biology, Biodiversity and Bioresources "3B", Cluj-Napoca, Romania — [3]Department of Applied and Environmental Chemistry, University of Szeged, Hungary — [4]INSPIRE Research Platform, Babes Bolyai University, Cluj-Napoca, Romania — [5]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Biomaterials are inovative systems used to solve medical issues. Daily, injuries produce major bleeding that affects people and, without proper care, leads to

other health problems. Traditional care methods are limited and outdated, so the focus is on natural materials with hemostatic properties, that are biocompatible and non-toxic. The aim of this work was to develop biomaterials based on pullulan, alginate and gelatin in various combinations, which could stop the bleeding and regenerate the wound. The developed sponge-like materials were characterized by FT-IR spectroscopy and X-ray diffraction. Then they were evaluated in vitro in terms of porosity, toxicity, swelling and charge on the surface, using SEM, cell viability assays, water up-take and mechanical tests. The investigations revealed good results as the synthesis was succesfull, the samples swell a lot, have good shape memory properties, are porous and non-toxic. These indicate their potential to stop bleeding, and therefore further in vivo tests will be carried out.

BP 13: Active Matter III (joint session DY/BP/CPP)

Time: Tuesday 9:30–13:00 Location: H47

BP 13.1 Tue 9:30 H47

From micro to macro: systematic coarse-graining of active particle models and implications on phase separation — •Sumeja Burekovic[1], Filippo De Luca[2], Cesare Nardini[1,3], Ananyo Maitra[4,5], and Michael E. Cates[2] — [1]CEA, Paris-Saclay, France — [2]DAMTP, University of Cambridge, UK — [3]LPTMC, Sorbonne Université, France — [4]LPTM, CY Cergy Paris Université, France — [5]LJP, Sorbonne Université, France

Significant insights into collective phenomena of active systems, such as phase separation, have been obtained through minimal field theories developed in a top-down manner. In contrast, the bottom-up approach seeks to link these continuum models to the microscopic dynamics of active particles, often formulated as Langevin equations for their position and orientation. This connection is typically achieved via explicit coarse-graining and allows active field theories to be expressed in terms of physically meaningful parameters. A major challenge in coarse-graining is the consistent elimination of irrelevant fast degrees of freedom to derive closed equations for the hydrodynamic variables or order parameters, such as the density field. We propose a systematic extension of standard homogenization/projection-operator techniques. As we show in minimal examples with few degrees of freedoms, our technique allows to go beyond the state of the art of homogenization in the mathematical literature. We then discuss the predictions of our coarse-graining methods for the large-scale phenomenology of non-aligning active particles, including cases in which microphase separation - rather than full phase separation - emerges due to activity.

BP 13.2 Tue 9:45 H47

Active Quadrupolar Dumbbells — •Margaret Rosenberg[1], Marco Musacchio[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf — [2]Università di Roma Sapienza, P.le Aldo Moro 2, 00185 Rome, Italy

The field of Active Matter has thrived in recent years, driven both by the insight that it underlies fundamental processes in nature, and by its vast potential for applications. Although the self-propulsion mechanisms of Active Matter allow us to consider and control a wide range of motions, there is - by default - no obvious control over the orientation and rotation of the particles. One approach to resolve this is the use of anisotropic particles and interactions. This contribution presents a computational study of a novel system composed of active, quadrupolar dumbbells, the phase behavior of which is determined by the competition between active motion and the orthogonal alignment favored by quadrupolar attraction. We explore the novel phase behavior unlocked by these anisotropic interactions, and discuss options for experimental realizations and applications.

BP 13.3 Tue 10:00 H47

Order by disorder in a swarm with obstacles — Pradeep Kumar[1], Sanjay Puri[1], and •Martin Weigel[2] — [1]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Simple models of swarming and active matter such as the Vicsek model [1] have been studied in detail, and the phase diagram as a function of noise strength and particle density is by now well understood. Real active systems are usually affected by impurities and random disorder, however. The presence of a quenched distribution of disc-like obstacles in the domain of the Vicsek model is observed to have a dramatic effect on the ordering behavior [2]: in contrast to the model without obstacles, where the strongest alignment is observed for the lowest noise, as soon as obstacles are added only the presence of a certain amount of noise leads to a global alignment of particles. This order by disorder phenomenon for active systems is traced back to the interplay of multiple length scales in the system: the typical inter-obstacle distance, the typical cluster size, and the resulting mean-free-paths of cluster-obstacle and cluster-cluster collisions. We present scaling arguments explaining these connections and provide an outlook towards similar phenomena in related systems.

[1] T. Vicsek, Phys. Rev. Lett. 75, 1226 (1995).
[2] O. Chepizhko, E. G. Altmann, and F. Peruani, Phys. Rev. Lett. 110, 238101 (2013).

BP 13.4 Tue 10:15 H47

Autonomous navigation in synthetic microswimmers: solving mazes with chemical echolocation — •Aritra K. Mukhopadhyay[1], Linhui Fu[2], Kai Feng[2], Ran Niu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems.

We propose and experimentally demonstrate a mechanism enabling synthetic microswimmers, such as autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, creating echoes that carry structural information about the environment. Remarkably, these echoes invoke automatic responses, such as synthetic chemotaxis, enabling the swimmers to avoid dead ends and autonomously find paths through complex mazes.

Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities, which could be useful for developing self-navigating micromachines with potential applications in targeted drug delivery and environmental sensing.

BP 13.5 Tue 10:30 H47

Active Particles in Tunable Colloidal Environments — •Abhimanyu Nowbagh[1], Venkata M.S.G. Tanuku[2], Thomas Palberg[2], and Ivo Buttinoni[1] — [1]Institute of Experimental Colloidal Physics, Heinrich-Heine University, 40225 Düsseldorf — [2]Institute of Physics, Johannes-Gutenberg University, 55128 Mainz

Active colloids are microscopic particles which propel through aqueous media by converting the externally available energy into directed motion. Using non equilibrium thermodynamics to understand biological systems: interactions of active colloids with crowded systems, and emergent phenomena of ensembles of active particles, remain an important and open question.

In this work, we investigate the dynamics of active particles in crowded environments subjected to alternating-current (AC) electric fields. The AC electric field is used to control: i) the velocity of active particles and ii) the inter-particle interaction between passive colloids. As we increase electric field strength, the velocity of active particles increases and the inter-particle interaction between passive colloids becomes stronger. We study the behaviour of active particles as a function of: i) the frequency of the applied AC electric field, ii) the area fraction of the passive crowd, iii) the active to passive particle number ratio, and iv) the velocity of the active particles.

Our experimental findings show that the active particles reorient faster with an increasing electric field strength. With an increase in the active to passive particle ratio, we show that cluster formation is non-monotonically sensitive to the passive crowd density.

Invited Talk BP 13.6 Tue 10:45 H47

Beyond spheres - active matter in new shapes — •Juliane Simmchen — University of Strathclyde, Cathedral street 295, Glasgow UK

Surface minimisation for a given volume is energetically favourable on the small scale - this is why most colloidal particles are spherical. In active matter they have the added advantage of facilitating comparison between experiment and theory, one of the reasons why spherical Janus particles dominate the field.

However, broadening the range of materials has led to interesting discoveries - behaviour that would not have been observable in the spherical regime. This talk will give an overview of the intriguing behaviour of non-spherical active materials at the microscale - from plates to truncated bipyramids and rods.

15 min. break

BP 13.7 Tue 11:30 H47

Modeling Filamentous Cyanobacteria — •Elias Fischer and Holger Stark — Institute Of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet, both in the present and the past. They triggered the great oxygenation event about 2.5 billion years ago, generating the atmospheric oxygen of our planet while contributing large parts of our fossil fuel record.

Filamentous cyanobacteria exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood. Furthermore, the gliding of cyanobacteria is strongly affected by external cues, most importantly light. They aggregate in regions with the highest light intensity, which means best environmental conditions for photosynthesis.

Following recent advances in understanding the self-organization of cyanobacteria, we present a novel approach for modeling the mechanical and behavioral aspects of individual cyanobacteria filaments, including force synchronization and response to light. Each filament is modeled as a bead-spring chain in 3D with bending and torsional elasticity, as well as a hard-core repulsion between the filaments. Notably, the propulsion forces that drive the individual parts of the filament forward are only considered locally where the filament comes into contact with another surface. First results on the 3D bending and twisting motion of a filament and its reaction to light are presented.

BP 13.8 Tue 11:45 H47

Self-assembly and control of active and passive triblock Janus colloids — •Juri Franz Schubert, Salman Fariz Navas, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Triblock Janus colloids belong to the family of patchy particles, interacting with hydrophobic attraction at opposite poles and electrostatic repulsion in the equatorial region. They are known to self-assemble into a colloidal kagome crystal from experiments [1] and theory [2,3,4]. However, investigating the self-assembly of such systems via Brownian Dynamics can result in timescales inaccessible to brute force simulations, often requiring complex sampling techniques [3]. Recently, it has been shown that introducing self-propulsion can significantly accelerate self-assembly and enhance the Kagome yield [4]. Here, we study the model introduced in [4] and further investigate the self-assembled structures in active and passive systems. Using simple time-dependent activity protocols, we are able to sample a temperature-density state diagram of the passive system. Our results closely match with earlier studies [2,3], where different triblock models and sampling techniques were used.

[1] Q. Chen, S. C. Bae, S. Granick, Nature 469, 7330 (2011).
[2] F. Romano, F. Sciortino, Soft Matter 7, 12 (2011).
[3] K. Bahri, H. Eslami, and F. Müller-Plathe, JCTC 18, 1870 (2022).
[4] S. A. Mallory, A. Cacciuto, JACS 141, 6 (2019).

BP 13.9 Tue 12:00 H47

Enhanced Diffusion and Universal Rouse-like Scaling of an Active Polymer in Poor Solvent — Suman Majumder[1], Subhajit Paul[2], and •Wolfhard Janke[3] — [1]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India — [2]Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India — [3]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

By means of Brownian dynamics simulations we study the steady-state dynamic properties of a flexible active polymer in a poor solvent condition. Our results show that the effective diffusion constant of the polymer D_{eff} gets significantly enhanced as activity increases, much like in active particles. The simulation data are in agreement with a theoretically constructed Rouse model of active polymer, demonstrating that irrespective of the strength of activity, the long-time dynamics of the polymer chain is characterized by a universal Rouse-like scaling $D_{\text{eff}} \sim N^{-1}$, where N is the chain length. We argue that the presence of hydrodynamic interactions will only have an insignificant effect on the observed scaling behavior.

BP 13.10 Tue 12:15 H47

A Pulsating Active Solid — •Umang A Dattani[1], Francesco Serafin[1], Jonas Ranft[2], and Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institut de Biologie de l ENS, Ecole Normale Superieure, CNRS

Active matter has garnered significant attention in recent decades due to its numerous parallels with biological systems. Inspired by recent studies of biological tissues, such as cardiac cells, where constituent cell sizes periodically vary, a new form of activity termed "pulsating active matter" has been introduced recently. We propose a model of a pulsating active solid, consisting of size-changing particles linked by a triangular spring network. Despite the fixed connectivity, our model exhibits a variety of patterns and topological phase defects, akin to previous studies. Additionally, we explore the elastic continuum limit, which successfully predicts several essential features of the microscopic model. We conclude by highlighting intriguing properties of this system and its different potential parallels.

Invited Talk BP 13.11 Tue 12:30 H47

Emergent correlations and boundary fluctuations in epithelial cell sheets — •Silke Henkes — Lorentz Institute, Leiden University, Leiden, The Netherlands

In soft active materials, the driving motion of individual constituents competes with their mechanical interactions, giving rise to active liquids, solids or glasses. An especially important example of this are epithelial cell sheets, which form a barrier function in the body and where the active crawling motion of cells over the substrate acts against cell-cell adhesion and repulsion.

I will show that a minimal model of cell sheets with uncorrelated activity, based on active Brownian dynamics and a vertex model, is a good quantitative match to data from two experiments on corneal and MDCK cell sheets. Its core feature is an emergent correlation length, arising from the diffusive spread of active forces through an elastic solid. This is a very general result that emerges in many active solids.

The boundary of such cell sheets exhibits a 'fingering instability' where the initially straight boundary develops large, spatiotemporally correlated fluctuations. Despite previous interpretations within many frameworks as an instability, I will show that it can be fully explained as arising from the active correlations of the cell sheets driving the boundary.

BP 14: Poster Session I

Bacterial biophysics, computational biophysics, membranes and vesicles, synthetic life-like systems and origin of life, systems and networks biophysics

Time: Tuesday 10:00–12:30 Location: P3

BP 14.1 Tue 10:00 P3

The Role of Localized Metabolic Activity in Streptomyces Hyphae: An Agent-Based Approach — •Ricardo Santander[1], Denis Iliasov[2], Thorsten Mascher[2], and Vasily Zaburdaev[1] — [1]Max-Planck Zentrum für Physik und Medizin, Kussmaulallee 2, Erlangen — [2]Institut für Mikrobiologie, Zellescher Weg 20b, Dresden

The filamentous bacterium Streptomyces undergoes complex multicellular development characterized by hyphal growth and branching. Recent discoveries of LpdA-containing fluorescent foci within the hyphae suggest localized sites of elevated metabolic activity and ATP production. To investigate their influence on hyphal morphogenesis, we developed an agent-based model simulating key cellular components and their interactions.

Simulations reveal that localized ATP production and high consumption rates near the tips create spatial heterogeneity in metabolic activity. By adjusting model parameters, the model replicates typical growth patterns and hyperbranching phenotypes observed experimentally.

Our findings suggest that the spatial distribution of metabolic foci and localized ATP production influence Streptomyces morphology and multicellular organization.

BP 14.2 Tue 10:00 P3

Optically driven thermofluidic assembly of bacteria — •Desmond Joseph Quinn[1], Selina Hanisch[2], Rohan Karande[3], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth Sciences, Leipzig University, Leipzig, Germany — [2]Helmholtz Center for Environmental Research (UFZ), Leipzig, Germany — [3]Biophysical Chemistry, Leipzig University, Leipzig, Germany

Bacteria in their planktonic state are known to assemble into biofilms in the vicinity of a solid surface. The complex cascade that results in the adhesion of the

bacteria to the surface is usually triggered by the diffusion of bacteria to its vicinity. We propose a method that makes use of temperature induced flow fields and depletion interactions for the localized assembly and manipulation of bacteria. In addition to the physical interactions that contribute to the assembly process, the motility of the bacteria affects the assembly and can be altered by the induced temperature and altered distribution of molecules. We try to disentangle these effects by studying passive and active bacteria independently. We look at how motility parameters change in response to the fields induced by the laser, and how this in turn affects assembly. Such controlled assembly of bacteria could be useful for technological applications in bioreactors. In addition, our method provides a way of experimentally probing the effect of localized temperature, osmotic pressure, and flow fields on the motility of bacteria.

BP 14.3 Tue 10:00 P3

Growth and characterization of MoS2 nanowalls on Ti-based bone implants — •Rania Ennaciri, Axel Printschler, Christof Neumann, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany

Antibiotic resistance presents an important issue in the medicine field particularly in the context of bone replacement surgeries, where infections from antibiotic-resistant bacteria can lead to severe health complications and even fatalities. While titanium (Ti) is the conventional choice for bone implants, there is a clear need for further improvements of this material to enhance its antimicrobial resistance. In this regard, hybrids based two-dimensional (2D) materials, such as molybdenum disulfide (MoS2), present a great promise due to their intrinsic antimicrobial activity and biocompatibility. These properties are generally manifested through biochemical reactions, by the generation of reactive oxygen species (ROS) that can lead to the damage of bacteria DNA, proteins and lipids. Also, mechanical actions, where the sharp edges of the nanowalls can cut the bacteria wall can lead to its death. To investigate these mechanisms, we use metal-organic chemical vapor deposition (MOCVD) technique to grow different morphologies and sizes of MoS2 nanowalls on Ti implants. We use scanning electron microscope (SEM), Raman spectroscopy and X-ray electron microscopy (XPS) to characterize the structural and chemical properties and to correlate them prospectively with the antimicrobial properties as well as with the growth bone cells.

BP 14.4 Tue 10:00 P3

Infrared Hyperspectral Mapping of Biofilms Growing in Confinement — •Felix Hermann Patzschke[1], Valentina Schmitz[2], Rohan Karande[2,3], and Frank Cichos[1] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig — [2]Leipzig University, Institute for Biochemistry, Johannisallee 21-23, 04103 Leipzig — [3]Helmholtz Centre for Environmental Research, Permoserstraße 15, 04318 Leipzig

Biofilms are microbial communities characterized by complex spatial organization and dynamic chemical composition. The formation and growth of biofilms in confined environments are of significant interest in fields such as medicine and bio-engineering. We seek to establish a clearer understanding of the interplay between physical confinement and microbial behavior by investigating whether specific quantifiable aspects of a cavity's geometry can influence the likelihood of biofilm initiation and the rate of its growth.

We utilize Photothermal Infrared (PTIR) hyperspectral microscopy to acquire infrared spectral data at sub-cellular spatial resolutions. Through spectral decomposition, we aim to map the chemical composition of biofilms and distribution of nutrients in space and time. Our results provide a detailed view of biofilm structure, metabolic activity, and growth dynamics in confined settings. This work underscores the potential of PTIR microscopy as an impactful tool for advancing the understanding of biological systems in scientifically and technologically significant domains.

BP 14.5 Tue 10:00 P3

Self-Organized Colonization Resistance without Physical Barriers — •Christian Westendorf[1], Valentin Slepukhin[1], Birgit Koch[1], Victor Peris[1], and Oskar Hallatschek[1,2] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University. — [2]Department of physics, University of California, Berkeley.

Small micrometer-scale cavities, such as gut crypts, soil pores, and plant apoplasts, represent key bacterial habitats, in which different strains compete for resources and space. Recent studies have shown that the physical structures of these microhabitats can influence the stability and resilience of bacterial colonizers by protecting local populations from invasion. Building on this, we experimentally and computationally investigate the dynamics of mixed bacterial populations within interconnected microfluidic cavities, examining the influence of geometric features and surface interactions on microbial organization and diversity. Our findings reveal that surface roughness and friction can drive self-organization into effectively isolated subpopulations, safeguarding slower-growing strains from competitive exclusion. By comparing velocity fields of growing populations with stochastic and analytical simulations, we demonstrate how local geometry and emergent microhabitats balance selective pressures, maintaining microbial diversity under competitive and evolutionary stress. Our work suggests that colonization-resistant microhabitats can form dynamically, even in the absence of physical barriers.

BP 14.6 Tue 10:00 P3

Comparing graphene and 2D MoS_2 nanopores for protein translocation and detection — •Peijia Wei, Mayukh Kansari, and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Nanopores, nanometer-scale openings in materials, have shown their strong potential in realizing ultra-fast, cost-effective, and real-time next-generation sequencing technology. These nanopores can electrophoretically drive charged biomolecules and detect these. Using computer simulations, we compare two-dimensional nanopores, namely graphene and MoS_2, to evaluate their effectiveness in protein detection. We modulate protein translocation and dynamics by adjusting the type and concentration of the surrounding solvent, using a typical monovalent salt solution and a molecular solution. Utilizing atomistic simulations, we assess the efficiency of both nanopores in threading proteins, based on measurable ionic current signals. Our results show that graphene nanopores strongly interact with proteins, hindering translocation under physiological conditions. This issue is addressed by introducing a denaturant, which creates a hydrophilic-cationic layer on the pore surface, facilitating the linearized threading of proteins. In contrast, MoS_2 nanopores facilitate protein passage even in physiological solutions, offering an alternative approach to controlling translocation speed. We analyze the two nanopore materials based on molecular interactions among the material, protein, and solvent, emphasizing their impact on protein dynamics and ionic signal enhancement for efficient 2D nanopore protein detection.

BP 14.7 Tue 10:00 P3

Exploring coarse graining RNA force fields via Machine Learning — •Anton Dorn[1] and Alexander Schug[1,2] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]KIT Scientific Computing Center, Karlsruhe, Germany

In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. Here we attempt to solve a modified version of the problem by determining a coarse-grained RNA force field for Molecular Dynamics simulations. The data sparsity can here be alleviated by atomistic RNA simulations using proven and established force fields. In a first step we show the viability of this approach with a limited scenario of only small RNA molecules. For this we adapt the invariant Graph Neural Network architecture, cgSchnett.

BP 14.8 Tue 10:00 P3

Parameterization of a dissipative particle dynamics thermostat (DPD) thermostat for coarse-grained molecular dynamics — •Karan Venkatesh, Viktor Klippenstein, and Nico F. A. van der Vegt — Technische Universität Darmstadt

Coarse-grained (CG) simulations represent a viable approach for modelling dynamics on long length and time scales inaccessible with atomistic simulations. In this work, we present a single-site coarse-graining method designed to match the dynamical and structural properties of a molecular liquid (cyclohexane).

We employ a DPD thermostat, in which the pairwise forces are decomposed into parallel and perpendicular components. An iterative optimization scheme is implemented to parameterize the parallel and perpendicular forces, aiming to match the diffusion coefficient and shear viscosity of the system, respectively. In our study, we find that matching the diffusion coefficient also leads to a match in the shear viscosity. However, this correspondence may not always hold, especially when dealing with structurally anisotropic molecules and soft potentials, as commonly encountered in soft matter systems. This approach can be further extended to simulate mixtures of CG molecular liquids, and study penetrant dynamics in CG polymer melts.

References: 1. V. Klippenstein; N F A van der Vegt; J. Chem. Theory Comput. 2023, 19(4), 1099-1110. 2. M. Tripathy; V Klippenstein; N F A van der Vegt; J. Chem. Phys. 2023, 159(9) 3. C. Junghans; M. Praprotnik; K. Kremer; Soft Matter 2008, 4(1), 156-161

BP 14.9 Tue 10:00 P3

Leveraging Experimental Vasculature Data for High Resolution Brain Tumor Simulations — •Eric Behle[1], Julian Herold[2], and Alexander Schug[1] — [1]NIC Research Group Computational Structural Biology, Jülich Supercomputing Centre, Jülich Research Center, Jülich, Germany — [2]Steinbuch Centre for Computing, KIT, Karlsruhe

Cancer remains a leading cause of mortality. Multidisciplinary studies probe its pathology to increase treatment options. Computational modeling of tumors on HPC resources offers insight into its progress and an avenue for advancing our understanding. However, initialization and parameterization of the underlying models require high-resolution data from real tissue structures. Here, we leveraged HPC resources and a massive dataset of a mouse brain's entire vascu-

lar network. We processed these image stacks into detailed 3D representations, identified brain regions of interest, and conducted a series of large-scale simulations to investigate how tumor growth is influenced by local vascular network characteristics. By simulating tumor growth with sub-cellular resolution, we can probe to which extent vessel density and network length influence growth. We determined that vessel density is the primary determinant of growth rate. Finally, our results allowed us to extrapolate tumor cell growth predictions for the entire mouse brain, highlighting the critical role of vascular topology in tumor progression. Such increasingly realistic simulations of cancer cells may enable researchers to bridge the gap between basic biology and clinical practice, supporting development of cancer therapies.

BP 14.10 Tue 10:00 P3

Boundary integral method for elastic solids in Stokes flow and applications in real-time deformability cytometry — •Thomas Mayr and Stephan Gekle — Universität Bayreuth, Deutschland

A Newtonian fluid at small Reynolds numbers can be described using the Stokes equation. A common choice to solve the Stokes equation numerically is the boundary integral method. Previously, this method was mainly used to describe rigid particles or capsules with an elastic membrane such as red blood cells. Here a technique is presented how to extend the boundary integral method to elastic solids discretized by the finite element method. This can be used as simple model to describe the stiffness of cells with a nucleus and a cytoskeleton, e.g. in some deformation experiments. In our case we will compare the simulations with an experimental technique called real-time deformability cytometry (RT-DC).

BP 14.11 Tue 10:00 P3

Mathematical Modeling of Intercellular Calcium Waves in Fibroblast Networks — •Kara Nachtnebel — Isarstr, 6, 93057 Regensburg

Inflammatory responses are essential for defending against pathogens but can result in tissue damage when not properly regulated. Resident tissue macrophages (RTMs) play a crucial role in maintaining immune homeostasis by modulating inflammatory cascades. Disruptions in these regulatory mechanisms can lead to heightened immune responses and may contribute to the development of autoimmune diseases. This study explores the role of fibroblast networks and their calcium signaling dynamics in maintaining tissue homeostasis. We aim to understand the mechanisms underlying these dynamics and predict calcium signal propagation in both healthy and pathological tissues. A mathematical model is developed to describe intracellular calcium ion diffusion and Inositol-1,4,5-triphosphate (IP3) signaling in fibroblast cells interconnected by gap junctions (GJs). This model incorporates intracellular calcium stores and IP3-sensitive receptor (IPR) dynamics, which significantly influence calcium release into the cytoplasm. IP3 generation is modeled as a function of phospholipase-C (PLC) activation, triggered either by external stimuli or by calcium, leading to calcium-induced calcium release (CICR). Our approach provides insights into how calcium signaling networks contribute to tissue homeostasis and how their dysfunction occurs in pathological conditions.

BP 14.12 Tue 10:00 P3

coarse-grained simulations of Lge1(1-80) peptide. — •Agaya Johnson[1], Anton Polyansky[2], Pedro Sanchez[1], Bojan Zagrovic[2], and Sofia Kantorovich[1] — [1]Computational and soft matter physics, University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]Department. of structural and computational biology, Campus- Vienna-biocenter 5, 1030 Vienna, Austria.

Biomolecular condensates in cells such as p-bodies, nucleoli and stress granules play an important role in regulating biological processes like transcription and ribosome biogenesis. Studying of such biomolecular condensates will give insight into the molecular basis of disease, like neurodegenerative diseases, cancer and diabetes. The main purpose of this study is to understand the main phenomenon, which leads to the formation of these biomolecular condensates such that we get a conclusion, whether is it phase separation, self-assemble or an aggregation. We use Lge1(1-80) peptide as a model for study because Lge1(1-80) is mostly disordered prone to form many cation - pi and pi - pi interaction (R, G and Y rich sequence) and because of its alternating net charge which are the prerequisites for the phase separation. Due to the limitations of high-resolution experimental techniques, we are using molecular dynamics simulation with coarse-grained approaches with the help of software package ESPResSo. Our goal is to develop a coarse-grained model for proteins that exhibit structural transitions and to understand fundamental mechanisms under those transitions.

BP 14.13 Tue 10:00 P3

Optimizing a Biomimetic Cross-Flow Microplastics Filter Inspired by Manta Rays — •Ioannis Gkekas[1] and Tim Robertino Baumann[2] — [1]Universität Bielefeld — [2]Universität Bielefeld

Microplastic pollution poses a significant threat to aquatic ecosystems, necessitating innovative filtration solutions. This study continues previous research on a biomimetic cross-flow filter inspired by manta ray feeding mechanisms. The objective is to optimize the filter's geometry and material properties to enhance efficiency and durability. Using COMSOL simulations, various geometrical configurations are being tested to identify an optimal design for maximizing filtration efficiency and clean water output. To address material durability, we reenforced PDMS (polydimethylsiloxane) with glass fibers to mitigate bursting under operational stress. Initial results indicate that the composite material significantly enhances durability compared to the original PDMS design. Once the simulations are complete, the optimal design will be fabricated for in-lab performance evaluation. This research advances the development of sustainable, high-efficiency microplastic filtration systems inspired by natural processes.

BP 14.14 Tue 10:00 P3

Autonomous, intrinsic circadian oscillator at cell membranes — •Mauro Ariel Forlino[1], Oreste Piro[2], and Martín García[1] — [1]Universität Kassel, Kassel, Germany — [2]Universtat de les Illes Balears, Palma, España

Circadian rhythms originated in endogenous cellular clockworks are the evolutionary solution that allows organisms to anticipate and synchronize their internal processes with the predictable changes in their environment on a daily basis. According to the conventional paradigm, eukaryotic cells generate circadian rhythms as outputs from gene-based biochemical oscillators comprised of transcription/translation feedback loops, necessarily involving processes occurring within the nucleus. However, mounting evidence has recently emerged indicating that circadian rhythms also exist in cells devoid of such nuclear clocks, notably seen in the circadian variation of red blood cell metabolism. Here, we demonstrate the existence of a completely different mechanism for generating endogenous circadian oscillations that solely involves processes within the cell membrane and its immediate vicinity, entirely independent of the nuclear clock. Rather than relying on the transcription/translation/repression loop as in nuclear oscillators, this membrane-located clock operates through an analogous regulatory circuit that involves the homeostatic regulation of ion channels and their gating kinetics.

BP 14.15 Tue 10:00 P3

Influence of the sapogenin gypsogenin on vesicles from 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) — •Melanie Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Small unilamellar vesicles (SUVs) composed of phospholipids, such as 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC), are commonly used as model membrane systems. DMPC bilayers undergo phase transitions from a gel to a fluid phase at around 24°C. While the effects of saponins on DMPC membranes are well-documented, the impact of their aglycones, sapogenins, remains less explored. Gypsogenin, a pentacyclic triterpenoid found in soapwort (Saponaria officinalis) and gypsum herb (Gypsophila oldhamiana), is of interest due to its anti-cancer potential. Gypsogenin shares structural features with cholesterol but has contrasting effects on membrane properties. While cholesterol increases membrane thickness and reduces fluidity, gypsogenin incorporation decreases the vesicle core radius and membrane thickness, as shown by small-angle X-ray scattering (SAXS) and cryo-TEM. UV-vis spectroscopy was used to monitor turbidity in solutions containing 0 to 25 mol% gypsogenin over a wide temperature range, showing a reversible increase upon cooling, indicating thermally reversible phase transitions. SAXS measurements revealed significant structural changes at 25 mol%. The core radius and membrane thickness decreased compared to pure DMPC vesicles. These findings suggest that gypsogenin alters DMPC membranes significantly at higher concentrations.

BP 14.16 Tue 10:00 P3

Properties of Long-Chain Lipid Enriched Regions in Biological Membranes: Insights from MD Simulations — •Annemarie Quas, Clara Rickhoff, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

Experimental studies of yeast plasma membranes reveal gel domains enriched in long-chain lipids and depleted in ergosterol [1]. To explore these findings, we perform coarse-grained molecular dynamics simulations of membranes with varying concentration of long-chain lipids. To enhance our understanding, we simulate both asymmetric membranes with long-chain lipids in the outer leaflet, as observed experimentally, and symmetric membranes containing long-chain lipids in both leaflets. Our analysis focuses on characterizing key membrane properties and examining the influence of long-chain lipids. The role of ergosterol is also investigated. Additionally, we assess non-affine lipid movements to provide insights into the dynamics within these gel domains. This study aims to bridge experimental observations with molecular-level mechanisms, advancing our understanding of gel-phase organization and its implications for membrane functionality.

[1] Aresta-Branco *et al.*, *J. Biol. Chem.* **2011**, 7, 5043-5054

BP 14.17 Tue 10:00 P3

G-FETs for label-free biosensing of protein interactions — •Florian Steinbach, Mykola Fomin, Margarete Schwirblat, and Carola Meyer — Institute of Physics, University of Osnabrück, Germany

Graphene field-effect transistors (G-FETs) offer a promising approach for label-free biosensing due to their sensitivity and compatibility with liquid environ-

ments. In this work, we investigate liquid-gated G-FETs functionalized with lipid monolayers for detecting protein interactions at membrane interfaces.

The fabrication process was refined to improve device stability and reduce measurement variability. To enable reusability, we employed tris-NTA-functionalized lipids, allowing reversible binding and elution of hexahistidine (H6)-tagged proteins while preserving device functionality for subsequent detection cycles. Adjustments to the functionalization protocol included histidine-based elution, which better preserved the passivation layer compared to standard imidazole methods. Electrical measurements were used to monitor functionalization steps and protein interactions. Using monomeric enhanced green fluorescent protein (H6-mEGFP) as a model system, we present characteristic shifts and changes in transconductance during each step of the protocol.

These developments contribute to the optimization of G-FETs for biosensing applications, with particular attention to the stability of functionalized interfaces under physiological conditions. The findings will be discussed in the context of improving sensor design and extending the approach to more complex biomolecular systems.

BP 14.18 Tue 10:00 P3

Theory of spatial aggregation and shell formation — •Pranay Jaiswal, Ivar Haugerud, and Christoph Weber — Institute of Physics, University of Augsburg, Augsburg, Germany

Many biological systems use coexisting phases composed of proteins and RNA to regulate chemical processes and molecular transport. In particular, the interface can act as a nucleation site for aggregation of proteins, leading to the formation of a solid-like shell. This shell provides a physical barrier for molecular transport of further biomolecules, giving rise to molecule-specific interface permeabilities. Here we propose a theoretical model for spatio-temporal protein aggregation in phase-separated systems. To this end, we use a phase-field of proteins and RNA combined with a phase-field characterising the solid-like, aggregated state. Our key finding is that aggregation is thermodynamically favored at the interface, making aggregation shells a likely phenomenon in phase-separated systems of aggregation-prone proteins. We show how such aggregation shells control molecular transport and shell permeabilities. Our theory can be applied to experimental systems undergoing irreversible aggregation to unravel the molecular mechanism underlying ageing in protein mixtures.

BP 14.19 Tue 10:00 P3

Cell-free protein synthesis measured in flowing nanolitre-droplets — Benno Schedler[1], Alexandros Katranidis[2], and •Jörg Fitter[1,2] — [1]AG Biophysik, I. Physikalsiches Institut (IA), RWTH Aachen University, D-52074 Aachen, Germany — [2]Forschungszentrum Jülich, ER-C-3, D-52425 Jülich, Germany

Cell-size confinement of biological reactions by utilizing microfluidic water-in-oil droplets has been widely used to revolutionize the field of biomolecular research. This approach capitalizes on the precise control and manipulation of nanoliter-sized droplets within microfluidic channels. The confinement facilitates reduced reagent consumption and improved scalability. Analysing cell-free protein synthesis (CFPS) is an ideal application of this approach and represents a complex multistep process which can be monitored in individual droplets if fluorescent proteins are synthesized [1]. Understanding the physicochemical principles underlying CFPS reactions, including the role of macromolecular crowding, is crucial for optimizing protein synthesis yields and functionality [2]. Here we present the results of our ongoing research using the example of the synthesis of green fluorescent protein (GFP), which we have analysed employing confocal fluorescence microscopy. Focus is set on the high throughput capability of the approach and thus the possibility of analysing several hundred parallel reactions. The latter provide important information about the average synthesis productivity and the distribution widths for reactions under different environmental conditions. [1] Hansen et al., 2016, Nature Nanotechnology, 11, 191; [2] Kempf et al., 2017, Scientific Reports, 7, 46753

BP 14.20 Tue 10:00 P3

Enhancing polymerization of prebiotic building blocks by wet-dry cycling — •Almuth Schmid and Dieter Braun — AG Braun, LMU Systems Biophysics, Munich, Germany

Prebiotic chemistry is limited by several factors as concentration or availability of starting materials on the early Earth. On top of that, many artificial and natural activation agents are too complex to have been a part of prebiotic reaction networks. To overcome this problem, amino acids might help reaching ideal environmental conditions, enhancing prebiotic reactions like polymerization of nucleotides. Preliminary experiments demonstrated, that in a wet-dry cycling system rel. yields of GC polymers are boosted up to 70% in the presence of amino acids.

By using wet-dry cycles and including other prebiotic plausible activating agents like volcanic rocks, a better control of the polymerization can be accomplished. Tracking the polymerization on tholeiite basaltic rock with SEM reveals first hints on where and how the polymers interact with the mineral.

BP 14.21 Tue 10:00 P3

Phase-separation enhances sequence selection via templated ligation — •Manav Koul, Ivar Haugerud, and Christoph Weber — Universität Augsburg, Universitätsstraße 2, 86159 Augsburg

The emergence of highly selective catalytic sequences was a crucial step towards the origin of life. templated ligation of RNA has been proposed as a pre-biotic mechanism to achieve self-replicating sequences without complex machinery. A question remains as to how sufficiently long and abundant templates can emerge from short nucleotides in a non-conducive prebiotic pool. As phase separation has been shown to provide versatile hubs of correlated sequences, we investigate its role in facilitating and directing templated ligation. To this end, we develop a non-equilibrium thermodynamic model to describe the oligomerization of sequences and their ligation at non-dilute conditions in phase-separated systems. We find that phase-separation enhances the selection pressure of this mechanism, resulting in a sequence distribution dominated by highly structured sequence of low entropy. Our results highlight that out-of-equilibrium condensed phases could provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de-novo life.

BP 14.22 Tue 10:00 P3

Phase Transitions in Non-Hydrated DPPC Lipid Bilayers Deposited on Silicon: Effects of Dry Nitrogen Atmosphere and Thermal Cycling — •Nicolás Moraga[1], Daniel Saavedra[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], María José Retamal[3], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Chile — [3]Facultad de Ingeniería, Universidad Finis Terrae, Santiago, Chile

This study investigates the phase behavior of DPPC lipid bilayers in a non-hydrated state, deposited on silicon substrates, under conditions that are both experimentally innovative and highly relevant for applied science and fundamental research. By assembling these bilayers in vacuum and exposing them to dry nitrogen atmospheres, we present a novel platform that extends beyond classical hydrated systems, with significant implications for biosensing technologies. Through controlled thermal cycling using high-resolution ellipsometry, a technique offering exceptional sensitivity to subtle changes, we analyze phase transitions, uncovering the impact of hydration-free environments on lipid bilayer organization. These findings provide new insights into the thermal resilience of DPPC bilayers, highlighting potential phase stability domains. Additionally, this approach simulates extraterrestrial-like conditions where water is absent, underscoring the adaptability of lipid-based structures and advancing our understanding of molecular organization under vacuum and inert atmospheres. Acknowledgements: ANID Fellowships (NM, DS, NGV); Puente UC 2024-25.

BP 14.23 Tue 10:00 P3

Cooperative Effects in Compartmentalized Irreversible Self-Assembly — •Severin Angerpointner, Richard Swiderski, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

From biomolecular compartments, protein patterns to porous rocks: Many biological and chemical systems like living cells or prebiotic chambers exhibit some form of spatial organization which separates biochemical processes. This is known to play a key role in the assembly of virus capsids or the enrichment of prebiotic chemicals. We systematically explore the effects of such spatial separation on the self-assembly of irreversibly binding identical particles. We show that already in a simplified model of two coupled biochemical compartments cooperative effects emerge through limiting compartment exchange. Further, these findings generalize to spatially extended systems like intracellular chemical gradients or membrane-assisted assembly.

BP 14.24 Tue 10:00 P3

Mathematical modelling of immune response on the example of psoriasis — •Nadezhda Esenkova[1,2], Lukas Pöschl[1,2], Gerard C. L. Wong[3], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]University of California, Los Angeles, USA

In recent years it was shown that antimicrobial peptides (AMPs) can contribute to the immune response by triggering Toll-Like Receptors (TLRs) on immune cells. Apart from natural AMPs it was suggested that proteolytic enzymes, secreted by neutrophils can digest other signaling molecules to AMP-like fragments, which can stimulate immune response and lead to disease progression. The goal of this work is to create a mathematical model of immune response by introducing this novel link of AMP-like fragments. To this aim we constructed a comprehensive signaling network of the immune response based on one of the best studied autoinflammatory diseases – psoriasis. Taking into account the key biological pathways we reduced it to the core network model, which we investigate using theoretical dynamical systems analysis and modern machine learning methods. We aim to understand how the hypothesized mechanism of autoinflammation due to AMP-like fragments augments the disease outcomes from full resolution, to chronification and rapid exacerbation.

BP 14.25 Tue 10:00 P3

Formation of thermally driven pH gradients from salts — •Riccardo Schiroli, Thomas Matreux, and Christof B. Mast — Systems Biophysics, LMU München, Munich, Germany

The impact of pH on biomolecule stability and chemical reactions suggests its crucial role in prebiotic chemistry. Thermophoresis, the movement of molecules along a thermal gradient, has been shown to accumulate and select a wide range of biomolecules, including RNAs and amino acids as well as different salt species leading in specific conditions to the emergence of pH gradients.

In this study, we investigated the formation of heat flow driven pH gradients in simulated rock fissures under various experimental conditions, including different salt solutions, initial pH values, and temperature gradients. Ion chromatography, combined with complexation techniques and fluorescent analysis, was used to analyze the distribution of ions and pH profiles within the fissures.

Our findings show that heat flows can efficiently induce pH gradients in solutions containing various salt species. We observed significant accumulation of common ions, leading to pH gradients in both alkaline and acidic solutions. Furthermore, we found that certain metal ions, such as lanthanides and iron, can significantly enhance the formation of pH gradients, even at micromolar concentrations. This study provides evidence for the role of heat flows in creating localized pH gradients under prebiotically plausible conditions. Our results highlight the ease with which pH gradients can form under a wide range of prebiotic plausible conditions, driven by simple heat flows.

BP 15: Cell Mechanics I

Time: Tuesday 11:45–13:00 Location: H44

Invited Talk BP 15.1 Tue 11:45 H44

Does Oncology Need Physics of Cancer? — •Josef Käs — Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnéstr 5, 04103 Leipzig

Cancer is a complex disease that accounts for nearly one in six deaths worldwide. More than 90 percent of deaths are due to metastasis * the process by which cancer cells spread from the primary tumor and seed a secondary tumor in a distant tissue. Despite advances in cancer treatment, metastatic recurrences remain a significant challenge. Understanding metastasis is crucial for a reliable predictive diagnosis needed for personalized oncology and to develop therapies that inhibit cancer spreading. The metastatic cascade routes in a mechanical problem for tumor cells on their way through the human body squeezing through dense tissues. Two clinical trials with more than 2000 breast cancer patients in each study prove that the onset of cancer cell motility can be explained as an unjamming transition and local cancer spreading of cancer cell clusters embedded in ECM must be described as active nematic droplets in a nematic phase. The gained physical parameters can be used a prognostic tumor marker for metastatic risk that improves breast cancer diagnosis by 26 percent. Beyond diagnostics the mechanical modulation of cancer cells by adipocytes points us towards migrastatic therapies to suppress metastasis.

BP 15.2 Tue 12:15 H44

Prostate cancer associated fibroblasts have distinct morpho-mechanical features that predict patient outcome — Antje Garside[1], Angela Jacobi[1], Shivakumar Keerthikumar[2,3], Michelle Richards[2], Birunthi Niranjan[2], Gail Risbridger[2,3], Mitchell Lawrence[2,3], and •Anna Taubenberger[1] — [1]BIOTEC, TUD, Dresden, Germany. — [2]Monash University, Victoria, Australia — [3]Peter MacCallum Cancer Centre, Melbourne, Australia.

Prostate cancer is among the most commonly diagnosed types of cancer. A key role in tumor progression has been attributed to the tumor stroma including its cellular components such as cancer associated fibroblasts (CAFs). Here we present a comprehensive study where we quantitatively assessed the morpho-mechanical properties of patient-derived prostatic CAFs and matched normal prostatic fibroblasts from a cohort of 35 patients, through combination of cell morphometric analysis and high-throughput mechanical probing of single cells by real-time deformability cytometry. CAFs comprised distinct morpho-mechanical features compared to their normal counterparts, including nuclear size and shape, cytoskeletal arrangement, cellular volumes and elastic properties. A combined score of these mechanical and morphological parameters distinguished patients with shorter and longer time to clinical relapse. Morpho-mechanical changes across patients were correlated with transcriptomic alterations in cellular components and pathways. In summary, our results suggest that high-throughput assessments of the biophysical properties of CAFs can serve as a complementary tool to predict patient outcome.

BP 15.3 Tue 12:30 H44

Viscoelasticity of Cancer Cells: New Insights from Magnetic Rotational Spectroscopy — •Jean-François Berret — Université Paris Cité, CNRS, Matière et systèmes complexes, 75013 Paris, France

Cell mechanical properties are linked to tumor progression and can serve as diagnostic biomarkers. Over the past two decades, numerous studies have shown that cancer cells are softer than healthy cells. While the viscoelastic nature of cells is well known, most studies focus on elasticity, with limited attention to viscosity. To address this, we developed Magnetic Rotational Spectroscopy (MRS), an active technique using non-toxic magnetic wires embedded in the cytoplasm and tracked via optical microscopy under a rotating magnetic field. This allows simultaneous measurement of viscosity η and elastic modulus G. MRS studies on 15 human and animal cell lines, both healthy and cancerous, uncovered a new finding: intracellular viscosity increases with wire size following a quadratic η(L)-relationship. Furthermore, in breast epithelial cells, only viscosity, not elasticity, could differentiate cells with low and high metastatic potential. A meta-analysis of literature on cell viscosity, covering whole-cell and intracellular data finally reveals that cancer cells have viscosities about 50% lower than healthy cells, suggesting that cancer cells are not only softer but also more fluid, offering potential for selective diagnostic tools in cell biomechanics. [1] A.M. Markl et al., Cancer Heterog. Plast., (2024). [2] J.-F. Berret, Nat. Commun. 7, 10134 (2016). [3] M. Dessard et al., Nanoscale Adv. 6, 1727 (2024).

BP 15.4 Tue 12:45 H44

Living Cells Feel the Surface Tension of Soft Solids — •Johannes Rheinlaender, Hendrik von Eysmondt, and Tilman E. Schäffer — Institute of Applied Physics, University Tübingen, Germany

For about 20 years it has been known that living cells actively respond to the stiffness of their microenvironment - most obviously - by a change in cell spreading area but also other properties such as stiffness, nucleus shape, and gene expression, denoted as mechanosensing. These effects are commonly investigated using hydrogels with a bulk Young's modulus in the kPa range, where cells respond to substrate stiffnesses typically between 1 and 100 kPa. On other soft materials such as elastomers, cell behavior has been shown to be different and weaker, plateauing below about 10 kPa, but the reason remained a matter of debate. On the microscale, surface properties such as surface tension are of increasing relevance, but probing interfaces with micro-indentation techniques such as atomic force microscopy is challenging due to adhesion effects. We therefore use scanning ion conductance microscopy (SICM), a unique scanning probe method benefiting from its non-contact measurement principle, to probe the surface tension of soft solids showing that elastomers exhibit surface tensions of about 10 mN/m, relatively independent of their bulk Young's modulus and surface treatment. Hence, cells mostly "feel" the bulk properties of elastomers for Young's moduli above about 10 kPa, but below mostly the surface tension, demonstrating that the substrate's surface tension is an important yet underestimated aspect in mechanobiology.

BP 16: Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 14:00–15:15 Location: H43

Invited Talk BP 16.1 Tue 14:00 H43

Mechanistic origins of temperature scaling in the early embryonic cell cycle — •Lendert Gelens — Laboratory of Dynamics in Biological Systems, Department of Cellular and Molecular Medicine, KU Leuven, Herestraat, 49, Leuven, Belgium

Temperature profoundly impacts organismal physiology and ecological dynamics, particularly affecting ectothermic species and making them especially vulnerable to climate shifts. Even though complex physiological processes usually involve dozens of enzymes, empirically it is found that the rates of these processes often obey the Arrhenius equation, which was originally derived for single enzyme-catalyzed reactions. Here we have examined the temperature scaling of the early embryonic cell cycle, with the goal of understanding why the Arrhenius equation approximately holds, and why it breaks down at temperature extremes.

Using experimental data from different frog, fish, fly, and worm species, we find that the apparent activation energies for the early embryonic cell cycle for diverse ectotherms are all similar. Computational modeling and experiments with frog egg extracts show that the non-Arrhenius scaling can be accounted for by biphasic temperature scaling in critical individual components of the cell cycle oscillator circuit, in combination with imbalances in the activation energies for different partially rate-determining enzymes. These findings provide mechanistic insights into the dynamic interplay between temperature and complex biochemical processes, and into why biological systems fail at extreme temperatures.

BP 16.2 Tue 14:30 H43

Reshaping morphogen gradients through porous tissue architecture — •Diana Khoromskaia[1,2] and Zena Hadjivasiliou[1,2,3] — [1]Francis Crick Institute, London, United Kingdom — [2]University College London, London, United Kingdom — [3]London Centre for Nanotechnology, London, United Kingdom

The morphogenesis of tissues during embryonic development is controlled by concentration gradients of morphogens – signalling molecules whose readout determines cell fate decisions. How the spread of morphogens is affected in tissues with complex geometry and spatially heterogeneous architecture is not well understood. To address this question, we introduce a porous vertex model, by explicitly considering the network of extracellular spaces between the cells. Morphogens produced by source cells disperse through the tissue via three modes of transport: extracellular diffusion, membrane-bound diffusion, and cell-based transport through recycling. With this model we investigate numerically and analytically how cell-scale geometry, such as cell size, cell shape anisotropy, and cell distance, influences effective diffusion and degradation of morphogens at tissue-scale. We further show that a non-linear coupling between cell packing and morphogen concentration renders the morphogen gradient robust to perturbations, for instance by locally buffering fluctuations in the production. Our characterisation of tissues as active porous materials provides new insights into how morphogenesis and cell fate determination may interact during embryonic development.

BP 16.3 Tue 14:45 H43

Active viscoelastic condensates provide controllable mechanical anchor points — •Oliver Paulin[1], Luise Zieger[2,3], Júlia Garcia-Baucells[5], Alexander Dammermann[5], Sebastian Aland[2,3,4], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]TU Bergakademie Freiberg — [3]HTW Dresden — [4]Center for Systems Biology, Dresden — [5]Max Perutz Labs, University of Vienna

Many biological materials must couple mechanical strength with the ability to rapidly self-assemble at a specific location. In particular, biomolecular condensates readily self-assemble via phase separation, but may also need to anchor external forces to fulfil their function. Spatial localisation of condensate formation can be controlled by active cores that preferentially drive the production of condensate material at a particular point, while resistance to external forces can be facilitated by viscoelastic material properties. Here, we develop a continuum model of viscoelastic growth around an active core, and investigate the results in a spherically symmetric geometry. We find that viscoelastic stresses restrict condensate growth, but also impart resistance to deformation. We investigate the effect of varying different mechanical properties on condensate growth and strength, and also study how strain-dependent material incorporation may limit the maximum rate of growth. Finally, we compare the predictions of our model to experimental data from centrosomes in C. elegans embryos, identifying a parameter regime in which rapid growth can be combined with appropriate mechanical strength.

BP 16.4 Tue 15:00 H43

Modelling cell crawling on different substrate stiffness — Sohei Nakamura and •Mitsusuke Tarama — Kyushu University, Fukuoka, Japan

Crawling cells sense the mechanical properties of the underlying substrate and change their dynamics accordingly. This ability called durotaxis is of great importance in various biological processes including development and homeostasis. In order to understand how intracellular chemical reactions and cellular mechanics give rise to durotaxis, we constructed a simple model from reaction diffusion equations for intracellular chemical compounds and force balance equations for the intracellular mechanics including the effect of the substrate stiffness. We found that within the model, the cell speed and diffusion coefficient change non-monotonically with the substrate stiffness, indicating the existence of an optimal substrate stiffness for migration. This non-monotonic behavior of the cell speed is consistent with experimental observations and can be understood to be caused by the competition between substrate adhesion and cell shape deformation. We further discuss cell migration on a patterned substrate.

BP 17: Poster Session II

Active matter, bioimaging, biomaterials and biopolymers, cell mechanics, cytoskeleton, protein structure and dynamics, single-molecule biophysics, statistical physics of biological systems, tissue mechanics, nonlinear dynamics in biological systems

Time: Tuesday 18:00–20:30 Location: P4

BP 17.1 Tue 18:00 P4

Effect of cilia length on the motility of confined microbes — •Tom Sosniok, Alexandros Fragkopoulos, Rodrigo Catalan, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Many microorganisms utilize their cilia or flagella to propel and navigate through their surrounding liquid environment. Often times though, the habitats of such microswimmers comprise confined spaces, and therefore, cell interactions with boundaries play an important role on their navigation. *Chlamydomonas rein-*

hardtii, a biciliated, green microalga that is commonly found in soil, typically swims in close proximity to curved boundaries [1]. We found that this near-wall swimming motility is controlled by gradients of wall curvature and steric interactions between the cilia and the surface [2]. Here we explore the effect of the cilia length on the motility and surface interactions of the cells using different *C. reinhardtii* mutant strains with different cilia lengths in quasi-2D circular confinement. We extract information about their motion from their mean squared displacements and visualize the wall-guided swimming via relative and radial probability densities. By comparing the results for the different strains we can directly analyse the influence of the cilia length on their swimming motility in confinement.

[1] T. Ostapenko, et al., *Phys. Rev. Lett.* **120**, 068002 (2018).
[2] J. Cammann et al., *Proc. Natl. Acad. Sci. U.S.A.* **118**, e2024752118 (2021).

BP 17.2 Tue 18:00 P4

Stochastic modeling of a two-component polymer engine — •Yasmin Abdelghaffar[1] and Marcus Jahnel[1,2] — [1]Cluster of Excellence Physics of Life, Technical University Dresden, Dresden, Germany — [2]Biotec, Technical University Dresden, Dresden, Germany

Long coiled-coil tethering proteins and small GTPases have recently been shown to form a new class of biomolecular motors driven by entropic collapse. The working principle of this motor is a cyclic flexibility transition of its filamentous tether, triggered by the GTPase unit. While a basic working model was proposed (Singh, 2023), many fundamental aspects of these two-component molecular motors remain unexplored. Here, we developed a stochastic model as an over-damped to-state semi-flexible polymer to describe the mechanochemical cycle that drives this motor. Using this model, we can predict how efficiency and power of this motor are affected by changes in model parameters such as persistence lengths. Additionally, by introducing force-dependent rates in the mechanochemical coupling of our model, we can potentially explain previous discrepancies in the measured hydrolysis rate of GTP between in bulk experiments, which occur under no force, and tweezer experiments, where the system is under tension. Our simulation study thus makes an indication on the chemical nature of the coiled-coil protein within the motor, identifying it as a potential GTPase-activating protein.

BP 17.3 Tue 18:00 P4

Modeling dynamics and density distribution of magnetotactic bacteria in traps — •Theo Richter, Sascha Lambert, and Stefan Klumpp — Institut für Dynamik komplexer Systeme, Universität Göttingen, Göttingen, Germany

Magnetotactic bacteria are microorganisms that navigate using internal magnetosomes, aligning them along magnetic fields. They represent an intriguing model system for studying active Brownian particle dynamics under an external alignment field. Previous studies have analyzed their movement through crowded channels, where the orientation along the magnetic field and their interaction with obstacles prove to be important mechanisms for navigation. In such complex environments, bacteria often find themselves trapped in corners, where the dynamics of how they escape these traps are crucial and remain mostly unexplored.

In this work, we aim to understand the density profiles, escape rate and general dynamics of single active Brownian particles under an alignment field inside trapping geometries. We investigate these quantities via simulations in varying trap geometries, with a focus on triangular traps, characterizing the effects of system parameters such as magnetic field strength and particle-wall interactions. We relate the behavior of the bacteria in these geometries to the sedimentation of active Brownian particles.

BP 17.4 Tue 18:00 P4

Light-switchable adhesion and clustering of *C. noctigama* at liquid-air interfaces — •Gustav Nolte, Alexandros Fragkopoulos, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Microalgae are unicellular photoactive organisms that are ubiquitous in liquid-infused natural environments. The biciliated microalga *Chlamydomonas reinhardtii* shows light-switchable adhesion and clustering at surfaces, a process so far exclusively observed for solid-liquid interfaces [1,2,3]. Here we report on the light-switchable formation of clusters by *Chlamydomonas noctigama*, a related species with increasing relevance in the field of optogenetics, at liquid-air interfaces. The morphology and dynamics of these clusters differ significantly from the clusters formed by *C. reinhardtii*. Apart from the average cluster size and polydispersity, the growth dynamics of individual clusters are studied for a wide range of cell densities. We find a critical cell density above which the number of clusters decreases over time. For the underlying principles of cluster formation and dynamics, we address potential mechanisms like preferential attachment and Ostwald ripening. Reversible clustering may provide an advantage for *C. noctigama* by allowing the cells to accumulate in locations optimal for photosynthesis while also increasing resilience to environmental stress within the cluster.

[1] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[2] R. E. Catalán, et al., *Soft Matter* **19**, 306 (2023).
[3] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).

BP 17.5 Tue 18:00 P4

The Dynamics of Spatiotemporal Self-organization in Active Turbulence — •Henri Jörn Schmidt — Max-Planck institute for self-organisation and dynamics, Göttingen, Germany

Spontaneous pattern formation in nature has been subject to extensive research in recent decades, with more and more emphasis being put on the dynamics of their creation processes.

In this work we investigate coherent structures in fluid flows. Specifically, this work concentrates on eddy currents found in the turbulent regime of active nematics. We analyse their formation and evolution as well as how their dynamics is affected by the cross-talk between different length scales. In doing so, we introduce a new methodology to record the overlaps of eluded structures in an agent-based approach. This allows for size changes in individual structures without inflicting biases in the computed intersection ratios.

Our results seem to indicate no particular cascade of different length scales. However, we do observe an universal evolution of the eddy currents, marked by a pronounced growing and shrinking phase. Usually, these stages take place within an encapsulating parent structure. Likewise, as the eddies have attained their nominal size, they give rise to new eluded structures themselves. These dynamics seem to be independent from both, the size ratio of clusters and their elapsed life time.

BP 17.6 Tue 18:00 P4

Macroscopic transports in cellular aggregates driven by dipole forces — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

The large-scale collective behavior of biological systems can be understood through macroscopic transport processes that emerge from the active interactions of individual components at the microscopic level. A striking example is the clustering and the associated transport slowdown observed in colonies of *Neisseria gonorrhoeae* bacteria, driven by active, contractile forces mediated by pili. In this study, we analytically derive the fluctuating hydrodynamics from the microscopic dynamics of a 2D model system representing an *N. gonorrhoeae* bacterial colony. The hydrodynamic current of cells involves two macroscopic transport coefficients: bulk diffusivity and conductivity, which generally depend on cell density and other microscopic parameters. Remarkably, our simulation results strongly support the analytical predictions of transport slowdown during the colony formation process. Beyond bacterial colonies, these findings offer insights into how contractile forces influence transport in other biological systems, such as tumor spheroids and neuronal organoids, and suggest experimental approaches for studying these phenomena.

BP 17.7 Tue 18:00 P4

Dynamics, stresses and cell fate in confluent cell monolayers — •Stefano Villa[1,2], Giorgio Scita[3], Roberto Cerbino[4], and Fabio Giavazzi[2] — [1]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — [2]Universitá degli Studi di Milano, 20090 Segrate — [3]IFOM-FIRC Institute of Molecular Oncology, 20139 Milan — [4]University of Vienna, 1090 Vienna

Confluent cell monolayers are 2D active systems exhibiting a variety of dynamical states, ranging from solid-like jammed systems to fluid-like flocking systems. Such a rich panorama results in different mechanical stresses the single cells within the monolayer are subjected to. Due to their impressive complexity, cells do not merely react to the mechanical stresses but actively interact with the environment, e.g. adapting their mechanical properties to the stimuli. The investigation of the close interplay between dynamical state and mechanical properties of tissues is therefore of paramount interest for unraveling how cells respond to mechano-physical stimuli. We present a detailed analysis based on cell segmentation performed on time-lapse microscopy videos showing the effect of motility-induced stresses on the single cell mechanics, comparing cell models mimicking healthy tissues and tumor-like tissues. We show how the increase in dynamics leads to larger cell deformations to which the cells respond by increasing the stiffness of the nucleus. Finally, we show how mechanical stresses within the monolayer can affect tissue morphogenesis in real systems, thus highlighting once again the relevance of mechano-physical stimuli for the cell and tissue development and fate.

BP 17.8 Tue 18:00 P4

Analysis of Wall-Torques for Rod-Shaped Active Particles — •Merle Duchêne, Sascha Lambert, and Stefan Klumpp — University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The motility of living things and synthetic self-propelled objects is often described using Active Brownian particle models. To account for interactions with complex environments, this model can be expanded with empirical forces or torques, such as those describing their alignment with an obstacle or wall after

a collision. Here, we evaluate the quality of these empirical models by comparing their output predictions with trajectories of rigid rod-shaped active particles that scatter sterically at a flat wall. Specifically, we analyze the torque reorienting the rod-shaped particle and compare it to predictions from a phenomenological model. We employ a classical least-squares method to evaluate the instantaneous torque and identify essential model parameters. In addition, a Bayesian inference procedure can be applied to construct the posterior distribution of plausible model parameters which provides a complementary perspective to the least-squares analysis.

BP 17.9 Tue 18:00 P4

Onset of bioconvection in a simple continuum model — •Marius M. Kaiser, Fabián Álvarez-Garrido, and Michael Wilczek — Universität Bayreuth

Dense suspensions of swimming micro-organisms show bioconvection, i.e.~the emergence of self-organized flow patterns much larger than the individual swimmers, under certain conditions. Here, we analyze the onset of bioconvection in a simple continuum model. The model is derived from the Fokker-Planck equation for the swimmer concentration field and the swimmer orientation field [Pedley, J. Fluid. Mech. 647, 335 (2010)] coupled to the Navier-Stokes equation, in which we only consider buoyancy effects (no cell stresses) and approximate higher-order moments in terms of the polar order parameter. A linear stability analysis in the idealized case of a prescribed polar orientation field shows that the system exhibits a type-II instability. The results of our linear stability analysis are in agreement with direct numerical simulations of our model. Simulations of the model, now with dynamically evolving polar orientation field, suggest that the type of spatial instability remains the same, albeit with shifted critical values. Our findings shed light on the mechanism driving pattern formation in this type of suspensions.

BP 17.10 Tue 18:00 P4

DNA origami laden with bespoke magnetic nanocubes: A route to programmable torques at the nanoscale — Florian Rothfischer[1], Yihao Wang[2], Lennart Weiss[1], Christopher Pauer[3], Kevin Lang[3], Susanne Kempter[3], Rabia Amin[2], Elena Eiwanger[3], Jan Lipfert[4], Tim Liedl[3], Friedrich C Simmel[1], Joe Tavacoli[3], and •Aidin Lak[2] — [1]Physics Department E14, Technical University Munich — [2]Institute for Electrical Measurement Science and Fundamental Electrical Engineering and Laboratory for Emerging Nanometrology (LENA), TU Braunschweig — [3]Faculty of Physics and Center for NanoScience, LMU Munich — [4]Institute for Physics, Augsburg University

Magnetic-field responsive actuators offer minimally-invasive and deep-tissue perturbation of cellular processes. Despite progress, the magnetic manipulation of cells at the single receptor level is still challenging; magnetic nanoparticles (MNPs) can only exert ~ fN forces. To achieve biologically relevant pN forces, it is necessary to assemble MNPs together in a controllable manner. This has not yet been achieved utilizing soft-synthetic templates, where control over the number, and orientation of MNPs remains a challenge. DNA origami (DNAO) can overcome this limit, specifically so for its capacity to arrange nanoparticles at high spatial resolution. Here, we demonstrate assembly of bespoke MNPs on 6 helix-bundle DNAO and show the controlled magnetic rotation of magnetic DNAOs under circulating magnetic fields of 8 mT. Our magnetic DNAOs are promising torque nanoprobes for activation of sub-cellular processes at high resolution.

BP 17.11 Tue 18:00 P4

Engineering Shear-Thinning Hydrogels: A Dynamic Scaffold for 3D Tissue Culture — •Bruno Schmelz[1], Fen Li[2], Kai Zhang[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Germany — [2]Sustainable Materials and Chemistry, Department of Wood Technology and Wood-based Composites, University of Göttingen, Germany

Extracellular matrix (ECM) scaffolds are essential for advanced 3D cell culture systems, providing structures for cell movement as well as physical and chemical cues that promote migration, proliferation, and differentiation. Hence, the ECM is crucial for functional tissue formation. However, natural ECM materials used in vitro, such as collagen and elastin, are difficult to control regarding elastic properties, polymer mesh size, and homogeneity. Our objective is to design a dynamic hydrogel tailored to meet the specific requirements of 3D tissue culture, such as viscoelastic properties and cell-binding sites, that initially supports tissue formation but can be dissolved and replaced by cell-generated ECM. We propose a hydrogel with non-covalent cross-linking moieties that allow for reorganization by embedded cells, similar to the reorganization of collagen fibers in physiological tissues. We present the rheological properties of the hydrogels and the initial findings of cell invasion into them. When subjected to stress, the hydrogels exhibit a transition to a more liquid-like state, with the potential to solidify again upon stress relaxation. This behavior allows cells to remodel their surrounding matrix and shape their environment, as evidenced by experiments with cells cultured on the hydrogels.

BP 17.12 Tue 18:00 P4

Supramolecular ordering in lipopolymer monolayers at the air/water interface — •Issam Assi, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald

Lipopolymers with covalently bound poly(ethylene oxide) (EO_N) bound to the head groups have been introduced to stabilize bilayer membranes. Langmuir monolayers of the lipopolymer DSPE-EO_N at the air/water interface show in the isotherm a transition from the liquid expanded to the liquid condensed phase, which is confirmed by in-situ Grazing Incidence X-ray Diffraction (GID at DESY, Hamburg). A laterally inhomogeneous film of condensed ordered alkyl chains embedded in a matrix of solvated polymers is formed. Small Angle GID shows these lipid domains are ordered in a hexagonal lattice (repeat distance about 12 nm). The films stay homogeneous on the micrometer scale as observed with Brewster Angle Microscopy. On transferred monolayers, these supramolecular phases were observed with AFM. Fast compression of DSPE-EO_{44} monolayers is necessary to maintain the hexagonal superstructure at relatively high lateral pressures, whereas slow compression induces a lamellar structure. Also, the superstructure of lipopolymers with shorter polymers (DSPE-EO_{11} and DSPE-EO_{22}) was explored.

BP 17.13 Tue 18:00 P4

Nanoscale drug delivery system aggregates controlably on graphite — •Henrik Siboni[1,2], Leonhard Grill[2], and Andreas Zimmer[1] — [1]Pharmaceutical Technology & Biopharmacy, University of Graz, Austria — [2]Single Molecule Chemistry, University of Graz, Austria

Nanoscale drug delivery systems are nanoparticles used to enhance the efficacy of drugs and their effectiveness depends on physical properties such as size, shape and aggregation behaviour. These parameters can be measured on a substrate with atomic force microscopy, but conserving the individual nanoparticles has proven challenging. In this study, we show that the substrate highly-oriented pyrolytic graphite allows for controllable imaging of single as well as aggregated protamine-oligonucleotide drug delivery systems. This approach can potentially be used to screen drug delivery systems and avoid unnecessary in vivo test.

BP 17.14 Tue 18:00 P4

Printed biometamaterials for mechanical regulation of cells — •Clara Schaefer[1], Alexander Berkes[2], Martin Wegener[2], Natalie Munding[1], and Motomu Tanaka[1,3] — [1]Institute of Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [2]Institute of Applied Physics, KIT, 76131 Karlsruhe, Gemany — [3]Kyoto University, Kyoto 606-8501, Japan

Ample evidence has shown that cells detect and respond to the mechanical properties of their microenvironment. Materials with non-conventional mechanical properties (mechanical metamaterials) have shown significant effects on human mesenchymal stem cells (Munding, et al. Adv. Funct. Mater. 2024). The key requirements are to make the unit cell size smaller than the cells and to make the materials deformable by cell traction forces. The anisotropic elastic properties lead to different responses in the traction force field that are distinct from those to bulk materials. To deal with multicellular systems and to follow cell migration, one of the challenges is to increase the lateral size to several hundreds of μm. To achieve this goal, we increased the printing speed by using a new multi-focus device in two-photon laser printing. This enables to fabricate even asymmetric metamaterial structures that can potentially be used to induce cell polarization.

BP 17.15 Tue 18:00 P4

Subcellular distribution of green-emitting carbon nanodots — •Mariell Gassen, Mine Polat, Carla Sprengel, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Carbon nanodots are promising fluorescent nanoparticles for biomedical imaging applications and drug delivery. They frequently show fluorescence in the blue range, which causes interference with the autofluorescence of the cell [1]. To circumvent this, we produced green-emitting carbon nanodots and incubated them in cells. We report tests about their subcellular distribution and studies of their suitability as carriers for active substances.

[1] S. Fasbender et al. The Low Toxicity of Graphene Quantum Dots is Reflected by Marginal Gene Expression Changes of Primary Human Hematopoietic Stem Cells. Sci Rep 9, 12028 (2019).

BP 17.16 Tue 18:00 P4

Red Blood Cells under brightfield microscopy — •Aaron Kreis, Sarah Tabea Hermes, Thomas John, and Christian Wagner — Experimental Physics, University Saarland

The observation of red blood cells under a conventional light microscope is a common practice in research and medicine. In many cases, the particular cell shape is the object of interest, see [1]. Red blood cells are composed mostly of hemoglobin, which shows its maximum absorption at ~ 420 nm. Nevertheless, the cells are mostly observed under white or red light. Furthermore, the refractive index of the cytosol is greater than that of water and refraction occurs. The combination of refraction and absorption leads to very different microscopy images at different focal points. We have quantified this using calculations by ray

tracing and we can explain the observed microscopy images, including the white 'halos' due to refraction at various focal positions. Diffraction isn't a major contribution in observed cell shapes. We demonstrate that the use of blue light results in a significantly better image contrast of the cell shapes without artifacts, compared to the usual observation with white light.

[1] Yoon at. al., Flickering Analysis of Erythrocyte Mechanical Properties, Biophysical Journal 97, 1606, (2009)

BP 17.17 Tue 18:00 P4

High-resolution chemical characterization of retinal pigment epithelium (RPE) using mid-infrared photo-induced force microscopy — •Maryam Ali[1,2], Robin Schneider[1], Patrick Then[1], Mohammad Soltaninezhad[1,2], Sebastian Unger[1,2], Christoph Krafft[1,2], Christine A. Curcio[3], Rainer Heintzmann[1,2], Thomas Ach[4], and Daniela Täuber[1,2] — [1]Leibniz Institute of Photonic Technology, Jena, Germany — [2]Friedrich Schiller University, Jena, Germany — [3]University of Alabama at Birmingham, United States — [4]University Hospital Bonn, Germany

Nanoscale infrared (IR) spectroscopic imaging methods fill a gap in bioimaging. Mid-IR photo-induced force microscopy (PiF-IR) combines powerful IR illumination with non-contact atomic force microscopy, resulting in high spectral and unprecedented spatial resolution (< 5 nm)[1]. We applied PiF-IR to a cross-section of the retinal pigment epithelium (RPE) layer of a human donor eye. The strongly polar RPE cells play a major role in the vision cycle. Several types of autofluorescent granules in RPE cells[2] contribute to fundus autofluorescence, a clinical imaging technique used for the diagnosis of retinal diseases. In spite of their importance, the chemical composition of these organelles is not fully known. A combined chemometrics analysis of three PiF-IR hyperspectra from locations across the RPE layer reveals variations in the protein content of the surfaces of granular organelles. –[1] J. Joseph et al., Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2024, 306, 123612. [2] K. Bermond et al., IOVS 2020, 61, 35.

BP 17.18 Tue 18:00 P4

Preparation of green fluorescent carbon nanoparticles — •Mine Polat, Carla Sprengel, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Carbon nanodots (CNDs) are promising materials for biomedical applications due to their unique fluorescent properties and biocompatible structure. However, many CNDs emit in the blue range, which is less favorable for specific applications. In this project, green-emitting CNDs were synthesized, their optical properties were analyzed, and the quantum yield was calculated. The results of absorption and emission spectra are presented.

BP 17.19 Tue 18:00 P4

Real-time monitoring of fluctuations in ATP levels and mechanobiological signatures in living cells — •Albina Nizamieva and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Living cells are genuine non-equilibrium systems with a typical energy turnover of roughly 10^8 times thermal energy in every second. This translates to about 10^7 ATP hydrolysis events per second, with which cells may fuel, for example, signaling cascades and/or contractions of the actomyosin cytoskeleton to probe and migrate on the substrate underneath. Here we have used fluorescent reporter molecules to quantify in living cells (1) the temporally fluctuating ATP levels, and (2) fluctuations of a key mechanosensory protein that connects cellular mechanics and signaling cascades. Our data reveal marked fluctuations on the scale of minutes and beyond, whereas short-term fluctuations appear to only report on fundamental and ubiquitous physico-chemical fluctuations that are rooted, for example, in the dyes' photophysics and diffusional motion.

BP 17.20 Tue 18:00 P4

Microscopic observation of red blood cell band patterns formed by centrifugation — •Luca Hastenteufel, Thomas John, Felix Maurer, and Christian Wagner — Experimental Physics, Saarland University

Percoll is a common medium composed of coated silica particles. It is widely used as the standard medium for the density separation of cells or subcellular compounds. The centrifugation of red blood cells in Percoll exhibits a heterogeneous structure characterized by discrete bands, however the density gradient is continuous. These band patterns have primarily been analysed using macroscopic images, such as photographs. We developed a microscopic scanning setup to examine these patterns in detail, from single cell level in μm-range up to the full pattern structure at 6 cm. This provides higher-resolution insights compared to traditional imaging methods. Additionally, high dynamic range (HDR) methods using multiple exposure levels lead to a more detailed pattern observation. Understanding these band patterns offers valuable information about red blood cell aggregation energy and the severity of related diseases.

BP 17.21 Tue 18:00 P4

Accessing local aggregation in phalloidin-stained Actin filaments using 2D Polarization Fluorescence Imaging — •Shangjun Cheng[1,2,3], Yutong Wang[1,2], Yunhao Mei[1,2], Hossein Zarei Oshtolagh[1,2], Lukas Spantzel[1,3], Patrick Then[1,4], Hans-Dieter Arndt[1], Adrian T. Press[1,3], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital — [4]Microverse Imaging Center, Jena, Germany

2-dimensional polarization-resolved fluorescence imaging (2DPOLIM) can discriminate between aggregated and non-aggregated protein forms independent of the sample's alignment by providing access to the full in-plane polarization properties of the sample. In combination with a semi-quantitative analysis of Förster Resonance Energy Transfer between similar fluorophores (homo-FRET) it can map the local aggregation in cells and tissue [1]. Actin assembly and disassembly is essential for cellular dynamics. A previous study has shown the direct link between infection and aggregation of F-Actin in hepatocytes [2]. Here, we present our speeded-up home-built 2DPOLIM setup [3] along with its calibration and image registration protocols allowing for an acquisition time in the range of a second. First results from application to the investigation of phalloidin-stained Actin filaments are presented. – [1] R. Camacho, et al., Advanced Materials, 31, 1805671, 2019. [2] P. Martinac, et al., Infection, 47, S6-S7, 2019. [3] Y. Wang, et al., Klosters, Switzerland, January 2023. doi:10.13140/RG.2.2.35169.79204

BP 17.22 Tue 18:00 P4

Liquid-cell Scanning Transmission Electron Microscopy (STEM) of isolated mitochondria and respective Au labels — •Eric Lieberwirth[1], Kevin Oldenburg[2], Anja Schaeper[3], Marcus Frank[4], Ingo Barke[1], Simone Baltrusch[3], and Sylvia Speller[1] — [1]Institute of Physics & LLM, University of Rostock — [2]ELMI-MV, University of Rostock — [3]Institute of Medical Biochemistry and Molecular Biology, Rostock University Medical Center — [4]Electron Microscopy Center, Rostock University Medical Center

In situ liquid-cell Scanning Transmission Electron Microscopy (STEM) holds the promise to observe biological organisms in a native state such as organelles, bacteria and eukaryotic cells [1,2]. In addition to acquisition of individual images, movies can be recorded during manipulation of tissue [3]. The potential radiation damage due to the transit of the electron beam through the sample is still under debate [4]. We imaged isolated mitochondria in Krebs-Ringer medium, and extracted imaging performance, and external features of radiation damage. We also study Au labels in the physiologic medium and show that atomic resolution of the nanoparticles is attainable. Such labelling is expected to increase resolution [1] and validate the presence of mitochondria in the STEM. One of the next challenges is validating the metabolic activity of the mitochondria during or upon the (S)TEM measurement.

[1] Kun He et al. (2019) J. Phys.: Condens. Matter 31 103001
[2] Frances M. Ross (2024) Micro. Tod. 32 17-22
[3] Elliot S. Pohlmann et al. (2015) Nano Lett. 15 2329-2335
[4] Yulian Wu et al. (2019) New J. Chem. 43 12548

BP 17.23 Tue 18:00 P4

Three-Axis Structured Illumination Lightsheet Microscopy — •Meelad Lalenejad and Alexander Rohrbach — University of Freiburg, Freiburg, Germany

Light-sheet microscopy (LSM) is known for increased image contrast and reduced photo-bleaching and toxicity since only those parts of the object are illuminated from the side that is in the focus of the objective lens. In addition, larger volumes are scanned plane-wise or line-wise by optimized laser beams, so LSM is significantly faster than point-wise scanning methods. However, for imaging a small number of cells, the spatial resolution is limited by the numerical aperture of the objective lens. We tackle the problem of limited resolution by combining holographically shaped illumination beams with three-axis interferometric arrangements. We use structured illumination microscopy (SIM) to obtain 3D super-resolved images in scattering media by generating interference fringes between every two beams from different illumination objective lenses.

BP 17.24 Tue 18:00 P4

Investigating Neutrophil dynamics using 200 Hz Rotating Coherent Scattering Microscopy — •Vera Obloh and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Neutrophils, the largest population of leukocytes in the human bloodstream, are initial responders in the rapid innate immune defense against most bacterial and fungal pathogens. They are activated before the complex humoral and lymphocyte-mediated processes of acquired immunity can effectively respond to an infection. To ensure effective defense, Neutrophils rapidly and efficiently move to areas of infection, based on highly dynamic processes of cytoskeleton reorganisation. Due to their ability to migrate rapidly and their availability and ease of cultivation, HL-60 Neutrophils are well suited for observations with Rotating Coherent Scattering (ROCS) microscopy, a novel 200 Hz label-free imaging technique with resolutions well below 200 nm. ROCS represents a powerful,

high-speed alternative to fluorescence microscopy, especially for observations over thousands of frames. We represent first images and analyses of so far unseen details and dynamics of Neutrophil migration.

BP 17.25 Tue 18:00 P4

Characterisation of fluorescent dyes and their uptake by M2 cells using FLIM — •Jana Sütterlin[1], Francisco Páez-Larios[1,2], Lukas Harder[1], Lea Klepsch[3,4], Vivien Bachmann[5], Antje Vollrath[3,4], Paul Jordan[5], Ulrich Schubert[3,4], Oliver Werz[5], Christian Franke[1], and Christian Eggeling[1,2] — [1]Institute for Applied Optics and Biophoysics, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [2]Department of Biophysical Imaging, Leibniz-Institut für photonische Technologien e.V., Jena, Deutschland — [3]Jena Center for Soft Matter, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [4]Institute for Organic and Macromolecular Chemistry, Friedrich-Schiller-Universität Jena, Jena, Deutschland — [5]Department of Pharmaceutical and Medical Chemistry, Friedrich-Schiller-Universität Jena, Jena, Deutschland

Polymeric nanocarriers are used to incorporate active substances into cells, that otherwise would have limited bioavailability. To study the particle-cell-interaction, the nano-particles contain a fluorescent dye, which allows monitoring by fluorescence microscopy. Since a dye's fluorescence lifetime depends on its environment, the dye's release from the nanoparticle into the cellular cytosol can be evaluated temporally and spatially by fluorescence-lifetime-imaging (FLIM). To that end, lifetime behaviour of Nile Red, ATTO 665 and ATTO Rhodamine 3B is characterised under different solvent conditions mimicking different cellular compartments. By this, a comparison with FLIM data of live cell uptakes is possible, which can yield insights into the dynamic interaction of drug-loaded nanoparticles and their target cell.

BP 17.26 Tue 18:00 P4

MINFLUX-derived particle traces reveal Mean Back Relaxation to study active systems — •Deisel Tobias, Muenker Till, Vos Bart, and Betz Timo — Third Institute of Physics, Georg-August Universität Göttingen, Göttingen, Germany

Living systems like cells exhibit dynamics far from thermodynamic equilibrium. In order to study such non-equilibrium systems, we need to use analytical methods beyond the classical methods developed in statistical physics. In order to quantify the activity in a living, we have recently introduced the Mean Back Relaxation (MBR), which exploits a three-point probability function and is solely derived from passive measurements. A main hurdle in using the MBR in the requirement of particle trajectories with high temporal and spatial precision, that are sufficiently long to detect activity. In normal flourescence microscopy this is not possible to achieve because of probe bleaching. To overcome this, we measure the MBR using MINFLUX nanoscopy, which is able to track fluorescent particles at a spatio-temporal resolution in the order of nanometers at a frequency in the order of a few kHz. We explore the MBR of fluorescent particles in living cells and study its change under the influence of cytoskeletal inhibition.

BP 17.27 Tue 18:00 P4

Thermal and directional motion of trapped particles in periodic potentials — •Ellen Hermle and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Molecular fiction can be considered as continuous on-binding and off-binding of molecules between two sliding surfaces. This complex process of energy dissipation to the environment, is important on most length scales, time scales and across disciplines. Usually, the relation between dynamic friction and velocity is quantified by a coefficient, which depends on various on- and off-binding parameters. Here, optical tweezers based Photonic Force Microscopy (PFM) has proven to be a suitable technique is used to analyse friction processes on mesoscopic length scales, specially at soft (-bio) interfaces. By 3D interferometric position tracking at 1 MHz we determine mean particle displacements and forces, as well as fluctuations of displacements and forces. Besides Brownian dynamic simulations, we present first experimental results of fluctuating particles dragged through a periodic potential, which can be generated by an optical potential from two interfering beams or by a specifically coated glass surface.

BP 17.28 Tue 18:00 P4

Investigating Ultrasonic Effects on Oral Cancer Cells Using Fluorescence Microscopy — •Wafa Tounsi, Amar Avdakovic, Vivian Maria Gulczynski, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Head and neck squamous cell carcinoma (HNSCC) is a challenging and often resilient cancer that affects many people globally. As conventional treatments sometimes fall short of effectively targeting these cancer cells without causing damage to surrounding healthy tissue, our research focuses on finding innovative alternatives. Our contribution explores the potential of using ultrasonic frequencies to selectively affect cancer cells while sparing healthy ones, offering a possible new avenue for treatment. In this study, we investigate how HNSCC cells respond to ultrasonic waves at frequencies between 20 and 250 kHz. We compare their reactions to benign oral keratinocytes, aiming to pinpoint acoustic conditions that might selectively disrupt cancer cells. In combination with Fluorescence Microscopy, we track various cellular responses, including changes in cell shape, membrane stability, and mitochondrial activity, using specific fluorochromes such as CellMask Green for plasma membranes, Hoechst for nuclear staining, and MitoTracker for mitochondria. By observing these differences, especially in the cytoskeleton, we gain valuable insights into the unique vulnerabilities of HNSCC cells, potentially paving the way for ultrasound-based, non-invasive treatments. Exploiting the distinct mechanical properties of cancer cells could enhance patient outcomes by enabling safer, more targeted treatments.

BP 17.29 Tue 18:00 P4

A flavin-based photoreceptor controls the photoactivation of ciliary adhesion in *Chlamydomonas*. — •Rodrigo E. Catalan[1,2], Antoine Girot[1,2], Alexandros Fragkopoulos[1,2], Olga Baidukova[3], Peter Hegemann[3], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [3]Humboldt University of Berlin, Institute of Biology, 10115 Berlin, Germany.

Light-activated proteins or photoreceptors play a crucial role on the behavior and, ultimately, the survival of photoactive microorganisms. The unicellular biciliated microalga *Chlamydomonas reinhardtii* has become a model organism to study light-mediated phenotypes, such as photosynthesis and phototaxis, among many others. Recently, we discovered that *C. reinhardtii* can reversibly switch on and off the adhesiveness of their cilia in blue and red light, respectively [1,2]. We characterized the action spectrum of this phenotype in wild-type (WT) *C. reinhardtii* cells via single-cell micropipette force measurements, and showed that it resembles the spectral sensitivity of a flavin-based photoreceptor. Further comparison of the ciliary adhesion forces between WT and photoreceptor-targeted mutants reveals that the deletion of two flavin-containing photoreceptors, namely animal- and plant cryptochromes, completely disrupts light-switchable adhesion.

[1] C. T. Kreis *et al.*, *Nat. Phys.* **14**, 45-49 (2018).
[2] R. E. Catalan *et al.*, *Soft Matter* **19**, 306-314 (2023).

BP 17.30 Tue 18:00 P4

Ciliary Adhesion of *Chlamydomonas reinhardtii* on Charge-Functionalized Surfaces — •Lea Rupprecht[1], Rodrigo Catalan[1], Christina Heinritz[2], Thomas Scheibel[2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Biomaterials, 95447 Bayreuth, Germany

Elucidating the physical phenomena underlying the interactions between microorganisms and surfaces is crucial for developing technologies to control the formation of microbial biofilms. While most studies use bacteria as model organisms, the principles of microbial adhesion remain rather elusive for eukaryotic photosynthetic microorganisms. Recently it was discovered that the model unicellular microalga *Chlamydomonas reinhardtii* adheres to surfaces by means of its two cilia under blue light [Kreis *et al.*, Nature Physics, 2018]. With *in vivo* single-cell micropipette force spectroscopy, the ciliary adhesion forces of *C. reinhardtii* on functionalized substrates were characterized to dissect the influence of surface energy, van der Waals and electrostatic interactions [Kreis *et al.*, Soft Matter, 2019]. The results suggest that the predominant nature of the protein-mediated cilia-substrate adhesion of *C. reinhardtii* is due to electrostatic interactions. Here we present adhesion force measurements of *C. reinhardtii* on poly-L-lysine- and recombinant spider silk-coated silicon, revealing no charge preference for ciliary adhesion. In contrast to prokaryotic microorganisms, our results show *C. reinhardtii* uses highly versatile cilia to achieve microbial adhesion to surfaces of a broad range of physicochemical properties.

BP 17.31 Tue 18:00 P4

Intracellular mechanics in migrating cells — •Jannis Fischer, Mohammad Amin Eskandari, and Timo Betz — Third Institute of Physics, Göttingen, Germany

To fulfill their incredibly large number of different tasks, biological cells have developed mechanisms to adapt their physical properties and appearance. The proper control of these changes is crucial, as they are not only essential for healthy cells, but can also distinguish healthy from diseased cells. Important examples related to such changes in mechanical properties are cell shape variation or cell migration. It is still not clear whether the changes in these mechanical properties are due to passive or active processes. Investigating and understanding these processes is the core of this work. For this, I will analyze the behavior of migrating cells, which are induced to move alternately on patterns and within channels. To connect the observed dynamics with the underlying mechanical properties and activities I will use the new quantity of mean back relaxation (MBR). Findings in this area could provide information for the big question of whether the mechanical properties of cells can be predicted by their activity.

BP 17.32 Tue 18:00 P4

Same, but different: Shared viscoelastic signature in hydrogels and cells — •Dorian Marx, Till M. Münker, Bart E. Vos, and Timo Betz — Third Institute of Physics - Biophysics, Georg-August-Universität Göttingen, Germany

We report the discovery of a striking "mechanical fixed point" in the response of polyacrylamide-based hydrogels to shear strain. Characterized by a pronounced and invariant relationship of parameters of the mechanical model, this leads to a convergence of the complex shear moduli of all measurements at a frequency of approximately 5 kHz. Intriguingly, reviewing existing literature reveals that this phenomenon is not unique to our simple hydrogel. Rather, there are many qualitatively similar observations in the distinct realm of (intra-)cellular mechanics, as probed by diverse techniques including optical tweezers and atomic force microscopy using many different cell types. Despite the fundamentally different natures of these systems - one being passive and at equilibrium (hydrogel), the other active and out-of-equilibrium (cell) - they show this peculiar viscoelastic signature. The existence of the mechanical fixed point hints at an unresolved constraint governing the mechanics across vastly different biological and synthetic systems.

BP 17.33 Tue 18:00 P4

: Identifying the proteins controlling the intracellular active mechanics — •Noémie Veyret, Till Münker, and Timo Betz — Third institute of Physics, University of Göttingen, Germany

Over the past few years, the study of cell mechanical properties has allowed new insights on the understanding of biological processes and life complexity. According to previous work, intracellular mechanical properties can be narrowed down to a fingerprinting of only 6 parameters. Through the use of active and passive microrheology measurements via optical tweezers, frequency dependent viscoelastic properties and intracellular activity were found to vary for different cell types. The aim of this project is to find a correlation between changes in protein expressions and mechanical fingerprint of cells. To do so optical tweezers measurements will be performed during the differentiation process of induced Pluripotent Stem Cells (iPSCs) into cell types derived from the three germ layers, namely neurons (ectoderm), skeletal muscles (mesoderm) and hepatocytes (endoderm). This measurement allows the characterization of the mechanics during the iPSC differentiation process. In parallel, the cell proteome will be studied using mass spectroscopy. Combining both, we hope to find the connection between proteins and their mechanical role, the intracellular "mechanome".

BP 17.34 Tue 18:00 P4

Investigating the rheology of intracellular transport by magnetic tweezers — •Katharina Beitzinger, Simon Wieland, and Holger Kress — Biological Physics, University of Bayreuth, Germany

Intracellular transport is an important part of phagocytosis, the cellular internalization of extracellular objects such as bacteria or microplastic particles. After uptake, the phagosome is transported mainly by dyneins along microtubules to the perinuclear region as part of the phagosomal maturation process. However, the kinetics of the recruitment of the motors to the phagosome is largely unknown. In order to investigate the mechanics of the transport, we use magnetic tweezers in combination with paramagnetic particles, internalized by mouse macrophages. By switching the tweezers on and off periodically, we exert alternating forces on the particle during the transport. The changes in the local viscoelastic cell properties are determined by modeling the creep compliance with a power law. First experiments show that the viscosity of the cells around the phagosomes remains almost constant, while the stiffness increases over time. The change in stiffness can be an indicator for a progressive adaption of the cell towards external stress by a recruitment of molecular motors to the phagosome. We expect that a quantification of the local viscoelastic cell properties during phagosomal transport can lead to a better understanding of this fundamental cellular process.

BP 17.35 Tue 18:00 P4

Optimizing Microfluidic Synthesis of Polymer Beads for In-Vivo Force Cell Sensing — •Jordan Dieter Groh, Alejandro Jurado Jiménez, and Timo Betz — Drittes Physikalisches Institut, Göttingen, Deutschland

Since the first use of deformable beads inside living tissue as force sensors about ten years ago, the technique has been refined with the introduction of new materials and methods to measure deformation. In many experiments, polyacrylamide beads have been used to assess forces in all kinds of in-vivo and in-vitro systems such as developing embryos, cancer spheroids, or reconstituted muscle tissue. However, using shear-induced emulsions as a fabrication method still shows two main limitations: a broad size distribution and small variations in polymer stiffness. We were able to optimize the production of polyacrylamide beads in two ways. First, by adoption of flow-focusing in a microfluidic setup. This technique is commonly employed in diverse fields, including drug delivery and food industry, for creating emulsions with precise control over droplet sizes. Second, by the use of a UV light-sensitive polymerization initiator that was triggered after the emulsion was created. The UV initiation of polymerization is instrumental in avoiding clogging of the microfluidic chips as polymerization happens only after emulsification. These improvements resulted in large beads with diameters of 93 um, which are still too large for many applications. Current approaches aim to reduce the bead size to around 5 um or even below.

BP 17.36 Tue 18:00 P4

Characterizing diffusion properties at liquid-liquid interfaces in microfluidic channels — •Eric Schneider, Eric Sündermann, Bob Fregin, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

Real-time deformability cytometry is a powerful and widely used method for investigating the mechanical properties of cells in suspension. Here, cells are deformed by hydrodynamic stress in a microfluidic system, that is comparable in size to the cells. Consequently, the range of cell sizes has to match the physical channel dimensions to ensure proper cell deformation. Virtual fluidic channels (VFCs) address this limitation, by allowing for the channel width to be adjusted within seconds. VFCs are formed by the liquid-liquid interface between two co-moving aqueous polymer solutions. The introduction of these two different polymer solutions generates a density gradient within the microfluidic channel, which can give rise to diffusive processes. We investigated the diffusive properties within VFCs and the influence of the liquid-liquid interface. For this, we examined the temporal behavior of a fluorescent dye distribution within the microfluidic chip. We modelled the diffusive behavior self-consistently by solving the kinetic diffusion equation, which accounts for the differential flow velocities within the microfluidic channel. Finally, by combining theoretical and experimental results, we determine the characteristic diffusion timescales in the VFC and across the liquid-liquid interface. With this we provide a general framework to investigate the diffusive properties along laminar flow boundaries.

BP 17.37 Tue 18:00 P4

A fast and quantitative method to study the membrane tension of suspended cells — •Eric Sündermann, Bob Fregin, Doreen Biedenweg, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

The development of high-throughput methods for cell mechanical research is becoming increasingly important as the analysis of large samples improves the statistical robustness to identify rare cell populations and transfer results from basic science into clinical applications. Various techniques are available for bulk mechanics, but none can analyse membrane tension with the throughput of a flow cytometer.

Here, we present membrane tension cytometry (MTC), that uses Flipper-TR, a fluorescent dye with a fluorescence lifetime being proportional to the tension inside a lipid bilayer. First, we established a calibration procedure using osmotically-stressed red blood cells. Next, we move to HL60 cells, a myeloid precursor cell line, which we exposed to various chemical and mechanical stresses. We find an increased fluorescence lifetime for increasing hydrodynamic stresses, as expected. Finally, we used methyl-β-cyclodextrin and Cytochalasin D to disturb cholesterol and filamentous actin levels, respectively. Our results show, that MTC is sensitive to membrane changes while being insensitive to cytoskeletal alterations.

BP 17.38 Tue 18:00 P4

Thermomechanical properties of bat erythrocytes as a blueprint for human hibernation — •Bob Fregin[1,2], Doreen Biedenweg[1], Oliver Otto[1,2], and Gerald Kerth[3] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]German Center for Cardiovascular Research, Partner Site Greifswald, Greifswald, Germany — [3]Applied Zoology and Nature Conservation, Zoological Institute and Museum, University of Greifswald, Greifswald, Germany

The ability to sustain efficient blood circulation at low body temperatures is a critical adaptation in hibernating mammals. Here, the mechanical properties of red blood cells (RBCs) could play a crucial role, which we studied for the hibernating common noctule bat, the non-hibernating Egyptian fruit bat, and humans. Using dynamic real-time deformability cytometry RBC elasticity and viscosity were measured at physiologically-relevant time scales (Milliseconds) and temperatures (37°C, 23°C, and 10°C).

Our findings reveal a temperature-driven increase in elasticity and viscosity, which is mainly influenced by membrane properties and not the cytosol. This effect is significantly enhanced in bats. Finally, our data demonstrate that RBC membranes of both bat species display a transition to a viscous-like state at lower temperatures, which is not explained by seasonal variations of environmental factors but seems to originate from physical properties of the cell membrane. Our results suggest RBC thermomechanical properties as a target for future research on human hibernation.

BP 17.39 Tue 18:00 P4

Passively Measuring Cell Activity via Mean Back Relaxation — •Sarah Louisa Lädke[1], Till Moritz Münker[1], Julian Schulz[1], Gabriel Knotz[2], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg-August-Universität Göttingen — [2]Institute of Theoretical Physics, Georg-August-Universität Göttingen

While many statistical methods are available for the characterization of passive motion in thermodynamic equilibrium, the investigation of active motion in liv-

ing systems remains a significant challenge. In particular, the study of intracellular mechanical properties requires techniques such as active microrheology to quantify the response of tracer particles to forces exerted via optical or magnetic tweezers. However, these methods often involve expensive and complex equipment, and their invasive nature can alter cellular behavior.

To address these limitations, we present an alternative approach to study intracellular mechanical properties and activity that relies only on passive measurements. To this end, we combine darkfield microscopy, highspeed imaging and image post-processing techniques to obtain trajectories of microparticles in Hela cells with nanometer and 300 microseconds spatial and temporal resolution. To filter noise that occurs in our particle tracking, we developed a new, Bayesian approach that can reliably differentiate between noise peaks and intrinsic fluctuations found in the frequency spectrum. Using the novel observable Mean Back Relaxation (MBR), we can link the particle tracks to intracellular activity and their mechanical properties.

BP 17.40 Tue 18:00 P4

Competition between deformation and free volume quantified by 3D image analysis of red blood cell — •Pavlik Lettinga[1,2], Mehrnaz Babaki[1,2], Dmitry Fedosov[1], Amirezza Gholivand[1], Remco Tuinier[3], and Joeri Opdam[3] — [1]Forschungszentrum Jülich — [2]KU Leuven — [3]TU Eindhoven

Cells in living organisms are subjected to mechanical strains caused by external forces like overcrowding, resulting in strong deformations that affect cell function. We study the interplay between deformation and crowding of red blood cells (RBCs) in dispersions of nonabsorbing rod-like viruses. We identify a sequence of configurational transitions of RBC doublets, including configurations that can only be induced by long-ranged attraction: highly fluctuating T-shaped and face-to-face configurations at low, and doublets approaching a complete spherical configuration at high, rod concentrations. Complementary simulations are used to explore different energy contributions to deformation as well as the stability of RBC doublet configurations. Our advanced analysis of 3D reconstructed confocal images of RBC doublets quantifies the depletion interaction and the resulting deformation energy. Thus, we introduce a noninvasive, high-throughput platform that is generally applicable to investigate the mechanical response of biological cells to external forces and characterize their mechanical properties.

BP 17.41 Tue 18:00 P4

Red blood cell membrane tension modulation by photo switchable molecules — •Tim Kutz[1], Bart Vos[1], Jan Bart Ravoo[3], Andreas Janshoff[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany — [2]Institute of Physical Chemistry, Georg August Universität Göttingen, Göttingen, Germany — [3]Organic Chemistry Institute and Center for Soft Nanoscience, University of Münster

Cellular stiffness and surface tension are fundamental determinants of cell behavior and function. However, the precise contributions of membrane and cortical components to overall cell mechanics remain unclear. Building upon our recently developed multi-modal approach, which combines atomic force microscopy, confocal spinning disk fluorescence microscopy, and micropipette aspiration, we investigated the mechanical properties of human red blood cells (hRBC) as a model system, with a focus on membrane manipulation. By incorporating photo switchable azobenzenes into the hRBC membrane, we created a dynamic system to modulate membrane properties through light-induced conformational changes.Comparisons were made between wild-type hRBCs and those containing azobenzenes in both the cis and trans states. This approach enabled us to directly correlate changes in membrane conformation with alterations in mechanical properties. Our results demonstrate the feasibility of using photo switchable molecules to modulate cellular mechanics in a controlled and reversible manner. This approach and novel platform advances our understanding of the contribution of the membrane to cellular tension.

BP 17.42 Tue 18:00 P4

Theoretical perspectives on controlling cells by ultrasound — •Niels Gieseler[1,2,3], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, Heidelberg 69120 Germany. — [2]BioQuant, Heidelberg University, im Neuenheimer Feld 267, Heidelberg 69120 Germany — [3]Max Planck Institute for Medical Research, Jahnstrasse 29, 69120 Heidelberg, Germany

Aside from the well-known use of ultrasound in medical imaging, there are many other biomedical applications of ultrasound, including enhanced bone healing, neurostimulation and sonogenetics. Different mechanisms have been implicated for these processes, including temperature changes, cavitation, radiation forces and acoustical streaming. In this work, we are interested in the interaction between ultrasound and tissue (including organoids) at the single-cell level. Combining concepts from hydrodynamics, elasticity theory and soft matter, we aim at theoretical predictions of the relative relevance of these different effects. In particular, we use the theory of viscoelasticity to predict whether intracellular streaming and organelle movement can be controlled by ultrasound.

BP 17.43 Tue 18:00 P4

Predicting mass density of eukaryotic nuclei and cells — •Omar Muñoz[1,2,3], Abin Biswas[1,3,4], Kyoohyun Kim[1,3], Jochen Guck[1,3], Vasily Zaburdaev[1,2], and Simone Reber[4,5] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany. — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Max Planck Institute for the Science of Light, Erlangen, Germany — [4]Max Planck Institute for Infection Biology, Berlin, Germany — [5]University of Applied Sciences Berlin, Berlin, Germany

Biophysical properties of the cell nucleus are important for various cellular processes from transcription to migration, but largely are still not well understood. The mass density is one such example, since we observed for a wide range of species that the cells maintain a certain nuclear to cytoplasmic mass density ratio with nuclear mass density being lower than its cytoplasmic counterpart. Moreover, in diseased states such as senescence we observed a breakdown of this density ratio where dilution of the cytoplasm made nuclei appear more dense, which suggests that the density ratio is a potential marker of proper cell functionality. Theoretical modeling can contribute to a better understanding of how this density ratio is established. There are two essential model components: a pump leak model to predict compartment volume and a model to determine the dry mass in the system, which is usually an active, dynamic process. Here we present the models for different systems such as human cells, nuclei in Xenopus egg extract and discuss their differences.

BP 17.44 Tue 18:00 P4

Modeling the endothelial cytoskeleton response to blood flow — •Berin Becic and Stephan Gekle — Biofluid Simulation and Modeling, University Bayreuth, Germany

As present in blood flow, it was observed that a shear flow leads to an alignment of endoethelial cells, which is connected to an alignment of its cytoskeleton. Understanding this behavior is important as its failure can lead to chronic inflammation which is one cause for the formation of artherosclerosis and other cardiovascular diseases. In order to do this we develop a three-dimensional model for the formation of the cytoskeleton based on the stress- and strain-dependency of the stress-fiber association and dissociation dynamics, as proposed by Deshpande et al (A bio-chemo-mechanical model for cell contractility , PNAS 2006). This model also offers the opportunity to study the spatially resolved formation of the cytoskeleton as observed in cells adhering to a substrate or the mechanic interactions between the cell and its nucleus.

BP 17.45 Tue 18:00 P4

Combining computational and experimental advances in microparticle traction force microscopy — •Bastian Kraus[1], Simon Brauburger[1], Tobias Walther[2], Kerstin Göpfrich[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany — [2]Center for Molecular Biology of Heidelberg University (ZMBH), Heidelberg University, 69120 Heidelberg, Germany

Traction force microscopy (TFM) infers cellular forces from the motion of fiducial markers embedded in soft elastic substrates. Over the last years, this approach has been extended to elastic microparticles, typically made from polyacrylamide. In contrast to flat substrates, this approach allows to infer forces either from the motion of embedded fiducial markers or from the deformation of the surface. Here, we compare these two different approaches from the viewpoint of elasticity theory and with computer simulations that include the image processing steps. We then apply the method to experimental data from DNA microbeads, for which one can implement markers for both bulk and surface deformations.

BP 17.46 Tue 18:00 P4

An FEM based framework to reconstruct cellular traction forces in arbitrary geometries — •Cornelis Mense and Ulrich Schwarz — Heidelberg University

In the last two decades, the reconstruction of cellular traction forces has been a valuable tool in mechanobiology and biomedical experiments. Traction forces are traditionally computed for displacements of soft elastic substrates, imaged using fluorescent micro-beads. These substrates have largely been planar surfaces, owing to the availability of methods by which to analyse such experimental data. But, as of late, a curiosity and drive has arisen to extend these experiments to arbitrary three-dimensional geometries. Here, a framework is proposed to inversely reconstruct tractions using the Finite Element Method. This method attempts to reduce noise and non-physical tractions by iteratively projecting experimental displacement fields onto force-balanced configurations using the principle of virtual work. The efficacy of the method is demonstrated through toy problems, wherein tractions are first prescribed onto a geometry to generate mock data sets of displacement fields. These fields are then artificially made noisy, after which the FEM software is tasked with retrieving the initially prescribed tractions. The experimental design space, that would be opened up by this framework, could prove a valuable tool in further understanding cell motility.

BP 17.47 Tue 18:00 P4

Investigating Particle Binding above Epithelial Cells with Photonic Force Microscopy — Nils le Coutre and •Alexander Rohrbach — IMTEK, Department for Microsystems Engineering, Freiburg, Germany

A significant portion of today's airborne particulates originates from human activities such as industrial processes and the combustion of crude oil-based fuels. This has been linked to an increased risk of diseases including asthma, lung cancer, and cardiovascular pathologies, correlating significantly with the inhalation of particulate matter. Here, we investigate the fluctuation-based interaction of single optically trapped particles with epithelial cells. Using photonic force microscopy, we trap the particles through a layer of epithelial cells and interferometrically track the thermal motions of the particle with the goal to recover binding and friction parameters in contact with the cell surface. This approach is challenging since the cell perturbs the phase of the trapping and tracking beam, such that the characteristic trajectories - obtained by interference and encoding the interactions - require a novel analysis method.

BP 17.48 Tue 18:00 P4

Investigating cell membrane tension — •Tina Boric[1,2], Julia Butzke[1,2], Eva Kreysing[2,3], and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

Cellular membranes are known to change their mechanical properties in response to external and internal mechanical stimuli, such as shear forces and changes in tissue stiffness. Membrane tension contributes to the transduction of these mechanical signals into intracellular responses via mechanosensitive ion channels. However, how and if a change in tissue stiffness affects the surface mechanics of the cell, which in turn would contribute to the activation of mechanosensitive ion channels, is not yet known. We are investigating the dependence of the effective membrane tension of HEK 293T cells on the expression levels of the mechanosensor Piezo1 using optical tweezers. Furthermore, we are comparing tether forces of cells grown on compliant custom-made substrates of biologically relevant stiffness. We also expose the cells to different pharmacological treatments that primarily affect the actin cortex to investigate how membrane-to-cortex attachment affects tether forces. Ultimately, our aim is to understand how changes in membrane tension lead to the activation of Piezo1. Our work will contribute to the understanding of how mechanosensitive ion channels are gated, which may have important implications for drug design in the future.

BP 17.49 Tue 18:00 P4

Revealing minimal cell particle interactions by thermal noise frequency decomposition — •Max Wechlin, Felix Jünger, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, Department of Microsystems Engineering (IMTEK), University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Nearly every interaction process in nano-scale soft materials, especially in living cells is governed by thermal noise. However, it is hardly known or often disregarded that many interaction processes take place only on specific timescales. This means that observing or measuring on the wrong timescale, can lead to wrong results or even no results. While interactions can be visible on one timescale, they can be completely invisible on another. Therefore, it is not only necessary to measure on a much broader frequency range than usually, but also to decompose the broadband fluctuation data with appropriate mathematical models. This way minimal or even hidden interactions can be revealed. We use optical tweezers based Photonic Force Microscopy with MHz-rate interferometric 3D particle tracking to approach 1*m-sized polystyrene beads to functional gels or to living cells. We demonstrate that interactions between particles and cells change in stiffness or friction over time and distance only on certain frequency bands, but not over the average fluctuations in energy and position.

BP 17.50 Tue 18:00 P4

Regulation of plasma membrane tension through the actin cytoskeleton and hydrostatic pressure — •Yogishree Arabinda Panda and Elisabeth Fischer-Friedrich — Excellence Cluster Physics of Life, TU Dresden, Dresden, Germany

The plasma membrane and its associated proteins serve as a critical signaling hub, transmitting information between the extracellular environment and the intracellular space. It plays essential roles in regulating the intracellular ion content, the membrane potential and processes such as endocytosis and exocytosis. Consequently, the plasma membrane is central to many physiological processes including cell differentiation, migration, and proliferation. Recent studies have shown that the activity of many transmembrane proteins is influenced by mechanical tension in the plasma membrane. Despite its importance in cellular signaling, the mechanisms by which cells regulate membrane tension remain poorly understood. In this study, we investigate the regulation of plasma membrane tension in mitotically arrested cells using FLIM in conjunction with the membrane dye FlipTR. Specifically, we explore how components of the actin cytoskeleton, intracellular hydrostatic pressure, and cell shape contribute to both actual and apparent membrane tension.

BP 17.51 Tue 18:00 P4

Single-cell physical phenotyping of blood and tissue biopsies — •Marketa Kubankova[1,2], Despina Soteriou[1,2], Martin Kräter[1,2], and Jochen Guck[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Deformability cytometry [1] is a microfluidic technique that allows the assessment of physical properties of single cells in a label-free and high-throughput manner, with up to 1000 cells analysed per second. Cell deformation and other physical phenotype parameters such as cell size and aspect ratio are obtained directly from brightfield cell images.

The diagnostic potential of deformability cytometry was previously demonstrated in various diseases [2, 3]. Here we show how deformability cytometry accurately discriminates between healthy and tumorous tissue in biopsies of mouse and human colons [4]. Cell deformation was a crucial parameter for the correct distinction of tumour tissue in colon cancer patients. Furthermore, we present new findings on how the physical properties of blood cells change during infectious diseases, and how they correlate with commonly used markers of infectious inflammation. Our findings pave the way for establishing deformability cytometry as a fast and marker-free diagnostic technique to sensitively detect pathological changes in solid and liquid biopsies.

[1] Otto et al., Nature Methods (2015), [2] Toepfner et al., Elife (2018), [3] Kubánková et al., Biophysical Journal (2021), [4] Soteriou and Kubánková et al., Nature Biomedical Engineering (2023)

BP 17.52 Tue 18:00 P4

Mechanobiology of immune cell confined migration — •Fatemeh Abbasi[1], Timo Betz[2], and Eva Kiermaier[1] — [1]LIMES Institute, University of Bonn, Bonn, Germany — [2]Third Institute of physics, University of Göttingen, Göttingen, Germany

In vivo, cells experience complex tissue environments and have to adjust their behavior and function based on their surrounding. Immune cells are the renowned examples. On their way from the bone marrow, where they are born, to the infection site, they have to cope with various physical challenges including geometrical confinement and different mechanical properties of the host tissues. To perform a successful confined migration, cells need to squeeze their nucleus, the most stiff and largest cell organelle, as well as reorganize their cytoskeleton. Despite the importance of this subject in immunology and pathology, it is still not well-understood how immune cells can adopt different nuclear morphologies and cytoskeleton organization while migrating through the small junctions and pores. Here, we use CFM (Confinement Force Microscopy), which was developed in the lab of Timo Betz, to confine immune cells in a 2.5D environment of various stiffness. We will study the role of centrosome, microtubule and nuclei morphology in innate immune cell confined migration. This study can help us to find out how nuclei and cytoskeletal organelles facilitate immune cell migration through confined microenvironments of different mechanical properties. Simultaneous measurement of the cell forces on the microenvironment will enable us to find out the mechanobiology of immune cell confined migration.

BP 17.53 Tue 18:00 P4

Processivity of myosin assemblies: ATP dependence and effect on network dynamics — •Jaskaran Singh and Stefan Klumpp — University of Göttingen, Institute for the Dynamics of Complex Systems, Göttingen,Germany

Motors proteins like myosin, kinesin are a major source of activity in cellular mechanisms like cell division and perform tasks such as maintaining cellular structure and transporting cargo within the cell. These motors form complexes of multiple motors and cooperate and give rise to complex behaviors not seen in single-motor dynamics. Myosin motors form medium sized (~100 motors) assemblies called myosin minifilaments that bind to and move along actin filaments. The mechano-chemical cycle of individual motors in the motor assembly is dependent on ATP. We are exploring the concentration of ATP as a control parameter for the processivity (walking distance) of myosin minifilaments through stochastic modelling. Here we propose processivity as a parameter to tune the activity in system. On the cellular scale, we explore the effect of processivity on cytoskeletal network structures at large. Preliminary results show that decrease in ATP concentration increases the processivity of myosin assemblies. However, the velocity of motor assembly decreases with decreasing ATP. Thus, an optimal trade-off between processivity and velocity must be maintained for efficient assembly performance. To study the effect of processivity on network level structures, we use the simulation package Cytosim. The simulation shows that higher processivity leads to a more pronounced contraction of the actin network.

BP 17.54 Tue 18:00 P4

Mechanosensing and shape adaption of cells on substrates of varying stiffness — •Pooja Yadav, Florian Rehfeldt, and Matthias Weiss — Experimentalphysik I,University of Bayreuth

Changes of characteristic cellular features with varying stiffness of the underlying substrate, e.g. shapes and sizes of cells and nuclei, are a hallmark of the complex interplay of mechano-biochemical feedback loops. To explore this in detail, we have quantified cellular features on polyacrylamide (PA) hydrogels of varying stiffness, from 2~kPa to 64~kPa, hence mimicking the diverse microenvironments found in vivo. In particular, we have quantified the areas of nuclei and cells, their aspect ratio, and the local order parameter of the cytoskeleton on different substrates, also in the absence and presence of cytoskeleton-severing drugs. As a result, we observed that cell and nucleus areas follow an isometric relation with both areas increasing with the stiffness of the substrate. In contrast, the aspect ratio of both show a non-trivial maximum at intermediate stiffnesses, which we attribute to the local nematic ordering of the cytoskeleton. Altogether, our data open up the way to investigate differential mechanical effects of nuclei and cells under perturbations.

BP 17.55 Tue 18:00 P4

Mechanical properties of microtubule in actin network — •Komal Bhattacharyya, Sarah Köster, and Stefan Klumpp — University of Göttingen, Göttingen, Germany

The cytoskeleton provides structural support and facilitates dynamic cellular processes such as growth and migration. Actin and microtubules are key components of the cytoskeleton. Actin, characterized by its semi-flexible nature, contrasts with the stiff, rod-like structure of microtubules. The synergy between these two elements plays a pivotal role in numerous biological phenomena. For instance, microtubules exhibit enhanced resistance to compressive forces when integrated into an actin network.

In our research, we use the simulation package Cytosim to study composite networks formed by actin and microtubules. Specifically, we analyze the buckling behavior of microtubules under compressive forces and thermal fluctuations and how it is affected by mechanical coupling to actin. We observe that long-range repulsive interactions between the filaments lead to very small elasticity and minimal suppression of microtubule buckling. As a consequence, the observed mechanical responses within composite networks can very likely not be explained without considering specific interactions between actin and microtubules.

BP 17.56 Tue 18:00 P4

Mechanical Properties of Intermediate Filament Networks — •Jonas Penning and Stefan Klumpp — Institute for Dynamics of complex systems, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The mechanical strength and dynamics of cells are essential for sustaining life. For instance, during simple activities such as breathing or walking, cells are subjected to significant tensile stresses as they are stretched, sheared, or compressed. The cytoskeleton - a cross-linked composite network of actin, microtubules, and intermediate filaments - plays a central role in determining the cells' mechanical properties. While actin and microtubule networks have been studied extensively, this work focuses on intermediate filaments, such as vimentin and keratin. Compared to actin, intermediate filaments exhibit much smaller persistence lengths, but are much more stretchable with highly nonlinear elasticity. Extedning the freely-jointed chain (FJC) model by nonlinear stretching elasticity, a simplified model has been developed to investigate the mechanical and physical properties of cross-linked intermediate filament networks. Analogous to experimental approaches, the mechanical properties of the model are tested by applying normal and shear strains or stresses and analyzing the resulting responses.

BP 17.57 Tue 18:00 P4

Infrared Spectroscopic Analysis of Structural and Thermal Dynamics in Cytochrome c-DNA Complex — •Berken Hamarat, Damla Melisa Balci, and Günnur Güler — Biophysics Laboratory, Department of Physics, Izmir Institute of Technology, Izmir, Türkiye

Cytochrome c (Cytc) plays a crucial role in cellular respiration and apoptosis, with potential for biosensor applications due to its electron transfer capabilities. The binding of Cytc to DNA enables its consideration as a target molecule in biosensors and facilitates the modulation of Cytc's electronic properties via protein-DNA interactions. Temperature-controlled FT-IR spectroscopy in the transmission mode was used to investigate the structural changes and thermal stability of Cytc upon DNA complex in oxidized and reduced forms. Deuterated samples of Cytc and DNA were used during the analysis. Structural changes were observed after DNA binding, with a reduction in α-helix content, particularly in the oxidized form. Thermal stability analyses showed that the Cytc-DNA complex lost structural integrity at lower temperatures compared to free Cytc. These results indicate that DNA binding not only alters Cytc's secondary structure but also reduces its thermal stability. While Cytc's high thermal stability makes it suitable for biosensor applications, the observed changes after DNA binding, particularly the decrease in thermal stability must be minimized and optimized to ensure effective biosensor functionality. (Supported by Scientific and Technological Research Council of Türkiye, TÜBITAK 2209-B Project, 1139B412200835).

BP 17.58 Tue 18:00 P4

Soft-landing Electrospray Ion Beam Deposition (ES-IBD) allows integration of native mass spectrometry and cryoEM to investigate membrane protein structure and function — •Carl von Hallerstein, Sophie Lawrence, Tarick El-Baba, Stephan Rauschenbach, and Carol Vivien Robinson — Kavli Institute for Nanoscience Discovery, University of Oxford, UK

Electrospray Ion Beam Deposition (ES-IBD) is an emerging sample preparation for the imaging of molecules (Esser et al. 2022, Faraday Discussions). Recently, using native mass spectrometry (nMS), the deposition and cryo-electron microscopy (cryoEM) imaging of soluble proteins was demonstrated (Esser et al. 2024, Sci. Adv.).

Here, we apply ES-IBD + cryoEM to membrane proteins, which only retain their native state while encased in lipid membranes or membrane-mimetics such as detergents or nanodiscs. ESIBD+cryoEM yields valuable information on lipid and surfactant interaction as well as hydration of the membrane protein.

BP 17.59 Tue 18:00 P4

Investigation into the dynamic structure of heat shock proteins using electrospray ion beam deposition and cryo-electron microscopy (ESIBD+cryoEM) — •Noor Naseeb, Lukas Eriksson, Jingjin Fan, Justin Benesch, and Stephan Rauschenbach — University of Oxford, Oxford, United Kingdom

The heat shock protein (HSP) family encompasses a wide variety of polydisperse proteins that act as chaperones in the cell as a means of preventing aggregation and misfolding of proteins under different forms of cellular stress. Standard methods, like X-ray crystallography (XRC), Nuclear magnetic resonance (NMR), and cryogenic electron microscopy (cryo-EM), lack the ability to properly study the structures of such dynamic and diverse proteins. To address this, we use electrospray ion beam deposition (ESIBD) that couples native mass spectrometry (MS), a chemically selective sample preparation technique, with cryo-EM. The combination allows for high-resolution visualization of a specific protein assembly by cryo-EM in their near-native state. Here we show that the chemically selective sample preparation technique via ESIBD enables structure determination of these dynamically assembled HSPs can be performed to better assess their structure, and therefore, function.

BP 17.60 Tue 18:00 P4

Hyperfine spectral diffusion in pulse EPR: theory and applications — •Sergei Kuzin[1,2], Gunnar Jeschke[1], and Maxim Yulkov[1] — [1]ETH Zurich, Zurich, Switzerland — [2]MPI for Multidisciplinary Sciences, G\"ottingen, Germany

Hyperfine interaction with nuclear spin bath and nuclear spin-spin interaction often dominate phase memory times of the electron spins in spin-diluted solids at cryogenic temperatures. Such an spin-ensemble effect also manifests is different EPR experiments as spectral diffusion.

Here, we present a new pulse EPR method called intermolecular hyperfine relaxation-induced dipolar modulation enhancement (ih-RIDME). This technique allows to investigate kinetics of spectral diffusion in amorphous solids. The sensitivity range of ih-RIDME lies within 1-3~nm around the spin centre. This makes it a powerful tool to probe nuclear spin arrangement at intermediate electron-nuclear distances. The quantification in ih-RIDME is based on a developed mathematical model of spectral diffusion resulting in a diffusion-like equation. With its help, ih-RIDME allows to quantify heterogeneous systems with a distribution of local proton densities.

We discuss the applications of ih-RIDME in dynamic nuclear polarization, structural biology, spin-labeled macromolecules and soft matter study.

BP 17.61 Tue 18:00 P4

Electron spin dynamics during MW pulses studied by 94 GHz chirp and phase-modulated EPR experiments — •Marvin Lenjer[1,2], Nino Will[3], Fabian Hecker[4], and Marina Bennati[1,2] — [1]MPI for Multidisciplinary Sciences — [2]Georg August University Göttingen — [3]Aarhus University — [4]Danish Technical University

Over the last decade, shaped microwave (MW) pulses have evolved into valuable tools for electron paramagnetic resonance (EPR) spectroscopy. They have been used to improve existing experiments by providing tunable broadband or band-selective frequency profiles as well as to design new experimental approaches. However, most applications were done at low fields (X- or Q-band) where high MW powers are available.

Here, we show the implementation of chirped and phase modulated pulses at a commercial Bruker E680 W-band (94 GHz) EPR spectrometer using a SpinJet arbitrary waveform generator. We apply these novel experimental tools to the analysis of spin dynamics during MW spin lock pulses. We measure inversion profiles in the intermediate regime between Rabi oscillations and saturation pulses via chirp echo EPR spectroscopy and analyze spin-spin relaxation during spin locking (i.e. $T_{2\rho}$) via phase modulation echoes during spin lock. Combination with density matrix simulations allows us to better understand electron spin evolution during long periods of MW irradiation. Altogether, these results promise future advances in design and applicability of hyperfine spectroscopy at high fields by use of spin locks and shaped pulses.

BP 17.62 Tue 18:00 P4

Human cardiac cadherin desmocollin 2 reveals ideal-, slip- and catch bonds in vitro — •Manuel Göz[1], Greta Pohl[2], Sylvia Steinecker[1], Volker Walhorn[1], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany — [2]Heart & Diabetes Center NRW, University Hospital of the Ruhr-University Bochum, Bad Oeynhausen, Germany

Desmosomal cadherins like DSC2 are known to associate in a strand-swap binding motif in which an N-terminal tryptophan residue binds into the hydrophobic binding pocket of opposing cadherins. Although this binding pattern is highly specific, it is of low affinity and exhibits decreased bond lifetimes at a single-molecule level. Using AFM-based SMFS, we show that the strand-swap dimerized DSC2 has two further binding modes, which may play a role in the integrity of the cardiac muscle. At short interaction times, the DSC2 monomers associate only short-lived and force-independent. These ideal bonds are probably a precursor state that stabilizes the formation of the strand-swap dimer. Tryptophan added to the measurement buffer acts as a competitive inhibitor, preventing the N-terminal strand exchange. Here, DSC2 dimerizes as an X-dimer and shows a triphasic slip-catch-slip type of dissociation. Within a force-activated transition (catch) regime, DSC2 dimers switch between brittle low force and strengthened high force adhesion states. So we can assume that desmosomal adhesion is mediated not only by strand-swap dimers (slip bond) but also by their precursor states (ideal bond) and force-activated X-dimers (catch bond).

BP 17.63 Tue 18:00 P4

Trajectories of particles trapped in double well potentials show new behavior in the Mean Back Relaxation — •Christian Muñoz[1], Mohammad A. Eskandari[1], Bart E. Vos[1], Till M. Münker[1], Dorian Marx[1], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Optical tweezers have been established as a powerful tool for studying microscopic particle dynamics in complex potentials. In this work, we investigate the behavior of a microparticle trapped in a double-well potential generated by optical tweezers. By systematically varying the laser power and the distance between the optical traps, we modeled the shape and depth of the potential. This approach allowed for a detailed analysis of the particle's stochastic transitions between the wells. Combining experimental measurements with Kramers' theory, we achieved accurate predictions of the transition rates between wells. Furthermore, we analyzed particle trajectories using the new quantity of Mean Back Relaxation (MBR), providing insights into the effects that a bistable system has on particle relaxation after defined fluctuations.

BP 17.64 Tue 18:00 P4

Cell-cell interactions of swimming ciliated microbes: from measured interaction dynamics to an effective potential — •Henrik Groh[1,2], Alexandros A. Fragkopoulos[1], Colin-Marius Koch[3], Michael Wilczek[3], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics I, 95447 Bayreuth, Germany — [3]University of Bayreuth, Theoretical Physics I, 95447 Bayreuth, Germany

In suspensions of living microorganisms the interactions of individual agents may result in large-scale collective effects. Frequently such phenomena are studied more extensively with the goal of linking them to the microscopic single-cell motility and cell-cell interactions. *Chlamydomonas reinhardtii* represents a unicellular eukaryotic model organism that is used to study collective phenomena of puller-type microswimmers, e.g., induced by a self-generated oxygen gradient [1] or by light (phototaxis). In order to complement these studies with a systematic cell-cell interaction analysis, we investigated the mutual interactions of *C. reinhardtii* in a quasi-2D suspension with high temporal and spatial resolution. Our measurements allow for deriving a pair-correlation function and an effective potential, which may eventually enter simulation studies. With our study we provide more detailed insights into the cell-cell interactions of *C. reinhardtii* and thus enable a better understanding of collective phenomena in living suspensions.

[1] A.A. Fragkopoulos, et al., *J. R. Soc. Interface* **18**, 20210553 (2021).

BP 17.65 Tue 18:00 P4

Quantum Physics Meets Epigenetics: Does Nature Harness Charge and Energy Transfer in Methylated DNA? — •Dennis Herb[1,2], Mirko Rossini[1,2], and Joachim Ankerhold[1,2] — [1]Institute for Complex Quantum Systems, Ulm University, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Ulm-Stuttgart, Germany

Charge transfer processes through DNA play a crucial role in gene regulation, including processes such as DNA methylation, an epigenetic modification essential for gene expression. However, the effects of methylation on excitonic energy transfer (EET) and coherent charge transfer (CT) in DNA remain poorly understood. Here, we theoretically investigate the effects of DNA methylation, as well as conformational changes, on biologically relevant DNA sequences. Using a Linear Combination of Atomic Orbitals (LCAO) approach, we compute the molecular electronic structure of nucleic acid bases and derive parameters for a computationally efficient tight-binding (TB) model. Our model incorporates intrinsic relaxation mechanisms for excited states, mimicking internal conversion (IC), and electron-hole Coulomb interactions. This framework provides physical insights into excited state lifetimes, charge separation dynamics, and dipole moments across diverse DNA sequences. By integrating quantum physics and physical chemistry methodologies with genetic and epigenetic analyses, this study offers a powerful interdisciplinary approach to investigate the quantum mechanisms underlying DNA charge dynamics and their modulation by epigenetic modifications.

BP 17.66 Tue 18:00 P4

Modeling host-pathogen interactions: infection process as a population dynamics problem — •Soham Mukhopadhyay[1], Jonathan Pollock[2], David Voehringer[2], and Vasily Zaburdaev[1] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Infection Biology, Uniklinikum Erlangen, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Helminth infections affect a large proportion of the world's population and cause significant morbidity. There are no vaccines against helminths, and the mechanisms by which the body fights off helminth infections are not well-understood. To better understand the immune system response we aim to develop a mathematical model describing the helminth load in different organs of the host as a function of time. As an experimental system, we use murine helminth infection by *Nippostrongylus brasiliensis*. We abstract infection progression as a state-transition process. The different host organs involved in the infection cycle act as the different states of the system, and the worms are treated as identical and independent particles transitioning from one state to another with fixed transition rates and delays. This allows simulation of the infection process via kinetic Monte Carlo and association of the infective dose of larvae to the number of eggs shed to the environment by adult worms from the intestine, which can then be compared against experimental data. Using simulations to generate training data, we employ Neural Network-based optimization to discover an optimal parameter set that can quantify the infection process.

BP 17.67 Tue 18:00 P4

Measuring activity from particle trajectories — •Lukas Abegg, Till M. Muenker, and Timo Betz — Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany

Is it possible to distinguish activity from thermal fluctuations just from observed trajectories? The newly introduced statistical quantity Mean Back Relaxation aims to achieve exactly this by using three-point correlation functions. This non-dimensional function yields a measure for deviation from equilibrium within a confined system. It is calculated as the average displacement of a tracer article under the condition of having moved the distance d in advance. For an equilibrium process, this quantity results in a long time value of $\frac{1}{2}$. However, deviation from this value is a marker for broken detailed balance. To gain deeper insight into this new statistical measure, we investigate this quantity inside a controlled system, namely a viscoelastic polyacrylamide gel. This probe was tuned to imitate the mechanical properties of cells, containing polystyrene particles with a size of one micron. To drive this system out of equilibrium, we use a movable optical tweezer to simulate active motion of the particle. The Mean Back Relaxation is calculated for all trajectories and fitted with an analytical solution for a viscoelastic system. The results are used to quantify the diffusion coefficient of the trapping laser and thus, the activity of the system tuned by our experimental realisation. Additionally, we can calculate the shear modulus $G^\star$ from this result.

BP 17.68 Tue 18:00 P4

Active Soft Glassy Rheology as a model for cytoskeletal mechanics — •Raffaele Mendozza and Peter Sollich — University of Goettingen, Institute for Theoretical Physics

The cytoskeleton plays a vital role in cellular processes like growth, migration, and division, owing to its unique mechanical properties [1]. Advanced microrheology techniques have revealed a complex power-law viscoelastic spectrum in this and other biopolymer networks, reflecting the presence of a broad distribution of relaxation timescales [2]. Coarse-grained trap models capture this phenomenology, suggesting a connection between cytoskeletal and soft glassy rheology (SGR) [3,4,5]; however, the original SGR model lacks explicit consideration of active processes, ubiquitous in living cells. We therefore explore how activity influences the rheological response of a soft glassy material, based on different working hypotheses. By introducing an activity-dependent effective temperature, the characteristic SGR viscoelastic spectrum is recovered, while modelling activity as an effective strain rate introduces a competing timescale that modifies the response. The resulting active SGR model provides insights into the mechanical behavior of cells independent of biochemical intricacies, serving as a foundation for future models incorporating more detailed structural information.

[1] P. Kollmannsberger and B. Fabry, 2011
[2] B. Fabry et al., 2001
[3] B. D. Hoffman1 and J. C. Crocker, 2009
[4] K. K. Mandadapu et al, 2008
[5] P. Sollich et al, 1997

BP 17.69 Tue 18:00 P4

Fluctuating liquid inclusions morphology in biomolecular condensates driven by fuel-dependent binding agents — •Leonardo Silva-Dias and Christoph A. Weber — Universität Augsburg, Augsburg, Germany

The presence of aggregation-prone proteins in non-dilute, multi-component solutions, such as the cellular environment, can lead to the formation of protein aggregates. In these environments, such proteins may also undergo phase separation, forming biomolecular condensates. Both processes are regulated by specialized molecules known as binding agents, examples of which include RNA, enzymes, and chaperones. These binding agents continuously consume biological fuels, driving the system out of equilibrium and enabling the emergence of complex behaviors, such as morphological changes in the condensates. Specifically, recent experimental evidence has shown that a system composed of aggregation-prone proteins and ATP-driven chaperones induces the formation of condensates with a fluctuating liquid inclusions morphology. Based on these observations, the present work provides a theoretical framework to describe the emergence of the fluctuating liquid inclusions state. The proposed description is developed through a mean-field model that accounts for chemical reactions and phase separation in the presence of stochastic fluctuations. In this system, we observed that local fluctuations trigger multiple nucleation events within the condensates, leading to the growth of many liquid inclusion structures, which ripen, dissolve, and renucleate.

BP 17.70 Tue 18:00 P4

Competitive resource sharing mechanism for synchronization and its energy cost — •Dongliang Zhang[1,2], Yuansheng Cao[1], Qi Ouyang[3], and Yuhai Tu[4] — [1]Department of Physics, Tsinghua University, Beijing, China — [2]Max Planck Institute for the Physics of Complex Systems — [3]School of Physics, Zhejiang University, Hangzhou, China — [4]IBM T. J. Watson Research Center, Yorktown Heights, New York, USA

Synchronization among a group of active agents is ubiquitous in nature. Although synchronization mechanism based on direct pairwise interactions between agents as exemplified by the Kuramoto model is well understood. The dynamics and energetics of another general mechanism based on indirect interactions among agents sharing a limited resource are less known. In this work, we proposed a simple thermodynamically consistent model for the resource-sharing (RS) mechanism.We find that synchronization relies on differential competence of agents for the limited resources.More advanced agents are less competent, which provides a negative feedback mechanism resulting in synchronization. We show that differential affinity breaks detailed balance and thus synchronization requires continuous energy dissipation in addition to the energy cost of the agents* processive motion. Our study reveals a tradeoff relation between the total energy dissipation rate and the performance of the system characterized by its average speed and synchronization accuracy. Different Pareto fronts with fixed dissipation or speed result naturally from the Energy-Speed-Accuracy (ESA) relationship.

BP 17.71 Tue 18:00 P4

Time irreversibility and effective temperature are independently regulated in the actin cortex of living cells — •N Narinder and Elisabeth Fischer-Friedrich — Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany

Living cells exhibit non-equilibrium dynamics driven by the intricate interplay between motor activity and their viscoelastic environment. The deviation from thermal equilibrium termed as irreversiblity is commonly characterized by an increased effective temperature and time-reversal symmetry breaking quantified through the Kullback-Leibler divergence (KLD). In this study, we determine entropy production as a measure of irreversibility both by the effective temperature and the KLD in the actin cortex of living cells using atomic force microscopy (AFM) with and without pharmacological treatments that modulate cellular activity and cortical mechanics. Surprisingly, we find that while the entropy production rate consistently increases with effective temperature, its time irreversibility estimated by the KLD can exhibit an opposite trend, depending on the mechanical properties of the cortex. Our findings underpin the role of mechanical properties on the irreversibility. Further, the findings are supported by a minimal model of the AFM tip as probe immersed in the viscoelastic environment of active cell cortex.

BP 17.72 Tue 18:00 P4

Triacylglycerols affect the water content and cohesive strength of collagen fibrils — •Martin Dehnert, Tiberius Klose, Yang Pan, Dietrich R. T. Zahn, Maximilian Voigtländer, Johannes F. Teichert, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Collagens, lipids, and water are among the major molecular components of connective tissue, but surprisingly little is known about their interactions in vivo. Here, we provide direct evidence that type I collagen fibrils extracted from chicken calcaneal tendon contain triacylglycerols (TAG), which influence the water content of the fibrils and act as plasticizers that affect the mechanical properties of the fibrils. We use organic solvents to dissolve lipids from native collagen fibrils and identify them as TAG using Raman spectroscopy and NMR spectroscopy. Using atomic force microscopy-based 3D depth profiling, we quantify the changes in volume, water content, and indentation modulus of the fibrils caused by the removal of TAG at the single fibril level. Based on these findings, we propose a molecular model for the intercalation of TAG into collagen fibrils. The discovery of the biomechanical function of TAG is fundamental to understanding the role of lipids in collagen fibrils during development, aging, and disease.

BP 17.73 Tue 18:00 P4

Cellular Potts Model links tissue surface tension to cell proliferation — •Kai Lennard Fastabend[1], Cécile M. Bidan[2], John W. C. Dunlop[3], and Philip Kollmannsberger[1] — [1]Biomedical Physics, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany — [2]Max Planck Institute of Colloids and Interfaces, Dept. of Biomaterials, Golm, Germany — [3]Paris Lodron University, Salzburg, Austria

The shape and growth kinetics of tissue depend not only on biochemical factors but also on the geometry of the extracellular environment. Cellular Potts Model simulations of tissue growth on different substrate geometries are a promising approach to investigate the role of adhesion forces, cell elasticity and tissue surface tension in the formation and organisation of tissue. To investigate how tension-dependent cell proliferation in tissues can explain the observed link between scaffold geometry and tissue growth kinetics, we implemented a growth rule based on the stretching of cells in CompuCell3D. Systematic parameter scans reveal the role of cell-substrate adhesion as the driving factor for monolayer formation, while cortical contractility introduces a surface tension to the tissue. The minimization of the macroscopic tissue surface leads to bulk tissue growth beyond the monolayer depending on the underlying substrate geometry. Our results highlight how cellular contractility and adhesion, together with geometric boundary conditions can determine the macroscopic growth patterns of tissues, independent of soluble growth factors.

BP 17.74 Tue 18:00 P4

Nanomechanical ultrastructure of native tendon tissue — Mario Zerson, Martin Dehnert, Paul Zech, Tiberius Klose, and •Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Tendon tissue is a natural, high performance material in which type I collagen fibrils act as the load-bearing elements. The collagen fibrils are embedded in the tendon ground substance, a hydrophilic gel. Using AFM-based nanoindentation measurements, we study the nanomechanical ultrastructure of collagen fibrils in native tendon tissue obtained from the calcaneus (Achilles) tendon of chicken. The sample is exposed to a flow of humid air with controlled relative humidity to maintain the water content close to physiological conditions. We reconstruct 3D depth profiles from measured force–distance data and analyze the tip–sample interaction with a recently developed hysteresis model with return point memory (Soft Matter 2024, *20*, 2831–2839). The latter describes the rate-independent nanoindentation response, which is dominated by an elasto-plastic deformation behavior. It allows us to quantify the elastic and dissipative contributions of the indentation response within individual collagen fibrils as well as in the contact regions between adjacent fibrils.

BP 17.75 Tue 18:00 P4

Adjustable tension in reconstituted heart muscle tissue to mimic physiological mechanical environment changes — •Anna Mukhina[1], Till Muenker[1], Mattias Luber[1], Arne Hofemeier[2], Bruno Schmelz[1], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, University of Goettingen — [2]Department of Pharmacology and Toxicology, University Medical Center Goettingen

The development of in vitro 3D muscle tissues is critical for studying muscle physiology, disease mechanisms, and drug responses. PMMA tissue chambers provide structural support for myogenic cells embedded in a 3D ECM scaffold, enabling organization into aligned myotubes resembling natural muscle tissue. Tissue self-organizes around posts of known stiffness, with muscle strength assessed via post-deflection during contraction. This project introduces a piezo-driven actuator into the PMMA chamber for external manipulation of tissue tension. Combining actuators with a direct readout of posts' positions enables feedback control to emulate diverse mechanical environments. This innovation investigates how varying mechanical loads influence muscle development, adaptation, and therapeutic responses.

The project involves: (1) design and integration of a piezo actuator system, using CAD and Labview for construction and feedback control; (2) validating the modified chamber with engineered human myocardium (EHM) derived from iPSCs, exposed to defined mechanical stresses to mimic physiological and pathological loads. Functional and morphological outcomes are assessed via post deflection analysis and fluorescence imaging, advancing insights into muscle biomechanics.

BP 17.76 Tue 18:00 P4

Illuminating forces in living tissues — •Lucia Baldauf[1], Anna Bajur[2], Katelyn Spillane[2], and Guillaume Charras[1] — [1]London Centre for Nanotechnology, University College London, UK — [2]Department of Life Sciences, Imperial College London, UK

How can epithelial tissues withstand large forces and support deformations that drastically increase their length? Adult epithelial tissues regularly experience forces that stretch them by up to 50 %, and deformations can reach several hundred percent during development. To fulfill their physiological barrier function, epithelia must accommodate such large deformations without fracturing. Consequently, cell-cell adhesions must be finely tuned, or pathologies like skin blistering or cancer metastasis can occur. However, the physical principles governing tissue integrity remain difficult to study, since tissue fracture is a multiscale process spanning up to 10 orders of magnitude in both size and force. Millimetre-sized tissues can withstand millinewton-forces, but tissue fracture results from the local failure of single nanometre-sized adhesion complexes that bear piconewton forces. New tools are needed to bridge these vastly different scales and understand what molecular processes lead to tissue failure. Here we develop a new experimental tool to study tissue integrity and force propagation across scales. We engineer living model tissues where DNA-based molecular force sensors in chimeric cell-cell junctions provide a local molecular-scale force readout, for the first time illuminating how forces propagate in living tissues under stretch.

BP 17.77 Tue 18:00 P4

Imaging cell mechanics of retina organoids using an oblique plane light-sheet microscope — •Achim Theo Brinkop[1,2], Florian Schorre[1], Stefan Stöberl[1], Elijah R. Shelton[1], Teresa Rogler[1,2], Michael Frischmann[1,2], Marie Lackmann[1], Kaustav Goswami[1], Alexander Zangl[1], Mythili Padavu[1], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Germany — [3]Munich Cluster for Systems Neurology (SyNergy) & Graduate School of Systemic Neuroscience (GSN), Munich, Germany

Retina organoids have become a powerful testbed for studying retina formation and neuronal development. Our current measurements of the creep compliance in retina organoids with magnetic droplets point towards soft glassy rheology of developing retinal tissue at second to hour timescales. As a next step, we explore whether the motion of cells agrees with predictions for glassy materials. For this purpose, we built a custom oblique plane microscope for long-term volumetric imaging of the cell movements during organoid development. Using a processing pipeline based on open-source python packages (Cellpose3, Ultrack), we segment and track individual cells. The tracks allow us to quantify cell dynamics and compare these with existing models for glassy materials. In the future, we will integrate magnetic droplet compliance measurements with volumetric imaging in one set-up to simultaneously probe organoid mechanics *in situ*. Combining tissue mechanics measurements with cell dynamic recordings, we aim to shed light on the mechanical cues that guide retina formation.

BP 17.78 Tue 18:00 P4

Investigating the mechanosensitive expression of sema3A and slit1 in hydrogel-embedded neuroepithelial cells — •Niklas Gampl[1,2] and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

During brain development, neurons extend long axons that grow along well-defined pathways to their destination. This axon pathfinding is regulated by chemical guidance cues, which are produced by neuroepithelial cells, and by tissue stiffness. To investigate whether environmental stiffness regulates the expression of chemical guidance cues in the developing brain, we developed a framework to culture Xenopus tissue explants in collagen-based hydrogels with tunable stiffness. We found an increase in sema3A and slit1 mRNA levels in hypothalamic neuroepithelial tissue cultured in stiff hydrogels (G' = 450 Pa) compared to soft hydrogels (G' = 40 Pa). Additionally, 3D traction force microscopy revealed that strain energy, generated by the explants and stored in the matrix, increased with stiffness. These findings highlight a mechanochemical mechanism linking tissue stiffness to chemical guidance cue expression. Further investigation could improve our understanding of the complex interplay between guidance cues and their integration by cells.

BP 17.79 Tue 18:00 P4

AFM imaging of epithelial basement membrane with and without molecular perturbations — •Karla Yanin Guerra Santillan[1], Christian Dahmann[2], and Elisabeth Fischer-Friedrich[1] — [1]Cluster of Excellence Physics of Life, Technische Universit\"at Dresden, Dresden, Germany — [2]School of Science, Technische Universit\"at Dresden, Dresden, Germany

Understanding the precise regulation of growth and form is fundamental to the healthy development of all organisms. The basement membrane is a specialized sheet of extracellular matrix that forms at the basal face of epithelial tissues. This biopolymer network plays a major role in structural support, proliferation regulation and biochemical signalling. Here, we present data of high-resolution images of the basement membrane in developing wing discs of the fruit fly Drosophila melanogaster using atomic force microscopy. We find that depending on the developmental stage, micron-sized ripple patterns of different amplitude are present on the surface of the basement membrane that depend on the presence of individual ECM proteins.

BP 17.80 Tue 18:00 P4

Species-specific biomineral pattern formation in centric diatoms — •Francesco Leone[1], Nils Kröger[1,2], and Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, 01307 Dresden — [2]B CUBE, TU Dresden, 01307 Dresden

Diatoms are unicellular algae known for their intricately patterned cell walls, primarily composed of amorphous silica (SiO2). Their hierarchically patterns biomineral architectures display outstanding material properties but also represent an ideal model system to study species-specific pattern formation during biomineralization by living organisms. In centric "barrel-shaped" diatoms, the "lids" display three prominent pattern features: branched rib patterns with radial symmetry, nano-pores and transverse connections. How these different pattern features evolve and mutually influence each other is not known. We are extending a mathematical model of branching morphogenesis, previously developed in our group for a single model species [1], to account for the variety of patterns in related species and mutants. To facilitate a rigorous quantitative comparison to electron microscopy images, we are developing automated image analysis pipelines for the morphometric characterization of different phenotypes. Through this research, we aim to reverse-engineer putative chemical and physical mechanisms taking place during diatom silica cell wall formation.

[1] Babenko et al. PNAS 121(10): e2309518121 2024

BP 17.81 Tue 18:00 P4

Self-stimulated growth of epithelial model tissues — •Maja Milas[1], Damir Vurnek[2], Narmin Abasova[2], Kevin Höllring[2], and Ana-Sunčana Smith[1,2] — [1]Group for Computational Life Sciences, Division of Physical Chemistry, Ruđer Bošković, Institute, Zagreb, Croatia — [2]PULS Group, Center for Advanced Materials and Processes, FAU Erlangen-Nürnberg

The growth of epithelium is one of the fundamental biological processes required for sustaining the life of multicellular organisms. This process can be studied in appreciable detail using model systems such as radially growing 2D MDCK colonies. Typically, epithelium grows from low densities to the homeostatic state while expanding laterally. This process has, in the past, been captured using Fisher Kolmogorov-like growth laws, where shortly after the establishment of homeostasis, the moving front reaches a constant velocity and density profile. However, in experiments presented herein, we show that the moving front continues to accelerate and expand for days after the steady state density is achieved in the center of the colony. This radial expansion cannot be captured by currently established models, even after introducing a highly non-linear growth term and recently proposed delays. We can, nonetheless, rationalize this growth scenario by introducing self-stimulation by an activator secreted and absorbed in a density-dependent manner and coupling it with the equation for the evolution of the density. Further work is necessary to identify the biochemical pathway regulating the effect of the activator.

BP 17.82 Tue 18:00 P4

Epithelial Tissue Response Under Solid Shear Stress — •Narmin Abasova[1], Annemarie Wirth[1], Kevin Hoellring[1], Rudolf Merkel[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Institute for Theoretical Physics, FAU Erlangen- Nurnberg (IZNF) — [2]Institute for Biological Information Processes (IBI), Forschungszentrum, 52428 Jülich, Germany — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epithelial cells are subjected to a diverse range of mechanical stresses in the human body, from the dynamic forces generated during physical activity to the rhythmic pulsations of blood flow. To better understand the mechanobiological processes due to various stress types, it is essential to investigate how they influence cellular responses and tissue functionality. Among the different forms of mechanical stress, solid shear stress transmitted through the extracellular matrix (ECM) remains a relatively underexplored side of tissue mechanics. Our research addresses this gap by utilising a custom-designed device that applies controlled shear stress to the substrate supporting epithelial cell cultures. By subjecting targeted cell clusters to solid shear stress, we observe and document the tissue's behavior under a microscope. This study examines key aspects of cellular response, including stress relaxation, proliferation, morphological alterations and topological changes at cell membranes, where neighboring cells exchange positions. Using stress-generating devices in this context allows us to better understand how distinct stress types influence tissue behavior.

BP 18: Tissue Mechanics

Time: Wednesday 9:30–13:00 Location: H44

Invited Talk BP 18.1 Wed 9:30 H44

Mechanical Imprints of Cell Competition — •Benoit Ladoux — Institut Jacques Monod, Université Paris Cité & CNRS

Epithelial tissues are dynamic communities of cells characterized by close intercellular communication and highly coordinated motion. The mechanical properties of these tissues are crucial for understanding key biological processes, such as homeostasis, morphogenesis, and metastasis, and are tightly regulated through cell-cell interactions. In this presentation, I will explore the role of mechanical forces in cell competition - a process where the expansion of one cell population drives the elimination of another. I will demonstrate how intercellular force transmission governs this competitive interaction, shedding light on the interplay between mechanics and cellular mechanisms.

BP 18.2 Wed 10:00 H44

Regulation of Homeostatic Tissue Composition and Self- Organization via Pressure-mediated Cell Cycle Control in Stem Cell-Derived Epithelial Tissues — •Johannes Krämer[1], Edouard Hannezo[2], Gerhard Gompper[1], and Jens Elgeti[1] — [1]Forschungszentrum Jülich, Institute for Advanced Simulations — [2]Institute of Science and Technology Austria

Tissue homeostasis relies on a precise balance between cellular proliferation and differentiation, with spatial cell distribution playing a critical role in effective replenishment. The mechanisms governing self-renewing cell types, including their proliferation rates, mechanical interactions, and spatial organization, remain incompletely understood. Here, we present a study of epithelial tissue dynamics using a descendant lineage model derived from slow-cycling, self-renewing stem cells. Through mean-field analysis, we establish conditions for cell cycle parameters that maintain a well-defined tissue configuration and demonstrate the influence of mechanical regulation on division control. To further explore spatio-temporal properties, we implement the lineage model in an agent-based computational framework, incorporating cell-cell mechanical interactions. Our findings reveal a regime in which stem cells exhibit long-range order, forming small, localized niche-like clusters with slow diffusion. These insights offer a novel perspective on the interplay between proliferation, differentiation, and the role of mechanical interactions on the spatial organization of cells, advancing our understanding of tissue homeostasis.

BP 18.3 Wed 10:15 H44

Spatiotemporal Analysis of Active Deformation of Patient-derived Colon Cnacer — •Shogo Nagai[1], Ryo Suzuki[2], Go Yamakawa[3], Akihisa Fukuda[3], Hiroshi Seno[3], and Motomu Tanaka[1,4] — [1]Physical Chemistry of Biosystems, Heidelberg University, Heidelberg, Germany — [2]Department of Biosciences and Informatics, Keio University, Tokyo, Japan — [3]Department of Gastroenterology and Hepatology, Kyoto University Graduate School of Medicine, Kyoto, Japan — [4]Center for Integrative Medicine and Physics, Kyoto University, Kyoto, Japan

Biomedical cancer research has relied on the investigation of fixed cells and tissues, in which the non-equilibrium dynamics of cancer have been largely overlooked. Extending the recent studies shedding light on the dynamics of the isolated cells, spatiotemporal analysis of cancer on a multicellular level is expected to reveal the dynamic mechanisms of cancer progression.

In this study, the time evolution of active deformation of growing colorectal cancer organoids (miniaturized organ model) was quantitatively evaluated by the Fourier expansion. Thereby, the larger deformation of malignant genetic mutated organoids was extracted, which was attributed to the slow effective viscoelastic relaxation. The simulation of the double-cell stage indicated the characteristic dynamics of organoids could be related to cell-cell junctions. In addition, biomedical evaluations showed lower cell-cell junctions of malignant colorectal cancer on a protein and RNA level.

BP 18.4 Wed 10:30 H44

a novel 3D platform for investigating cancer cell migration and tissue organization under mechanical load — •Mattias Luber, Bruno Schmelz, Mahboubeh Farajian, and Timo Betz — Third Institute of Physics - University of Göttingen - Germany

Recent advances in tissue engineering and mechanobiology have highlighted the critical role of mechanical forces in guiding cellular organization and extracellular matrix (ECM) remodeling. Building on these findings, we introduce a novel platform for engineering connective tissues that facilitates high-resolution live imaging of self-organization and ECM remodeling under diverse experimental conditions. This platform employs controlled mechanical loading to induce fibroblast alignment, resulting in the formation of highly organized tissue structures. By enabling both global and localized measurements of tissue tension and providing precise control over mechanical load, it allows for the detailed investigation of ECM remodeling, cellular dynamics, and nuclear deformation. A key application of this platform is in uncovering how mechanical properties of the tissue environment influence cancer cell behavior. By integrating models of MDA-MB-231 breast cancer cells, we demonstrated how variations in tissue tension and ECM structure directly modulate cancer cell migration patterns. These findings highlight the critical interplay between mechanical forces and cellular invasiveness, providing insights into the biomechanical drivers of cancer progression.

BP 18.5 Wed 10:45 H44

Bridging the gap between single cell and tissue mechanics — •Mathilde G. Lettinga[1], Antje Garside[1], Vaibhav Mahajan[1], Franziska Baenke[2], Valeria Lozovanu[2], Daniel Stange[2], Ingolf Sack[3], and Anna V. Taubenberger[1] — [1]Center for Molecular and Cellular Bioengineering (CMCB), BIOTEC, Dresden University of Technology, Germany — [2]Department of Visceral, Thoracic and Vascular Surgery, University Hospital Dresden, Germany — [3]Department of Radiology, Charité - Universitätsmedizin Berlin, Germany

Tumours exhibit altered biophysical properties across spatial scales. Compared to healthy tissue, solid tumours are typically stiffer, while individual cancer cells are more compliant. The increased tissue stiffness can partly be attributed to the extracellular matrix. However, the contributions of single cell mechanics and collective cell behaviour to the emergent tissue properties remain unclear.

To bridge this gap between single cell and tissue mechanics, we have established a 3D in vitro tumour model, based on patient-derived colorectal liver metastasis organoids grown in hydrogels mimicking the extracellular matrix. Cells retrieved from dissociated organoids were mechanically characterised with real-time deformability cytometry and AFM. These data were benchmarked to the morphometric and mechanical properties of intact organoids, which were assessed in situ by confocal and Brillouin microscopy. The bulk mechanical properties of our model system were investigated using tabletop magnetic resonance elastography. Our data contribute to a better understanding of the mechanical coupling between single cells and tissues.

BP 18.6 Wed 11:00 H44

Exploring glassy dynamics in retina organoids through time-series imaging — •Alexander Johann Zangl[1], Achim Theo Brinkop[1,2], Elijah R. Shelton[1], Marie Lackmann[1,2], Teresa Rogler[1,2], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Ulm, Germany — [3]Munich Cluster for Systems Neurology (SyNergy) & Graduate School of Systemic Neuroscience (GSN), Munich, Germany

Quantifying cell dynamics and the mechanical forces guiding such movements can provide crucial insights for understanding tissue development and disease progression. Stem cell derived neuronal organoids provide an accessible system for studying nervous tissue development in the laboratory. Recently, magnetic droplet based mechanical measurements in retina organoids revealed a weak power-law scaling in the mechanical properties, suggesting that the retinal tissue is a glassy material. While the mechanical observations are consistent with predictions of soft glassy rheology, whether the movements of the individual cells making up those tissues are also in agreement with a glassy material is still unknown. Using confocal fluorescent time-series imaging, we observe the movements of nuclei in the forming retina. By tracking cells, we can determine whether cellular movements also point to the retina as a solid-like material just above a glass transition. We characterize the cell dynamics of the tissue by analysing the scaling of the mean-square displacements of the nuclei. This will help us understand how mechanical cues guide retina formation.

15 min. break

BP 18.7 Wed 11:30 H44

Statistical Inference and Selection of a Mechanistic Model during Tissue Specification in Beetle Embryogenesis — •Zoë Lange[1,2], Franziska Krämer[3], Frederic Strobl[3], Ernst H.K. Stelzer[3], and Franziska Matthäus[1,4] — [1]Frankfurt Institute for Advanced Studies — [2]Fachbereich Physik, Universität Frankfurt am Main — [3]Buchmann Institute for Molecular Life Sciences — [4]Fachbereich Informatik und Mathematik, Universität Frankfurt am Main

During development of the beetle Tribolium castaneum, the blastoderm differentiates into embryo and extra-embryonic serosa tissues with distinct morphologies. Using statistical inference, we estimate effective cell tensions and pressures based on cell geometry and a force-balance assumption. Our analysis reveals an inverse relationship between tension and cell shape with characteristic slopes for serosa and embryo tissues. We identify and parametrize a mechanistic vertex model that captures the differing properties of serosa and embryo cells. This study demonstrates how statistical inference can guide the selection and refinement of mechanistic models to understand tissue dynamics during embryogenesis.

BP 18.8 Wed 11:45 H44

Dynamics and mechanics of germband extension in *Drosophila* — •Maryam Setoudeh[1,2,3], Giulia Serafini[3], Pavel Tomancak[3,4], and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Center for Systems Biology Dresden — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Cluster of Excellence Physics of Life, TU Dresden

During *Drosophila* development, cell intercalations and cell divisions drive the extension of the germband on the dorsal side of the embryo towards its anterior. We and others [1] have recently observed that the shape of the germband is often curved, even in the wild-type, contrary to the textbook picture of a straight germband. Here, we develop a mechanical model in which the germband midline appears as an elastic line pushed by an effective force resulting from germband extension. Its motion is resisted by frictional forces from surrounding tissues and attachment at the tip mediated by the integrin scab. In this model, we discover an instability of the straight shape that explains the observed variability in the wild-type as well as the twisting phenotype observed in embryos in which scab is depleted. We also find that an alternative model of a growing rather than pushed elastic line cannot explain the observed instability. This highlights the mechanical role of these pushing forces in germband extension.

[1] Smits *et al.*, Curr. Biol. **33**, 3536 (2023)

BP 18.9 Wed 12:00 H44

A mechanical model of the symmetry breaking of the shape of the primordial hindgut — Daniel S. Alber[1,2], Shiheng Zhao[3,4,5], Eric F. Wieschaus[2,6], Stanislav Y. Shvartsman[2,6,7], and •Pierre A. Haas[3,4,5] — [1]Department of Chemical and Biological Engineering, Princeton University — [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University — [3]Max Planck Institute for the Physics of Complex Systems — [4]Max Planck Institute of Molecular Cell Biology and Genetics — [5]Center for Systems Biology Dresden — [6]Department of Molecular Biology, Princeton University — [7]Center for Computational Biology, Flatiron Institute

During early *Drosophila* morphogenesis, as the germband extends and the midgut invaginates, the initially circular primordial hindgut moves from the posterior pole of the embryo to its dorsal side and folds into a characteristic keyhole shape. Here, we develop a minimal model of this symmetry breaking in which the hindgut appears as an inextensible elastic ring in the plane. We discover that, as the area enclosed by the ring decreases (midgut invagination) while a diameter is held fixed (germband extension), the circular shape bifurcates robustly into the observed keyhole shape. Moreover, we show how embryonic curvature breaks symmetry further to select the observed orientation of the keyhole shape. This demonstrates that morphogenesis of the primordial hindgut can be a passive mechanical consequence of active deformations of the tissues that surround it.

BP 18.10 Wed 12:15 H44

What mouse embryos can teach us about tissue spreading — •María-José Franco-Oñate[1], Ricard Alert[1], and Kate Cavanaugh[2] — [1]MPI for the Physics of Complex Systems, Dresden, Germany — [2]University of San Francisco in California, United States

Processes such as embryogenesis, tissue repair and cancer metastasis are dependent upon the migration of large groups of cells through changes in group morphogenesis or collective migration. These processes entail both molecular and mechanical interactions between cells and their surrounding environment. Several attempts have been made to create models of these interactions [1].

In this study, we focus our attention on mouse embryos during implantation. In this process, the embryo adheres to the substrate and extends along it. The results of ongoing experiments indicate that embryos derived from older mice are unable to implant, resulting in a lack of spreading of the tissue that adheres to the substrate. The objective of this study is to gain insight into the mechanisms underlying the spreading process and its dependence on the age of the embryo. To this end, we employ a coarse-grained approach, in which the tissue is conceptualised as an active polar fluid, to investigate the dynamics of a spreading tissue [2]. To validate our theoretical model, we utilise traction force microscopy, which enables us to quantify the forces exerted by the tissue.

[1] R. Alert and X. Trepat. Ann. Rev. 11: 77-LF1 (2020)
[2] C. Pérez-González, R. Alert, et al. Nat. Phys. 15: 79-88 (2019)

BP 18.11 Wed 12:30 H44

Growth control in development and regeneration in the zebrafish pectoral fin — •Maximilian Kotz[1,2], Lucas de Oliveira Petrocchi Ribas[1,3], Shivani G. Ramkumar[1,3], Rita Mateus[1,3], and Benjamin M. Friedrich[1,2] — [1]PoL, Dresden, Germany — [2]cfaed, Dresden, Germany — [3]MPI-CBG, Dresden, Germany

Although all multicellular organisms can develop from a single cell, only few organism can regenerate lost body parts in adulthood. If it as an open question whether the mechanisms controlling growth in regeneration are the same as those in development. We combine theory and experiment to address this question using the pectoral fin of zebrafish as a model system. As a novel paradigm, we compare unperturbed development and regeneration after partial amputation during development. To quantify growth, we developed machine learning-based image analysis pipelines and introduce a curvilinear coordinate system to describe the geometry of the tissue. Tissue samples from different individuals became comparable by defining diffeomorphisms that minimize an elastic pseudo-energy, which enables a rigorous statistical comparison of proliferation rates, shape changes and even morphogen gradients. This quantification revealed that volume growth is driven by distinct processes. In particular, growth along the different body axes is markedly different, with thickness growth apparently uncoupled from in-plane growth. To identify the underlying mechanisms of growth control, we probe predictions from different mathematical models by investigating different amputation scenarios, along with genetic or pharmacological perturbations.

BP 18.12 Wed 12:45 H44

Model of growth arrests and proportional growth inspired by axolotl limb regeneration — •Natalia Lyubaykina[1,2], Dunja Knapp[3], Pietro Tardivo[4], Tatiana Sandoval-Guzmán[3], Elly Tanaka[4], and Benjamin M Friedrich[1,2] — [1]Cluster of Excellence 'Physics of Life', Technical University Dresden, Dresden, Germany — [2]Center for Advancing Electronics, Technical University Dresden, Dresden, Germany — [3]CRTD/Center for Regenerative Therapies TU Dresden, Germany — [4]Research Institute of Molecular Pathology, Vienna Biocenter (VBC), Campus Vienna Biocenter, Vienna, Austria

Axolotl can regenerate lost limbs even as adults, posing the question of how the size of a regenerating limb is matched to a variable animal size. Two interacting morphogens, SHH and FGF8, regulate limb development and regeneration. Inspired by this biological example, we theoretically investigate general mechanisms of morphogen-controlled growth arrest and proportional growth. In the proposed model, tissue growth increases the spatial distance between both morphogen gradients, thus providing negative feedback that eventually arrests growth. We propose two distinct scaling scenarios of morphogen gradients: either dynamic scaling with regenerating blastema size, or static scaling with animal size. We show that only the latter ensures robust growth arrest and proportional growth. We compare theory predictions to experimental quantification of SHH and FGF8 dynamics at different time points of regeneration in different-sized animals, suggestive of scaling with animal size.

BP 19: Membranes and Vesicles II

Time: Wednesday 9:30–13:00 Location: H46

BP 19.1 Wed 9:30 H46

Atomistic Insights into pH-Dependent Structural Transitions in Lipid Mesophases: A Combined MD/SAXS Approach — •Akhil Sudarsan[1], Julian Philipp[2], Joachim Rädler[2], and Nadine Schwierz[1] — [1]University of Augsburg, Augsburg, Germany — [2]Ludwig Maximilians-University, Munich, Germany

Lipid nanoparticles (LNPs) are crucial delivery vehicles for mRNA-based therapeutics, enabling the encapsulation and release of negatively charged nucleic acids through ionizable lipids that exhibit pH-dependent fusogenic activity. This study investigates ionizable DLin-MC3-DMA (MC3) lipid/cholesterol mesophases that mimic the core structure of LNPs, focusing on the inverse hexagonal (H_{II}) and inverse micellar (L_{II}) phases, both featuring an internal water domain surrounded by ionizable lipids. By combining experimental SAXS data and molecular dynamics (MD) simulations, we show that the L_{II} phase, which is stable at higher pH, transitions to H_{II} at lower pH. We also calculate the water content of the simulated core phases through comparison with scattering data and elucidate the distribution of lipids in these mesophases. We further developed an approach to compute scattering profiles directly from MD simulations, which corrects for artifacts arising from periodic boundary conditions, enabling direct, model-free comparisons between experimental and simulated data enhancing the reliability of the structural interpretations. In summary, integrating SAXS experiments and MD simulations offer molecular insights into the dynamic behaviour and pH-dependent structural transitions of ionizable lipid mesophases.

BP 19.2 Wed 9:45 H46

The effect of long-chain sphingolipids on lipid bilayers — •Clara Rickhoff, Annemarie Quas, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Münster, Germany

Lipid bilayers are found to form microdomains, so called rafts, that support a

sorting of compounds in the bilayer, and that way are thought to be essential for cellular processes, such as vesicular traffic. One type of raft that is found in lipid bilayers of e.g. yeast cells in experiments are sphingolipid-enriched and sterol-depleted domains, that seem to form gel-like domains. In our work, we conduct MD simulations of lipid bilayers containing different concentrations of long-chain sphingolipids in order to investigate their effect on the membrane at the atomistic level. The remaining part of the lipid bilayer is chosen close to experimental results (Wedlich-Söldner group, University of Münster). From these simulations we gain insight into structural properties such as of e.g. the order parameter, the RDF or the interdigitation. This allows a deeper understanding of the order of the long-chain spingolipids, their effect on the overall membrane structure and the coupling between the leaflets.

BP 19.3 Wed 10:00 H46

Engineering asymmetric lipid vesicles for protein delivery — •Kevin Jahnke, Chenjing Yang, and David Weitz — Harvard University, Cambridge, USA

The delivery of therapeutics to cells is crucial for the treatment and prevention of diseases. To enhance targeting and protect therapeutics from degradation, they are often encapsulated into drug delivery vehicles like lipid nanoparticles, liposomes and viral vectors. However, there is no universal vehicle for all cargo types including small molecules, nucleic acids and proteins. Here, we present a method for engineering lipid vesicles with asymmetric leaflets and demonstrate their ability to deliver mRNA and proteins to cells (Yang,.., Weitz, Jahnke; biorxiv 2024). We show that leaflet asymmetry modulates the biophysical properties of lipid vesicles, leading to an enhanced vesicle uptake by cells, and an up to 5-fold increased transfection efficiency with mRNA. Additionally, we show that asymmetric vesicles can deliver a variety of proteins, including the gene-editing protein Cas9 and Cas9/sgRNA complexes. By modifying lipid vesicles with polysaccharides (Jahnke et al.; PNAS 2024) or the engineering of lipid-polymer hybrid vesicles, we further achieve the targeted delivery to specific cell types. Our method and findings expand the parameter space for engineering drug delivery vehicles and demonstrate the pivotal role of leaflet asymmetry in determining the biophysical properties of lipid vesicles. Consequently, our work leads to many applications, including the formation of more efficient, universal drug carriers that enable the delivery of proteins to cells.

BP 19.4 Wed 10:15 H46

Vesicle to bicelle decomposition can be correlated with the lipid's main phase transition: a direct evidence using chain-deuterated lipid — •Carina Dargel[1,2], Lara H. Moleiro[2], Aurel Radulescu[3], Tim J. Stank[2], and Thomas Hellweg[2] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]University of Bielefeld, Physical and Biophysical Chemistry, Bielefeld, Germany — [3]FZ Jülich, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Mixtures of the phospholipid 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and the saponin β-aescin form bicelles above a critical saponin concentration. Modification of the membrane's phase state by temperature increase induces a structural growth of the bicelles resulting in membrane-like DMPC-aescin aggregates or mixed small unilamellar vesicles.

The temperature-induced transition is fully reversible, independent of the aescin content. Furthermore, the decomposition of the mixed vesicles back to bicelles shows a prominent hysteresis effect, which is correlated with the main phase transition temperature T_m of the lipid. This correlation was demonstrated for the first time by taking advantage of the shift of the membrane's T_m due to chain-deuteration and thus the use of d54-DMPC by both turbidimetry and small angle neutron scattering (SANS)[1].

[1] Dargel *et al.* (2025), Journal of Colloid and Interface Science, 679, 209-220.

BP 19.5 Wed 10:30 H46

Exploring DNA Linkers for Biomimetic Cell Adhesion of Red Blood Cells — •Sebastian W. Krauss[1], Roger Rubio-Sánchez[1], Bortolo M. Mognetti[2], Lorenzo Di Michele[1], and Pietro Cicuta[3] — [1]CEB, University of Cambridge, UK — [2]ULB, Brussels, Belgium — [3]Department of Physics, University of Cambridge, UK

Ligand-receptor interactions are fundamental to cellular membrane dynamics, influencing a range of processes like cell-cell signaling and viral infections. These interactions govern how adjacent membranes recognize, bind, and respond to one another. To better understand these mechanisms, we developed a biomimetic approach that grants precise control over the strength of interactions between opposing membranes. Our strategy employs short membrane-anchored amphiphilic DNA nanostructures featuring single-stranded 'sticky-ends', which are designed to bind through complementary sequences, providing an adaptive platform for membrane-membrane interactions [Chem. Comm. 57, 12725 (2021)]. We implemented our platform to functionalize red blood cells (RBCs), creating cellular aggregates with programmable morphologies, ranging from doublets to star-like geometries. Additionally, we used DNA-functionalized particles to selectively bind RBCs. By tuning the sequence, we precisely controlled interaction strength, enabling RBCs to progressively envelop beads. Furthermore, we employed optical tweezers to observe the rapid formation of strong bonds in situ [manuscripts in preparation]. This system offers insights into the forces and dynamics of RBC aggregation and their interactions with pathogens, such as Plasmodium species responsible for malaria.

BP 19.6 Wed 10:45 H46

Investigating Endosomal Escape Mechanisms of PEI-DNA Polyplexes with Computer Simulations — •Jonas Lehnen[1], Friederike Schmid[1], and Giovanni Settanni[2] — [1]Physik, Johannes Gutenberg Universität, Mainz — [2]Physik, Ruhr-Universität Bochum

Nucleic-acid-based therapeutics have recently demonstrated their potential thanks to the successful COVID-19 vaccination campaign. They have been already approved or in the latest stages of clinical trials as remedies for a broad range of pathologies, including cancer and genetic diseases. These approaches make use of complex delivery vehicles to take the nucleic acids to the target tissues. The presently used lipid-based nanoparticles still face a relatively low delivery rate and side effects. Polyplexes, formed by the aggregation of cationic polymers with the anionic nucleic acids, may provide a valid alternative. The transfection mechanism for these polyplexes is an ongoing topic of research. We use coarse grained molecular dynamics simulations to investigate contributing factors to the endosomal escape process which is a crucial limiting step in the transfection process. Our simulations model an endosome containing a polyplex, evaluating key factors such as the surface tension of the endosome caused by osmotic swelling and the interactions between the polyplex and the endosomal membrane, which are key factors in the predominant theories.

BP 19.7 Wed 11:00 H46

Modeling endosomal membrane budding patterns — •Felix Frey and Andela Saric — Institute of Science and Technology Austria, Klosterneuburg, Austria

Lipid membranes define cells and structure their interior. Endosomes, which are organelles that host molecular cargo sorting processes, are enclosed by flexible membranes from which small vesicles continuously pinch off. The reshaping of the endosomal membrane is mediated by filamentous proteins of the ESCRT-III family. Strikingly, in endosomes of flowering plant cells, arrays of concatenated membrane vesicles can form, which are connected either in parallel or in series with the membrane base. Here we combine coarse-grained molecular dynamics simulations and continuum theory with electron tomography to study the budding patterns at plant endosomal membranes [1]. We find that changes in ESCRT-III filament properties, such as curvature and membrane binding energy, determine the formation pathways and shapes of the emerging vesicle networks.

[1] E. Weiner*, E. Berryman*, F. Frey*, A. González Solís* et al., Proc. Natl. Acad. Sci. U.S.A. 121.44 (2024): e2409407121. *Equal contributions.

15 min. break

Invited Talk BP 19.8 Wed 11:30 H46

Rolling vesicles: From confined rotational flows to surface-enabled motion — •Laura R. Arriaga[1], Paula Magrinya[1], Pablo Palacios[1], Pablo Llombart[1], Rafael Delgado-Buscalioni[1], Alfredo Alexander-Katz[2], and Juan L. Aragones[1] — [1]Department of Theoretical Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autonoma de Madrid, 28049, Madrid, Spain — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA

Friction forces are essential for cell movement, yet they also trigger numerous active cellular responses, complicating their measurement in vivo. In this talk, we will introduce a synthetic model designed to measure friction forces between biomimetic membranes and substrates. The model consists of a vesicle with precisely controlled properties, fabricated via microfluidics, encapsulating a single ferromagnetic particle that is magnetically driven to rotate. The rotation of the particle generates a confined rotational flow, setting the vesicle membrane into motion. By adjusting the magnetic field frequency and vesicle size, the rotation frequency of the vesicle can be finely controlled, resulting in a rolling vesicle that functions as an effective tribological tool. At low frequencies, molecular contact between the membrane and substrate dominates frictional interactions, providing a measurement of the contact friction coefficient. Adjusting membrane fluidity within this model will enable the study of frictional processes in more complex biomimetic systems.

BP 19.9 Wed 12:00 H46

Dynamics of a microswimmer near a deformable boundary — •Sagnik Garai, Ursy Makanga, Akhil Varma, and Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We study the hydrodynamic interactions of swimming microorganisms with nearby deformable boundaries omnipresent in their natural habitats. The boundary, characterized by its surface tension and bending rigidity, is deformed by the disturbance flow produced by the microswimmer and thereby modifies its swimming velocities. Describing the far-field flow of the agent as a combination of a

force and torque dipole, we compute small deformations of the boundary. We further use the Lorentz reciprocal theorem to obtain leading-order corrections of its swimming velocities and compute a phase diagram based on the swimmer's initial orientation and the material properties of the deformable boundary. Our results reveal that pushers can both re-orient away from the boundary, leading to overall hydroelastic repulsion, or hover near the boundary, while pullers exhibit enhanced attraction. These findings demonstrate that the complex elastohydrodynamic interactions can generate behaviors that are fundamentally different to swimming near planar walls.

BP 19.10 Wed 12:15 H46

Uptake of microgels by membrane wrapping — •Tanwi Debnath[1], Jiarul Midya[1,2], Thorsten Auth[1], and Gerhard Gompper[1] — [1]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]School of Basic Sciences, IIT Bhubaneswar, 752050, India

The interaction of nano- and microcarriers with lipid-bilayer membranes plays a key role for cellular engulfment and drug delivery [1]. The physico-chemical parameters of the particles that control engulfment are their size, shape, and deformability [2]. Microgels are particularly versatile because their elasticity can be tuned in a wide range by changing the density of crosslinkers. Using a mass-spring model for the microgel and a continuum model for the membrane, we study microgel wrapping at lipid-bilayers. We use the Hertz theory to characterize the microgel's Young's modulus and Poisson's ratio. With the help of triangulated membranes and energy minimization, we determine the interplay of microgel and membrane deformation. We predict wrapping diagrams for microgels with various Young's moduli at membranes with various tensions. A higher microgel deformability increases the stability of partial-wrapped states; there is a transition from oblate at low wrapping fractions to cup-like shape at high wrapping fractions. Our results on this tunable and responsive system will allow the design of the microgels with optimal elastic properties for biomedical applications. [1] S. Dasgupta et al., J. Phys. Condens. Matter **29**, 373003 (2017). [2] J. Midya et al., ACS Nano **17**, 1935 (2023).

BP 19.11 Wed 12:30 H46

Shaping Cellular Interfaces — •Susanne Liese[1], Xueping Zhao[2], Tiemei Lu[3], Marcel Mokbel[4], Sebastian Aland[4], Evan Spruijt[3], Frank Jülicher[5], and Christoph Weber[1] — [1]Universität Augsburg — [2]University of Nottingham Ningbo China — [3]Radboud University, Nijmegen — [4]TU Freiberg — [5]Max Planck Institute for the Physics of Complex Systems

The interaction between liquid droplet-like coacervates and biological membranes is central to cellular organization and drives essential processes including endocytosis, intracellular transport, and signaling. In our research, we uncover the complex dynamics underlying these interactions, demonstrating how non-equilibrium processes, chemical activity, and mechanical deformations dictate the behavior of droplet-membrane systems. We demonstrate that non-equilibrium binding of biomolecular condensates to membranes gives rise to rich physical phenomena, and we also reveal how membrane reshaping contributes to behaviors such as anomalous wetting and deformation-driven uptake. By integrating experiments, theoretical models, and computational simulations, our work provides new insights into the mesoscale physics of cellular systems and reveals the intricate interplay of chemical and mechanical forces at the droplet-membrane interface. This understanding advances both fundamental biology and potential applications in synthetic biology and intracellular delivery.

BP 19.12 Wed 12:45 H46

Biomolecular condensates wetting membranes - dynamical insights from numerical simulations — •Sebastian Aland — HTW Dresden — TU Freiberg

Biological cells use membranes and condensates (liquid-like droplets) to compartmentalize their interior. As every structure within a cell is either enclosed by a membrane or by a liquid interface it is fundamental to understand what happens if these two come into contact. Recent studies suggest that membrane-droplet interactions are involved in various key biological processes. As experimental image resolution is limited at the corresponding length and time scales, numerical methods are essential to shed light on the dynamics of the process. Using a combination of sharp and diffuse interface models, we derive a mathematical model to describe the interplay of a thin elastic membrane with a two-phase fluid. We demonstrate that the wetting interaction by capillary forces leads to a range of fascinating phenomena like droplet wrapping, endocytosis and an inverted cheerios effect.

BP 20: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Wednesday 15:00–18:00 Location: H44

BP 20.1 Wed 15:00 H44

Separating bio-condensates with surfactant-like proteins — Jannik Kindermann and •Tyler Harmon — Leibniz Institute for Polymer Research, Dresden, Germany

Biocondensates are prevalent in cells as individual compartments that separate material and reactions in space. Many condensates share similar components and/or chemical interactions that drive their formation. This would suggest that the condensate:condensate interface would have a very low surface tension compared to the condensate:solvent interfaces. Supported by in vitro results, this leads to condensate-inside-condensate or dumbbell-like architectures which minimize the condensate:solvent interfaces. However, in vitro, condensates are most often isolated in space from each other. This could play important roles such as limiting the direct flow of material from one condensate to another. The mechanism in cells that separates droplets in space is unknown.

We show using simulations and theory that proteins or other biopolymers that have surfactant like molecular architectures can separate condensates in space. We show how robust this mechanism can be with respect to condensate specificity and the expression levels of surfactant-like molecules in cells.

BP 20.2 Wed 15:15 H44

Phase separation in membranes and compartments with binding reactions — •Riccardo Rossetto, Gerrit Wellecke, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization

Biological cells exhibit a hierarchical spatial organization, where various compartments and membranes harbor condensates that form by phase separation. Cells can control the emergence of these condensates by affecting the physical interactions of the involved biomolecules, thus also tuning the binding affinity to the compartments. We describe this situation with a thermodynamically-consistent kinetic model considering passive and active binding reactions to elucidate their role in controlling the occurrence and timescales of phase separation in compartments. On the one hand, binding reactions can lead to the emergence of new equilibrium phenomena, such as re-entrant phase transitions and multistability. On the other hand, they can also affect the kinetics of phase separation. As a particular example, we consider protein droplets in cellular membranes when proteins can also unbind to the cellular bulk. For fast bulk diffusion, this leads to effective nonlocal transport, which fundamentally affects droplet dynamics. For instance, the seminal Lifshitz-Slyozov coarsening can be abolished. Furthermore, active binding reactions can both accelerate or fully suppress coarsening, leading to protein patterns on the membrane. The general conclusions from our model unveil fundamental mechanisms of phase separation in membranes and compartments, and will help us explain more biological observations in the future.

BP 20.3 Wed 15:30 H44

Reconciling conflicting selection pressures in the plant collaborative non-self recognition self-incompatibility system — Amit Jangid[1], Keren Erez[1], Ohad-Noy Feldheim[2], and •Tamar Friedlander[1] — [1]Faculty of Agriculture, food and environment, The Hebrew University of Jerusalem, Rehovot, Israel — [2]Einstein Institute for Mathematics, The Hebrew University of Jerusalem, Jerusalem, Israel

Complex biological systems should often reconcile conflicting selection pressures. Specifically, in systems relying on molecular recognition, molecules should recognize particular partners, but avoid others. Here we study how such selection pressures shape the evolution of the self-incompatibility system in plants. This system inhibits self-fertilization using specific molecular recognition between proteins, expressed in the plant female and male reproductive organs. We study the impact of these opposing selection pressures on the amino acid frequencies in these proteins' recognition domain. We construct a theoretical framework enabling promiscuous recognition between proteins and multiple partners each, as found empirically, and employ stochastic simulations. We find asymmetric responses to selection affecting mostly the female, but not the male protein composition. Using large deviations theory, we well-approximate the simulated frequencies and find agreement with genomic data. Our work offers a general theoretical framework to study the impact of multiple selection pressures, applicable to additional biological systems.

BP 20.4 Wed 15:45 H44

Learning the Equilibrium Free Energy from Non-Equilibrium Steady States with Denoising Diffusion Models — •Daniel Nagel and Tristan Bereau — Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg, Germany

Estimating accurate free energy profiles is crucial for predicting the behavior of complex molecular systems. While biased molecular dynamics simulations enhance the sampling of rare events, extracting reliable free energy landscapes from these simulations remains challenging. On the other hand, stochastic thermodynamics, i.e. the concept of entropy production, provides valuable insights into the dynamics of complex systems in non-equilibrium states. However, its computational complexity, due to dependence on time-dependent probability distributions, limits its application to smaller systems.

This work presents a novel approach that combines stochastic thermodynamics with the established machine learning technique of denoising diffusion models to efficiently estimate free energy profiles from biased non-equilibrium steady states. By linking the diffusion and simulation times, we show that the training objective, known as the score, can be decomposed into a non-trivial conservative contribution from the equilibrium potential and a trivial non-conservative part determined by external driving forces. To showcase the effectiveness of our approach and its ability to learn equilibrium free energy profiles, we apply it to a driven toy model and a Martini force field molecular dynamics simulation of a small molecule biased through a lipid bilayer.

BP 20.5 Wed 16:00 H44

Multiple Pareto-optimal solutions of the dissipation-adaptation trade-off — •Jorge Tabanera-Bravo and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen

Adaptation refers to the ability to recover and maintain "normal" function upon perturbations of internal or external conditions and is essential for sustaining life. Biological adaptation mechanisms are dissipative, i.e. they require a supply of energy such as the coupling to the hydrolysis of ATP. Via evolution the underlying biochemical machinery of living organisms evolved into highly optimized states. However, in the case of adaptation processes two quantities are optimized simultaneously, the adaptation speed or accuracy and the thermodynamic cost. In such cases one typically faces a trade-off, where improving one quantity implies worsening the other. The solution is no longer unique but rather a Pareto set—the set of all physically attainable protocols along which no quantity can be improved without worsening another. We investigate Pareto fronts in adaptation-dissipation trade-offs for a cellular thermostat and a minimal ATP-driven receptor-ligand reaction network. We find convex sections of Pareto fronts to be interrupted by concave regions, implying the existence of distinct optimization mechanisms. We discuss the implications of such "compromise-optimal" solutions and argue that they may endow biological systems with a superior flexibility to evolve, resist, and adapt to different nvironments.

15 min. break

Invited Talk BP 20.6 Wed 16:30 H44

Centrosome positioning in cell migration and immune response — •Heiko Rieger — Department of Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Leukocytes are the key players of the immune system in eliminating pathogen-infected or tumorigenic cells. During these processes centrosome positioning plays a crucial role for establishing cell polarization and directed migration, targeted secretion of vesicles for T cell activation and cellular cytotoxicity as well as the maintenance of cell integrity. Here, we give an overview over microtubule organization and dynamics during immune processes and present models for centrosome repositioning during the formation of the immunological synapse and during cell migration. We focus particularly on actin-myosin crosstalk, which is involved in regulating the polarity and morphology of migrating cells and encompasses mechanical interactions, mediated by crosslinkers and molecular motors, as well as cytoskeletal regulators. Based on recent experimental results we develop a computational whole-cell model involving dynamical microtubules that interact not only mechanically but also via signaling with an active cell boundary. A rich self-organized dynamical behavior emerges, comprising varying positions of the microtubule organizing center relative to the nucleus in the migration direction, varying migration characteristics and cell shapes, and complex migratory behavior in obstacle parks and microfluidic setups. Specific dependencies of these behaviors from parameters like the average microtubule length or the cell-boundary stiffness are predicted and compared with experimental observations.

BP 20.7 Wed 17:00 H44

Modelling neuron growth dynamics and role of extra-cellular matrix — •Pritha Dolai, Federica Furlanetto, Sven Falk, Marisa Karow, and Vasily Zaburdaev — Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, Erlangen

Biological tissues are composed of cells embedded in extracellular matrix (ECM) and extracellular fluid. We study the role of cell-matrix interactions in the context of brain tissues and the mechanism of neuron growth through this matrix. We consider two modes for the neurite growth: linear growth by tip extension and growth by the traction force at the tip of the neurite with the ECM. In the second mechanism, growth happens solely due to the interaction of the growing appendages with the particles modeling the matrix. With an agent based model we recapitulate experimentally observed neuron growth patterns in healthy neurons and neurons with mutations corresponding to a disease state performed in organoid models. In experiments, neuron growth is quantified by the dynamics of the growing tips. Additionally we compare further growth characteristics such as track length and velocity of the tip, tortuosity, and angular correlation of growth direction. Our model provides mechanistic description of the neurite growth and can be useful in describing neuronal network formation during early development.

BP 20.8 Wed 17:15 H44

Cellular morphodynamics as quantifiers for functional states of resident tissue macrophages in vivo — •Miriam Schnitzerlein[1,2], Eric Greto[3,4], Anja Wegner[3,4], Anna Möller[3,4], Oliver Aust[3,4], Oumaima Ben Brahim[3,4], Stefan Uderhardt[3,4], and Vasily Zaburdaev[1,2] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — [4]Deutsches Zentrum für Immuntherapie, FAU

Resident tissue macrophages (RTMs) perform essential tasks such as clearing cellular debris to ensure tissue homeostasis. Such actions are accompanied by morphological changes in cell shape which reflect their functional states. Until now, RTMs were mostly studied *in vitro*, even though their dynamic behaviour *in vivo* is fundamentally different.

We employed a high-resolution, intravital imaging protocol to generate dynamic data of *in vivo* peritoneal RTMs of mice. Next we built a custom image processing pipeline to assess RTM morphodynamics via a set of human-interpretable cell shape and size features. Those features could quantitatively and also qualitatively differentiate between cells in different activation states. Furthermore, we showed that unperturbed RTMs exhibit a wide range of morphodynamical phenotypes, constituting a naive morphospace of behavioural motifs. Analysing cells challenged by chemical stimulations or due to aging gave us insights into how RTMs respond and adapt to inflammatory stimuli.

BP 20.9 Wed 17:30 H44

Slimming down through frustration — •Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France — PMMH, CNRS, ESPCI Paris, PSL University, Sorbonne Université, Université Paris-Cité, F-75005, Paris, France

In many disease, proteins aggregate into fibers. Why? One could think of molecular reasons, but here we try something more general. We propose that when particles with complex shapes aggregate, geometrical frustration builds up and fibers generically appear. Such a rule could be very useful in designing artificial self-assembling systems.

BP 20.10 Wed 17:45 H44

RNA fitness prediction with sparse physics based models - A way to explore the sequence space — •Christian Faber[1], Francesco Calvanese[2], Alexander Schug[1], and Martin Weigt[3] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Sorbonne-Université, Paris, France — [3]CNRS, Paris, France

The field of medicine uses macromolecules as a means of therapeutic intervention. Consequently, the functional attributes of these novel molecules are assuming greater significance. To complement the wet-lab experiments, we have devised a series of statistical physics based models that are capable of predicting the fitness of RNA molecules based on one- and two-point mutation scans. The experimental data were employed as training data to fit models of increasing complexity, commencing with an additive model and concluding with a model that accounts for global and local epistasis. The models were validated using fitness data from scans with higher order mutations of the wild-type. In contrast to conventional AI algorithms, the parameters of our models were designed for direct interpretation. In examining more distant sequences, we can distinguish the corresponding RNA family from random sequences with a high degree of accuracy. Moreover, the models facilitate interpretations of evolutionary processes and the significance of epistatic terms. Our model can be used to create a fitness landscape far beyond the experimental sequence space, thus identifying promising RNA molecules. Furthermore, the extension to the entire sequence space can be used as a blueprint for other molecules, providing a novel avenue for questions in biomolecular design.

BP 21: Networks, From Topology to Dynamics (joint session SOE/BP/DY)

Time: Wednesday 15:00–17:30 Location: H45

BP 21.1 Wed 15:00 H45

Self-organized transport in noisy dynamic networks — •Frederic Folz[1], Joshua Rainer Ganz[1], Kurt Mehlhorn[2], and Giovanna Morigi[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Algorithms and Complexity Group, Max-Planck-Institut für Informatik, Saarland Informatics Campus, 66123 Saarbrücken, Germany

We present a numerical study of multicommodity transport in a noisy, nonlinear network. The nonlinearity determines the dynamics of the edge capacities, which can be amplified or suppressed depending on the local current flowing across an edge. We consider network self-organization for three different nonlinear functions: For all three we identify parameter regimes where noise leads to self-organization into more robust topologies, that are not found by the sole noiseless dynamics. Moreover, the interplay between noise and specific functional behavior of the nonlinearity gives rise to different features, such as (i) continuous or discontinuous responses to the demand strength and (ii) either single or multistable solutions. Our study shows the crucial role of the activation function on noise-assisted phenomena.

BP 21.2 Wed 15:15 H45

Critical properties of Heider balance on multiplex networks — •Krishnadas Mohandas, Krzysztof Suchecki, and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, PL-00-662 Warsaw, Poland

Heider's structural balance theory has proven invaluable in comprehending the dynamics of social groups characterized by both friendly and hostile relationships. Extending this understanding to multiplex networks, we investigate Heider balance dynamics in systems where agents exhibit correlated relations across multiple layers. In our model, intralayer interactions adhere to Heider dynamics, while interlayer correlations are governed by Ising interactions, using heat bath dynamics for link signs. This framework reveals a multifaceted equilibrium landscape, with distinct phases coexisting across layers. Starting from a paradise state with positive links in all layers, increasing temperature induces a discontinuous transition to disorder, similar to single-layer scenarios but with a higher critical temperature, as verified through extended mean-field analysis and agent-based simulations.

We extend this analysis to Erdös-Rényi random graphs in noisy environments. We predict a first-order transition with a critical temperature scaling as p^2 for monolayers and follow a more complex behavior for bilayers. To replicate dynamics observed in complete graphs, intralayer Heider interaction strengths must scale as p^{-2}, while interlayer interaction strengths scale as p^{-1} in random graphs. Numerical simulations confirm these analytical predictions for dense graphs.

BP 21.3 Wed 15:30 H45

Functional Motifs in Food Webs and Networks — •Melanie Habermann[1,2,3], Ashkaan Fahimipour[4], Justin Yeakel[5,6], and Thilo Gross[1,2,3] — [1]Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Oldenburg, GER — [2]Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven, GER — [3]Carl-von-Ossietzky University, Institute for Chemistry and Biology of the Marine Environment (ICBM), Oldenburg, GER — [4]Florida Atlantic University, Boca Raton, FL, USA — [5]University of California Merced, Merced, CA, USA — [6]The Santa Fe Institute, Santa Fe, NM, USA

It is interesting to ask when the presence of a small subgraph in a complex network is sufficient to impose constraints on system dynamics that are independent of the broader network structure. We refer to these subgraphs as functional motifs. A classic example can be found in ecology with the competitive exclusion motif in food webs, where two species compete for the same resource without regulation. The presence of this motif precludes any stable equilibrium for the entire system. However, examples of other motifs with similarly definitive implications for system stability are rare. But our usual notion of asymptotic stability is just one among many different concepts of stability. Another one, reactivity, captures a system's immediate response to small perturbations. In this talk, we explain why functional stability motifs are rare and show that every subgraph is a functional reactivity motif. This highlights reactivity as a promising concept for exploring a vast range of networked phenomena.

BP 21.4 Wed 15:45 H45

Infecting Apex Predators Could Lead to Their Extinction — •Fakhteh Ghanbarnejad[1] and Hooman Saveh[2] — [1]SRH University of Applied Sciences, Leipzig, Germany — [2]Sharif University of Technology, Tehran, Iran

Food webs have been extensively studied from both ecological and mathematical aspects. However, most of the models studied in this area do not capture the effects of infectious diseases simultaneously. Recently, the idea of including an infectious disease in a food web model has been investigated. We study and simulate a small food chain consisting of only prey, predators, and apex predators governed by the generalized Lotka-Volterra equations and we implement the Susceptible-Infected-Recovered (SIR) model on only one of the species at a time in the food chain. To study the effects of an infectious disease on the food chain, we introduce a new parameter that increases predation rate by a factor of w and decreases hunting rate by a factor of $1/w$ for infected species. When the infectious disease is in our predators we observe that predators do not extinct under any set of parameters, however, an oscillation in its population size occurs under some circumstances which we do not observe in ordinary SIR or the generalized Lotka-Volterra equations alone. When an infectious disease is present in apex predators, oscillations in the population size do not happen; but if the set of parameters is in a specific range the apex predators may extinct. Furthermore, the chance of survival of the community, known as community persistence, increases for the predators and decreases for the apex predators.

15 min. break

BP 21.5 Wed 16:15 H45

Behavioral Heterogeneity in Disease Spread: Contrasting Effects of Prevention Strategies and Social Mixing — •Fabio Sartori[1,2] and Michael Maes[1] — [1]Chair of Sociology and Computational Social Science, Karlsruhe Institute of Technology, Karlsruhe — [2]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany

Despite mounting evidence of behavioral heterogeneity in response to disease threats, the majority of epidemiological models assume uniform behavior across populations for mathematical tractability. We analyze three distinct mechanisms of behavioral response to disease threat: susceptibility reduction (e.g., mask-wearing), active testing, and vaccination propensity. Through extensive numerical analysis, we demonstrate that the impact of behavioral heterogeneity strongly depends on the specific mechanism involved. While heterogeneous susceptibility-reducing behaviors generally decrease disease spread, heterogeneity in testing rates and vaccination propensity typically amplifies epidemic severity. Furthermore, we show that non-homogeneous mixing patterns, particularly when correlated with behavioral traits, exacerbate disease spread across all three mechanisms. These findings reveal fundamental principles about the interplay between behavioral heterogeneity and epidemic dynamics, challenging the conventional homogeneous assumption and providing important implications for public health interventions and policy design.

BP 21.6 Wed 16:30 H45

Modelling retweet cascades using multivariate Hawkes processes on sparse networks — Alexander Kreiss[1] and •Eckehard Olbrich[2] — [1]Leipzig University, Germany — [2]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

We apply a model that considers vertices in a network who are able to cast events, e.g. users of the online social media platform Twitter. Furthermore, there is a directed edge from vertex A to vertex B if A takes note of the events cast by B and changes its own behavior accordingly. More precisely, the model assumes that the activity of B increases the activity of A and likewise its other neighbors. This is called peer effects. However, there might also be other information, which also influences the activity of the vertices, e.g. the time of the day for social media posts. This is called global effects. We use a Hawkes model that incorporates, both, peer and global effects. This allows for the estimation of the network, that is, the influence structure while controlling for network effects or the estimation of the global effects while controlling for peer effects. The estimation is based on a LASSO strategy, which respects sparsity in the network. We apply this model to retweets on Twitter in order to reconstruct potential retweet cascades and identify accounts that are influential in sharing information.

BP 21.7 Wed 16:45 H45

Influence, Incidence, Imitators and Individualists: Comparing social influence models of protective behavior in an epidemic — •Andreas Reitenbach — Karlsruhe Institute of Technology, Karlsruhe, Germany

To manage a pandemic, it is critical that citizens voluntarily engage in protective behavior (e.g. masking or vaccinating). Voluntary behavior is subject to complex dynamics of social influence, however. While various models couple social influence dynamics with disease spreading, assumptions about how individuals influence each other differ markedly. Models assuming herding implement that agents imitate their peers. On the contrary, rational agents (individualists) engage in protective behavior when their peers are not and vice versa, potentially free-riding on others' contributions to herd immunity.

Here, I study whether and why these competing behavior models translate into different disease dynamics. Following a recent call to abstract from psychological mechanisms underlying social influence, I translate the behavior theories into influence-response functions.

I find that individualists self-coordinate on a moderate level of protection and

experience long-lasting but flat incidence curves. Herding, in contrast can result in rapid cycling through waves of high incidence and strong collective efforts to mitigate. Whether herders or individualists navigate an epidemic better can depend on the population's hospital capacity and disease parameters.

BP 21.8 Wed 17:00 H45

Formalism and Physical Principles of Human Mobility and Routine — •Marlli Zambrano[1], Ashish Thampi[2], Alejandra Rincon[2], Andrzej Jarynowski[1], Steven Schulz[2], and Vitaly Belik[1] — [1]Freie Universität Berlin, Germany — [2]Machine Learning Unit, NET CHECK GmbH, Berlin, Germany

The physical principles underlying human mobility have been extensively studied in recent years, enabled by the availability of large-scale mobile phone data. While significant progress has been made in understanding general mobility patterns, capturing the dynamics of individual trajectories, specifically how mobility varies from person to person and day to day, remains challenging due to the need for highly detailed and persistent data. This study addresses this challenge by examining sequences of individual daily mobility motifs, as defined by Schneider et al., from a stochastic process perspective. The analysis uses a persistent mobile phone user panel in Berlin, with high-frequency GPS data collected over four years. Twenty motifs were identified, covering 96% of all observations. The extent of inter- and intra individual variability is explored, focusing on how motifs change within individuals over time and differ between individuals in various contexts (e.g., weekends, seasons). Additionally, sequences of motifs are modeled as a stochastic process, and properties such as transition probabilities are analyzed. These findings provide deeper insights into the variability and structure of human mobility, contributing to a better understanding of individual mobility dynamics.

BP 21.9 Wed 17:15 H45

The world air transportation network: import risk of diseases, pandemic potentials and passenger routes — •Pascal Klamser[1,2], Adrian Zachariae[1,2], Benjamin Maier[3], Olga Baranov[4], and Dirk Brockmann[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Robert Koch-Institute, Berlin, Germany — [3]University of Copenhagen, Copenhagen, Denmark — [4]LMU München, München, Germany

Disease propagation between countries strongly depends on their effective distance, a measure derived from the world air transportation network. It reduces the complex spreading patterns of a pandemic to a wave-like propagation from the outbreak country, establishing a linear relationship to the arrival time of the unmitigated spread of a disease. However, in the early stages of an outbreak, what concerns decision-makers in countries is understanding the relative risk of active cases arriving in their country*essentially, the likelihood that an active case boarding an airplane at the outbreak location will reach them. While there are data-fitted models available to estimate these risks, accurate mechanistic, parameter-free models are still lacking.

We (i) introduce the "import risk" model, which defines import probabilities using the effective-distance framework, (ii) show its application to estimate the pandemic potential of emerging variants of COVID-19 and (iii) show that the effective distance shortest path tree, on which the "import risk" model is based on, is an extremely accurate representation of true passenger routes.

BP 22: Bioimaging

Time: Wednesday 15:00–17:45 Location: H46

Invited Talk BP 22.1 Wed 15:00 H46

From DNA Nanotechnology to biomedical insight: Towards single-molecule spatial omics — •Ralf Jungmann — LMU and MPI of Biochemistry, Munich, Germany

Super-resolution fluorescence microscopy is a powerful tool for biophysical and biological research. The transient binding of short fluorescently labeled oligonucleotides (DNA-PAINT) can be leveraged for easy-to-implement multiplexed super-resolution imaging that achieves molecular-scale resolution across large fields of view. This seminar will introduce recent technical advancements in DNA-PAINT including approaches that achieve sub-10-nm spatial resolution and spectrally unlimited multiplexing in whole cells followed by recent developments in novel protein labeling probes that have the potential to facilitate DNA-barcoded labeling of much of the proteome within intact cellular environments. Applications of these new approaches will be discussed in cell surface receptor imaging and neuroscience. Visualization and quantification of cell surface receptors at thus far elusive spatial resolutions and levels of multiplexing yield fundamental insights into the molecular architecture of surface receptor interactions thus enabling the future development of more refined *pattern*-based therapeutics. A key approach in implementing these methods has been to leverage standard off-the-shelf fluorescence microscopy hardware as a tool for spatial omics, thus democratizing the ability to visualize most biomolecules and probe their network-wide interactions in single cells, tissues, and beyond with single-molecule-based "Localizomics".

BP 22.2 Wed 15:30 H46

3D Single-Nanoparticle Tracking with Fluorescence Lifetime Imaging for Investigating Lipid Nanoparticles Endosomal Pathways — •Thomas Kellerer[1,2], Judith A. Müller[2], Tanja Grawert[1], Lukas Moser[1], Joachim O. Rädler[2], and Thomas Hellerer[1] — [1]Multiphoton Imaging Lab, Munich University of Applied Sciences, 80335 Munich, Germany — [2]Faculty of Physics and Center for NanoScience, Ludwig Maximilians-University, 80539 Munich, Germany

Lipid nanoparticles (LNPs) are vital for delivering mRNA in drug delivery systems, but the kinetics and intracellular pathways of their cargo release remain often unclear. To address this, we developed a microscopy technique to track single nanoparticles in 3D over extended periods. This approach integrates a lock-in amplifier for simultaneous image based 3D tracking and fluorescence lifetime measurement, enabling analysis of the microenvironment, such as pH changes. Achieving a frame rate of 7.6 fps at 1024x1024 resolution and lifetimes measured within 102 ns, our method provides novel insights into LNP dynamics and endosomal acidification in live cells. This technique was applied to study the acidification kinetics of endosomes during transfection. By measuring pH changes in real time, we provided insights into the intracellular behavior of LNPs and their role in mRNA delivery. This approach establishes a new standard for tracking nanoparticles and analyzing their microenvironments with high spatial and temporal resolution.

BP 22.3 Wed 15:45 H46

The dynamics of binding and uptake of SARS-CoV-2 viruslike particles investigated by ROCS and fluorescence microscopy — •Alexander Rohrbach and Dominik Huber — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

Viruses such as coronavirus SARS-CoV-2 are challenging to observe during interactions with sales in life-cell imaging to their small size and remarkable speed. Techniques like fluorescence microscopy often struggle to visualize these interactions, especially due to their susceptibility to bleaching and the difficulty to label different structures without altering their function.

In our research we use 200 Hz Rotating Coherent Scattering (ROCS) microscopy in order to visualize the diffusion of 100 nm sized virus-mimicking particles (VLPs) and their interactions with macro*phages or epithelial cells. ROCS is a label-free imaging technique at 160 nm resolution, using coherent backscattering of a rotating laser. By tracking VLPs with ROCS and with fluorescence, we are able to analyze their fluctuations and thereby the dynamics of diffusing VLPs close to A549 lung epithelial cells. Using spatiotemporal and spectral analysis methods, we can investigate for the first time diffusion, binding and uptake events of single VLPs at the cell periphery.

BP 22.4 Wed 16:00 H46

Visualising immune cell interactions in lymph nodes — •Anna Schepers[1], Joannah Fergusson[1], Helena Coker[1], Robert Kochl[2], and Marco Fritzsche[1] — [1]Kennedy Institute of Rheumatology, Oxford, UK — [2]King's College London, UK

The inherently multiscale immune response is regulated by diverse cell interactions, relying on cues from tissues down to single cells and subcellular structures. The intricate dynamics of the immune system present challenges for the observation of the immune response. A technological advance has been achieved with the introduction of lattice light sheet microscopy (LLSM), allowing fast and gentle imaging of live samples while achieving subcellular resolution. By complementing LLSM-based volumetric imaging with advanced sample handling of *ex vivo* tissue samples and perfusion imaging chambers, we provide a system that preserves critical physiological complexity. The perfusion system ensures oxygen and nutrient supply to maintain and sample viability while, at the same time, enabling imaging of the perfused samples. We show that in our setup, we can follow single cells and their interactions in volumes several cell layers deep in living samples within their environment, providing nuanced insights into the immune response.

15 min. break

BP 22.5 Wed 16:30 H46

Platelet biomechanics in biochemical confinement — •Vincent Gidlund, Aylin Balmes, and Tilman Schäffer — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Platelets, as part of the human blood, play a critical role in wound healing, hemostasis, and thrombotic diseases. When platelets accumulate and form plugs during wound healing, they can experience confining microenvironments. For a deeper understanding of platelet biomechanics, it is important to investigate the effects of a confining microenvironment on platelets. It is known that platelets can adapt to line-shaped microenvironments, but the mechanical properties of platelets subjected to two-dimensional confining microenvironments remain unexplored. We use microcontact printing of fibrinogen patterns of different shapes (circles, triangles) and areas to create a biochemically confining microenvironment for platelets. We then apply epifluorescence microscopy and scanning ion conductance microscopy (SICM) to measure F-actin distribution, topography, and stiffness of platelets confined to these shapes. We found that platelets adapt their morphology to match the shape of the underlying fibrinogen pattern. They show a redistribution of F-actin towards the periphery, as has been observed in other cell types. Additionally, a reduced shape area leads to decreased platelet stiffness.

BP 22.6 Wed 16:45 H46

Near infrared fluorescent silicate nanosheets for Bioimaging — •Bjoern F. Hill and Sebastian Kruss — Physical Chemistry II, Ruhr-University Bochum, Bochu, Germany

Fluorophores emitting in the near-infrared (NIR) are highly advantageous in photonics and biosensing due to reduced light scattering, low phototoxicity, and minimal autofluorescence in this spectral region.

Egyptian Blue (CaCuSi4O10) combines properties that make it a promising material for bioimaging and -photonics: It exhibits bright and stable NIR fluorescence (λ_em=935 nm), its layered structure enables exfoliation into 2D nanosheets (EB-NS), additionally it features a high quantum yield, proven biocompatibility and low production costs.

We present a surfactant-assisted exfoliation route to produce monodisperse EB-NS, tailored to nm-scale diameters, with thicknesses as low as single monolayers, while retaining their NIR fluorescence [1].

Addidionally, we demonstrate the integration of EB-NS with single-walled carbon nanotubes (SWCNTs) to create a ratiometric fluorescence sensor for dopamine. This sensor achieves robust, non-invasive imaging of neurotransmitter release from live cells, while the remarkable stability of the EB-NS fluorescence compensates for environmental fluctuations and enhances measurement reliability [2].

In summary, EB-NS represent a novel, accessible, and highly stable NIR fluorescent nanomaterial with broad applications in bioimaging and -photonics.

[1] B. Hill, et. al., RSC Adv., 2023,13, 20916-20925

[2] B. Hill, J. Mohr, et.al., Nanoscale, 2024,16, 18534-18544

BP 22.7 Wed 17:00 H46

Lysosomal activity in response to incubation of pristine and functionalized carbon nanodots — •Carla Sprengel[1], Céline David[2], Lena Berning[2], Cathrin Nollmann[1], Björn Stork[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Institute of Molecular Medicine I, Medical Faculty and University Hospital Düsseldorf, Heinrich Heine University, Düsseldorf, Germany

Fluorescent carbon nanodots (CNDs) have emerged as promising carriers for drug delivery systems due to their high biocompatibility and functionalizability. We could not find an influence of CNDs on cellular lysosomal functions, as characterized via the cathepsin B and L activity and autophagic markers p62 and LC3B-II, even under high CND concentrations. Functionalization of CNDs with branched polyethylenimin (bPEI) as a model drug conjugate leads to a greater accumulation of bPEI-CND compounds within lysosomes compared to native CNDs. Here, changes in the lysosomal size and function can be explained exclusively by bPEI. This leads us to conclude that CNDs are highly efficient and inert carriers for delivering functional molecules into lysosomes as target while minimizing lysosomal escape and therefore preventing unintended side effects on other cell organelles.

BP 22.8 Wed 17:15 H46

Grating Based X-ray Phase Contrast CT with Laboratory Setups — •Luka Gaetani[1,2], Josef Scholz[1,2], Lorenz Birnbacher[2,3], and Julia Herzen[1,2] — [1]Research Group Biomedical Imaging Physics, Department of Physics, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Chair of Biomedical Physics — [3]Institute for Diagnostic and Interventional Radiology, TUM Klinikum rechts der Isar, 81675 München, Germany

Grating-based X-ray Phase Contrast Computed Tomography (CT) represents a significant advancement in imaging, offering enhanced sensitivity to soft tissues and low-density materials by capturing phase information complementary to absorption contrast. This technique utilizes a series of optical gratings to measure phase shifts introduced by the sample, enabling the reconstruction of high-resolution phase contrast images. Laboratory-based implementations of this method, facilitated by compact X-ray sources and precise grating alignment, have extended its accessibility and applicability to diverse fields. However, optimizing these setups necessitates addressing challenges such as coherence management, efficient data acquisition, and advanced reconstruction algorithms to maximize their performance in non-synchrotron environments. This presentation will demonstrate how a grating-based interferometer enables the quantitative determination of electron density, a physical property of the sample, by accurately correlating the sample's influence on the gray values in the recorded X-ray images.

BP 22.9 Wed 17:30 H46

Nanomaterials: A Versatile Sensitizer for Enhanced Singlet Molecular Oxygen Generation — •Zahid Ullah Khan[1], Latif Ullah Khan[1,2], Hermi Felinto Brito[1], and Paolo Di Mascio[1] — [1]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [2]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan

Singlet molecular oxygen (1O2) plays a crucial role in various fields, including optoelectronics, photooxygenation reactions, and biomedical therapies, particularly as a major contributor to the success of photodynamic therapy (PDT). Since direct excitation of oxygen from the triplet ground state (3O2) to the singlet-excited state is spin-forbidden, thus, making the design of heterogeneous sensitizers crucial for efficient 1O2 production. For this purpose, nanomaterials, such as quantum dots (QDs) and rare earth fluoride nanoparticles (NPs), have emerged as versatile sensitizers for 1O2 generation, either individually or in combination with other inorganic or organic materials. Hence, conjoining the photophysical properties of QDs and rare earth NPs with other materials, e.g., coupling/combining with other inorganic materials, doping with the transition metal ions or lanthanide ions, and conjugation with a molecular sensitizer provide the opportunity to achieve high-efficiency quantum yields of 1O2 which is not possible with either component separately. Hence, the current work focuses the development of semiconductor QDs and rare earth-based nanosensitizer for efficient production of 1O2.

BP 23: Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)

Time: Wednesday 18:00–20:00 Location: P2

See O 75 for details of this session.

BP 24: Members' Assembly

Time: Wednesday 18:15–19:15 Location: H46

All members of the Biological Physics Division are invited to participate.

BP 25: Cell Mechanics II

Time: Thursday 9:30–13:00 Location: H44

Invited Talk BP 25.1 Thu 9:30 H44

Oncogenic signaling and stiffness sensing — •Johanna Ivaska — University of Turku

Tissue homeostasis is dependent on the spatially controlled localization of specific cell types and the correct composition of the extracellular stroma. Integrin-mediated adhesions, in conjunction with the actin cytoskeleton and signaling by receptor tyrosine kinases, regulate cell fate and identity and allow cells to migrate and invade the surrounding extra-cellular matrix (ECM). We have previously uncovered key differences between normal and cancer-associated stroma, whereby the mechanical and architectural features of normal stroma inhibit tumour growth and may epigenetically reprogram aggressive breast cancer cells towards a more benign phenotype. Recently, we turned our attention to other putative crosstalk mechanisms between cancer cells and the tumor microenvironment as well as tumor cell interactions with distinct tissue borders during systemic dissemination in the body. I will describe different control mechanisms guiding cancer cell invasion across physiological borders and their relevance to cancer progression and metastasis.

BP 25.2 Thu 10:00 H44

Perfect stabilization of biomolecular adhesions under load — •Anton Francis Burnet[1,2] and Benedikt Sabass[1,2] — [1]Department of Veterinary Sciences, Ludwig-Maximilians-Universität München, 80752 Munich, Germany — [2]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80752 Munich, Germany

Cell focal adhesions are complex molecular assemblies that demonstrate the remarkable capability to adapt to mechanical load by changing their size. Drawing from the molecular mechanisms believed to drive this behavior, we present a minimal adhesion model for mechanically induced aggregation of adhesion molecules. If the internal states of adhesion molecules are coupled to their aggregation dynamics sufficiently strongly, the system becomes instable and unbounded growth ensues. Unexpectedly, the very same type of instability can lead to perfect stability under mechanical load, where adhesions adapt their size to withstand arbitrarily large load without rupturing-a phenomenon we term perfect stabilization. We derive state diagrams characterizing adhesion stability under stationary load and show that perfect stabilization also occurs for dynamic loads on physiologically relevant timescales. Finally, we show that perfect stabilization is a generic phenomenon that can be realized in many different ways by coupling aggregation rates with internal molecular states and argue that the phenomenon has broad implications for understanding cellular mechanics.

BP 25.3 Thu 10:15 H44

Environmental stiffness regulates neuronal maturation via Piezo1-mediated TTR activity — •Eva Kreysing[1,2,3], Hélène Gautier[1], Leila Muresan[1], Sudipta Mukherjee[1,2,3], Alexander Winkel[1], Xiaohui Zhao[1], Ragnhildur Thóra Káradóttir[1], and Kristian Franze[1,2,3] — [1]University of Cambridge, UK — [2]FAU Erlangen — [3]MPZ Erlangen

During the development of the nervous system, neurons grow axons and dendrites to connect with other cells. As neurons become integrated into the neural network, they mature and develop electrical activity. While mechanical interactions between neurons and their environment are critical for axon growth and pathfinding, the role of mechanical cues in the electrical maturation of neurons, and thus the formation of circuits in the developing brain, remain unexplored. Here, we cultured rat hippocampal neurons on substrates with different mechanical properties and found that electrical activity developed earlier on soft hydrogels compared to stiff hydrogels. This stiffness-dependent neuronal maturation was mediated by the mechanosensitive ion channel Piezo1. Using RNA sequencing, pathway analysis and Western blots, we identified a downstream signalling cascade responsible for the differential expression of neurotransmitter receptors. Finally, we found that stiffening of the developing Xenopus brain leads to impaired synapse formation in vivo. Our findings highlight the critical role of mechanical signals in neuronal maturation and suggest that local brain tissue stiffness is a critical parameter for circuit formation in the developing brain.

BP 25.4 Thu 10:30 H44

The positioning of stress fibers in contractile cells minimizes internal mechanical stress — •Valentin Wössner[1,2], Lukas Riedel[3,4], Dominic Kempf[3], Falko Ziebert[1,2], Peter Bastian[3], and Ulrich S. Schwarz[1,2,3] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]BioQuant, Heidelberg University, Heidelberg, Germany — [3]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany — [4]Institute for Environmental Decisions, ETH Zürich, Zürich, Switzerland

Stress fibers are contractile bundles of actin filaments found in the cytoskeleton of animal cells. They play crucial roles in force generation, mechanical adaptation, shape control and mechanosensing. While the physical description of single stress fibers is well-developed, much less is known about their spatial distribution on the level of whole cells. Here, we combine a finite element method for one-dimensional fibers embedded in a two-dimensional elastic bulk medium with dynamical rules for stress fiber formation based on genetic algorithms [1]. We postulate that their main goal is to achieve minimal mechanical stress in the bulk material with as few fibers as possible. We find that stress fibers typically run through the cell in a diagonal fashion and that they cross each other under biaxial stretch. In the future, our approach can be extended to three dimensions and to stress fibers with viscoelasticity.

[1] Riedel et al., J. Mech. Phys. Solids 195 (2025) 105950

BP 25.5 Thu 10:45 H44

Towards a better understanding of the cytokinetic contractile ring — •Francine Kolley-Köchel[1] and Sebastian Aland[1,2] — [1]Faculty of Mathematics and Informatics, TU Freiberg, 09599 Freiberg, Germany — [2]Faculty of Informatics/Mathematics, HTW Dresden, 01069 Dresden, Germany

The dynamics of viscoelastic surfaces plays an important role in biological systems. One prominent example is the actin cortex, with elastic properties on short time scales and viscous on long time scale. Numerical simulations of such a system can provide a better understanding of the real biological system. Here we present a novel monolithic model of viscoelastic surfaces within a dominant surface rheology, capturing both, shear and dilational dynamics. We demonstrate that these full three dimensional simulations are numerically stable for low and high surface viscosities and show spontaneous pattern formation, induced by active stress regulation. We discuss how this model can guide future work towards a betters understanding of complex viscoelastic surface dynamics and the formation of the cytokinetic contractile ring.

BP 25.6 Thu 11:00 H44

Using microfluidics for measuring microplastic particle-cell interactions — •Matteo A. Kumar[1], Simon Wieland[1,2], Anja F.R.M. Ramsperger[1,2], Christian Laforsch[1,2], and Holger Kress[1] — [1]Biological Physics, University of Bayreuth, Germany — [2]Animal Ecology I and BayCEER, University of Bayreuth, Germany

The growing presence of microplastic particles (MPs) in the environment increases human exposure to these contaminants, which can accumulate in tissues and spread throughout the body. Various MP properties, such as shape, size, charge and surface morphology, influence their interactions with cells. We have recently shown that the zeta-potential of MPs significantly affects their adhesion to and internalization into cells*. However, the question, whether the zeta-potential directly or another underlying parameter influencing it (e.g. the number of functional surface groups) plays the decisive role, remains unsolved.

To address this, we use a microfluidic platform and combine it with a convolutional neural network to allow the measurement of hundreds of interactions in parallel. By allowing MPs with different surface functionalizations to sediment onto the cells, we determine their binding kinetics. We subsequently exert a well-defined flow force on the MPs to quantify their adhesion to the cells. Our work contributes to understanding which properties of MPs are determining particle-cell interaction and therefore identifying potential drivers for their biological impact.

*Wieland, S., Ramsperger, A.F.R.M., Gross, W. et al. Nat Commun 15, 922 (2024).

15. min. break

BP 25.7 Thu 11:30 H44

Direct mechanical communication of cellular to nuclear shape in oocytes — •Bart Vos[1], Yamini Vadapalli[2], Till Muenker[1], Peter Lenart[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Mechanics play a crucial role in a wide range of cellular processes, from differentiation to division and metastatic invasion. Additionally, mechanical signaling can regulate protein expression. Although the mechanical properties of the cytoskeleton, providing shape, motility and mechanical stability to the cell, have been extensively studied, remarkably little is known about the mechanical environment within the nucleus of a cell and the exact mechanisms of force transduction between the cytoplasm to the nucleus.

To address these questions, we apply external deformations to oocytes of different species to observe how cellular deformations can be transmitted to the nucleus, leading to nuclear deformations. We combine this with optical tweezers-based microrheology in the cellular nucleus, allowing a direct comparison between intracellular and intranuclear mechanics. The observed viscoelastic behavior of the nucleoplasm on various time scales is profoundly different from the cytoskeleton. In addition, we probe the role of activity in the mechanics of the nucleus. Depending on the mechanical properties of the cytoplasm and nucleoplasm, nuclei can be highly susceptible to external strain or be largely

shielded, suggesting a mechanical communication that might be relevant for proper oocyte function.

BP 25.8 Thu 11:45 H44

Robust mitotic events in C. elegans embryos with and without mechanical perturbations — Vincent Borne and •Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Early embryogenesis of the nematode Caenorhabditis elegans proceeds in an autonomous fashion within a protective chitin eggshell. Cell-division timing and the subsequent mechanically guided positioning of cells is virtually invariant between individuals, especially before gastrulation. By mechanically perturbing the embryo without breaking its eggshell, we have probed the limits of this stereotypical and robust developmental program. Compressing embryos to half of their native diameter frequently resulted in a loss of cytokinesis, yielding a non-natural syncytium that still allowed for multiple divisions of nuclei. The orientation of mitotic axes was strongly altered in the syncytium, but key features of division timing and spatial arrangement of nuclei remained surprisingly similar to those of unperturbed embryos in the first few division cycles. Our data suggest that few very robust mechanisms govern the progress of early embryogenesis of C. elegans.

BP 25.9 Thu 12:00 H44

Density and viscosity Measurements of the cytosol of human red blood cells — •Thomas John and Christian Wagner — Experimental Physics, Saarland University

We present a method to determine the viscosity of the intracellular liquid - the cytosol - of human red blood cells (RBCs). Our method combines the measurement of the mass density distribution of RBCs and the viscosity of the cytosol as a function of the water content. The density distribution is measured through buoyant density centrifugation combined with cell counting. By correlating this Gaussian distribution of cell population densities with the viscosity-density relation of the cytosol, we obtain a log-normal distribution of the cytosol viscosity of healthy RBCs. The viscosity contrast λ, defined as the ratio of viscosities between the RBC cytosol and the blood plasma under physiological conditions, is determined to have a mean value of $\bar{\lambda} = 10$. This value is significantly larger than those used in the literature for numerical simulations.

BP 25.10 Thu 12:15 H44

Aggregation and disaggregation of red blood cells — •Kirill Korneev[1], Nicolas Moreno[2], Thomas John[1], Christian Wagner[1], and Dmitry Fedosov[3] — [1]Experimental Physics, Saarland University — [2]Basque Center for Applied Mathematics, Bilbao Spain — [3]Theoretical Physics of Living Matter, Forschungszentrum Jülich

Laser tweezers (LT) are devices for manipulating, trapping and force measurement on particles into optical traps. Red blood cells (RBCs) are the majority of blood cells. Those cells are very deformable and show spontaneously forming complex structures at rest state, due to aggregation. The mechanisms of RBCs aggregation are not fully understood, however there are currently two main hypotheses that can explain it: the bridging model based on mobile and immobile bonds, and the depletion layer model. In this work, experimental values of the RBCs disaggregation force were obtained by stretching RBC aggregates. We will show, that the mechanism of RBCs disaggregation involves these two hypotheses. We will also show that the bridging model with mobile bonds reproduces well the corresponding experimental data, offering insights into the interplay between bridging and depletion interactions and providing a framework for studying similar interactions between other biological cells.

N. Moreno, et al., Aggregation and disaggregation of red blood cells: depletion versus bridging, bioRxiv 2024.11.20.624311 (2024)

BP 25.11 Thu 12:30 H44

Dynamic states of P. falciparum infected erythrocytes adhering in shear flow - a qualitative study of rolling and flipping motions — •Katharina Scholz[1], Leon Lettermann[2], Jessica Kehrer[3], Michael Lanzer[3], Ulrich Schwarz[2], and Motomu Tanaka[1] — [1]Institute for Physical Chemistry, University of Heidelberg, Germany — [2]Institute for Theoretical Physics, University of Heidelberg, Germany — [3]Center of Infectious Diseases, Heidelberg University Medical School, Germany

As surviving strategy, the malaria parasite remodels the red blood cell by causing the expression of adhesive proteins on its surface. The modification allows the infected cell to adhere to the endothelial cells in the blood stream, thereby avoiding clearance by the spleen.

This transformation also alters cell shape and movement behaviour during development. We used Reflection Interference Contrast Microscopy (RICM) in quantitative flow chamber experiments and employed a high-speed camera to gain more information about the contact footprint of cells. With this setup, we tracked parasitised erythrocytes individually, label-free and non-invasively. Early-stage trophozoites exhibited flipping behaviour, while late-stage schizonts showed a steady rolling motion. Our results provide a quantitative understanding of how parasite development affects dynamic cytoadhesion behaviour and shed light on understanding endothelial cell activation.

BP 25.12 Thu 12:45 H44

Deformability cytometry for large-scale mechano-genomic screening in interphase and mitosis — •Laura Strampe[1], Katarzyna Plak[2,3], Christine Schweitzer[1], Cornelia Liebers[1,2], Buzz Baum[3], Jona Kayser[1], and Jochen Guck[1,2] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Biotechnology Center of TU Dresden, Dresden, Germany — [3]MRC Laboratory of Molecular Biology, Cambridge, United Kingdom

We demonstrate the scalability of real-time fluorescence and deformability cytometry (RT-FDC) for large-scale cell cycle-resolved mechano-genomic screening. Using RNA interference, we screened 215 kinase and phosphatase genes on their effects on cell mechanics in interphase and mitosis. RT-FDC combines high throughput (up to 100 cells per second) with fluorescence-based cell cycle classification, enabling single-cell mechanical phenotyping of entire populations. We show that cell cycle resolution is essential for identifying genetic regulators of cell mechanics, as stiffness differences between interphase and mitotic cells can obscure genuine knockdown effects or generate false-positive hits. Genes regulating mitotic mechanics or softening cells upon knockdown are particularly likely to be masked. Of the 81 genes identified as affecting cell stiffness, 22 were detected only through cell cycle resolution. These include *PRL-1*, a cancer metastasis marker with opposing effects across the cell cycle: stiffening interphase cells and softening mitotic cells. This suggests that *PRL-1* overexpression in metastatic cells expands the range of mechanical phenotypes during cell cycle progression, facilitating tumor adaptability.

BP 26: Synthetic life-like systems and Origins of Life

Time: Thursday 9:30–12:15 Location: H46

BP 26.1 Thu 9:30 H46

Heat flows through rock cracks purify life's building blocks and protect RNA from hydrolysis — •Paula Aikkila[1], Thomas Matreux[2], Dieter Braun[1], and Christof Mast[1] — [1]Ludwig-Maximilians-Universität München — [2]ESPCI Paris

The emergence of biopolymer building blocks is a crucial step during the origins of life. However, their synthesis pathways usually require feedstocks of pure reactants and defined purification and mixing steps to suppress unwanted side reactions, which is required for high product yields. We show that heat flows through thin crack-like compartments purify complex mixtures of prebiotically relevant building blocks and drive prebiotically relevant reactions such as the dimerization of glycine. In these same compartments, we furthermore study how heat-flows can locally switch on and off pH gradients, thereby enabling or disabling RNA hydrolysis depending on their hybridization state. We seek to explore how this enables spontaneous symmetry breaking in the sequence and folding space, possibly facilitating the emergence of functional ribozyme.

BP 26.2 Thu 9:45 H46

Membraneless protocell confined by a heat flow — •Alexander Floroni[1], Noël Yeh Martín[2], Thomas Matreux[1], Laura Weise[3], Sheref Mansy[4], Hannes Mutschler[5], Christof Mast[1], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich; München, Germany — [2]Institute of Biotechnology HiLIFE, University of Helsinki, Helsinki, Finland — [3]MPI of Biochemistry; Martinsried, Germany — [4]Department of Chemistry, University of Alberta; Edmonton, Canada — [5]Department of Chemistry and Chemical Biology, TU Dortmund; Dortmund, Germany

In living cells, a complex mixture of biomolecules is assembled within and across membranes. This state is maintained by a sophisticated protein machinery. It imports nutrients, removes waste, and orchestrates cell division. Here we show how the molecular contents of a cell can be coupled in a coordinated way to the non-equilibrium of a heat flow. A temperature difference across a water-filled pore accumulated the core components of a modern cell to make a functional reaction. The mechanism arose from the interplay of convection and thermophoresis. Protein synthesis was triggered as a direct result of the up-concentration. The same non-equilibrium setting continued to attract nutrients from an adjacent fluid stream, while keeping the cellular molecules confined. Our results show how a simple and archaic non-equilibrium physical process can assemble the many different molecules of a cell and trigger its basic functions. The framework provides a membrane-free environment to bridge the long evolutionary times from an RNA world to a protein-based cell-like proto-metabolism.

BP 26.3 Thu 10:00 H46

A game of life with dormancy — •Daniel Henrik Nevermann[1], Claudius Gros[1], and Jay Lennon[2] — [1]Institute for Theoretical Physics, Goethe-University Frankfurt, Germany — [2]Department of Biology, Indiana University, Bloomington, IN 47405, USA

The factors contributing to the persistence of life are fundamental for understanding complex living systems. Many species contend with harsh environments by entering a reversible state of reduced metabolic activity, a phenomenon known as dormancy. Here, we develop Spore Life, a model to investigate the effects of dormancy on population dynamics. It is based on Conway's Game of Life, a deterministic cellular automaton where simple rules govern the metabolic state of an individual based on its neighborhood. For individuals that would otherwise die, Spore Life provides a refuge in the form of an inactive state. These dormant individuals (spores) can resuscitate when local conditions improve. The model includes a parameter $\alpha \in [0, 1]$ that controls the survival probability of spores, which yields stochastic dynamics between the limits $\alpha = 0$ (Game of Life) and $\alpha = 1$ (Spore Life). In addition to identifying the emergence of unique periodic configurations, we find that spore survival increases the average number of active individuals and buffers populations from extinction. Contrary to expectations, the population stabilization does not require large and long-lived seed bank. Instead, the demographic patterns in Spore Life only require a small number of resuscitation events. Spore Life can be interactively explored at `https://itp.uni-frankfurt.de/spore-life/`.

BP 26.4 Thu 10:15 H46

Continuous Evolving Game of Life with Diversity — •Alexandre Guillet and Frank Jülicher — MPI-PKS, Dresden, Germany

The complex phenomenology of J. Conway's "Game of Life" cellular automaton, in particular its gliders, has been translated into continuous fields in space and time in a 2011 preprint by S. Rafler. The striking organic feel associated with these artificial life simulations in isotropic space has attracted the attention of a growing online community at the intersection of citizen science and computer art, which has recently culminated in the exploration and classification of the diverse morphologies of the "Lenia" gliders by BWC. Chan and others.

Our research focuses on a minimal variant of these continuous nonlinear dynamical systems that is capable of generating gliding, self-replicating and vanishing patterns, with striking resemblance to cell division, motility and death. Elaborating upon the governing partial integro-differential equation, we allow each cell to carry individual variations of the parameters, thus introducing a spatial diversity of rules. A conservation law is enforced on the resources of the cells as a selection pressure, together with a mutation process as a random source of diversity. The spontaneous evolution of the system from a single cell leads to a rich phenomenology, ranging from mycelial growth to epithelia and amoeboid motion.

This continuous and evolving model with diversity raises the Game of Life into a toy model for the morphogenesis and evolution of primordial lifeforms.

BP 26.5 Thu 10:30 H46

Cooperative effects in compartmentalized irreversible self-assembly — •Richard Swiderski, Severin Angerpointner, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

From biomolecular compartments, protein patterns to porous rocks: Many biological and chemical systems like living cells or prebiotic chambers exhibit some form of spatial organization which separates biochemical processes. This is known to play a key role in the assembly of virus capsids or the enrichment of prebiotic chemicals. We systematically explore the effects of such spatial separation on the self-assembly of irreversibly binding identical particles. We show that already in a simplified model of two coupled biochemical compartments cooperative effects emerge through limiting compartment exchange. Further, these findings generalize to spatially extended systems like intracellular chemical gradients or membrane-assisted assembly.

15 min. break

Invited Talk BP 26.6 Thu 11:00 H46

Theory for sequence selection via phase separation and oligomerization — •Christoph Weber — University of Augsburg, Universitätsstr. 1, 86159 Augsburg

Non-equilibrium selection pressures were proposed for the formation of oligonucleotides with rich functionalities encoded in their sequences, such as catalysis. Since phase separation was shown to direct various chemical processes, we ask whether condensed phases can provide mechanisms for sequence selection. To answer this question, we use non-equilibrium thermodynamics and describe the reversible oligomerization of different monomers to sequences at non-dilute conditions prone to phase separation. We find that when sequences oligomerize, their interactions give rise to phase separation, boosting specific sequences' enrichment and depletion. Our key result is that phase separation gives rise to a selection pressure for the oligomerization of specific sequence patterns when fragmentation maintains the system away from equilibrium. Specifically, slow fragmentation favors alternating sequences that interact well with their environment (more cooperative), while fast fragmentation selects sequences with extended motifs capable of specific sequence interactions (less cooperative). Our results highlight that out-of-equilibrium condensed phases could provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de novo life.

BP 26.7 Thu 11:30 H46

Prebiotic RNA Replication through Templated Ligation by Humidity and pH Cycles — •Felix T. Dänekamp and Dieter Braun — Systems Biophysics LMU, Munich, Germany

To replicate long RNA strands, templated ligation from 2',3'-cyclic phosphate RNA is a promising pathway. Preliminary screenings suggest that through tuning of monovalent salt content and through adding Lysine or other amino acids to the solution, no additional catalysts are required to attain yields of 50% ligation product in one day. Cycling physical conditions such as pH and salt/RNA concentration likely solves the strand inhibition problem. This opens up the possibility of prebiotic ligation chain reactions and thus open-ended evolution from short RNA strands.

BP 26.8 Thu 11:45 H46

Gravitationally induced oscillations of active droplets — •Advait Thatte[1], Judit Sastre[2], Alexander Bergmann[2], Michele Stasi[2], Marta Tena-Solsona[2], Job Boekhoven[2], and Christoph Weber[1] — [1]Faculty of Mathematics, Natural Sciences, and Materials Engineering, and Institute of Physics, University of Augsburg, Universitätsstrasse 1, 86159 Augsburg, Germany — [2]Department of Bioscience, School of Natural Sciences, Technical University of Munich, Lichtenbergstrasse 4, 85748 Garching, Germany

Oscillations in the formation and dissolution of compartments inside living cells are pivotal in orchestrating various cellular functions and processes. Recent experiments on synthetic cells showed the spontaneous emergence of spatio-temporal oscillations in the number of droplets, their size, and position. Oscillations occur because droplets grow via gravitationally induced fusion above their stationary size. As a result droplets shrink, feeding the nucleation of new sedimenting droplets, restarting the cycle. The stationary droplet size is a consequence of deactivating droplet material inside and activating outside. Here we present a theoretical model for phase separation with non equilibrium chemical fuelling including a sharp interface model for many active droplets. The model quantitatively describes the stationary droplet size and the oscillation frequency observed experimentally.

BP 26.9 Thu 12:00 H46

Linking fitness landscape topography to the characteristics of the underlying genotype-phenotype map — Malvika Srivastava[1,2], Ard A. Louis[3], and •Nora S. Martin[4] — [1]Institute of Integrative Biology, ETH Zurich, Zurich, Switzerland — [2]Swiss Institute of Bioinformatics, Lausanne, Switzerland — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, UK — [4]CRG (Barcelona Collaboratorium for Modelling and Predictive Biology), Dr. Aiguader 88, Barcelona 08003, Spain

The topographies of fitness landscapes are central in models of evolutionary processes. Key topographical features include the prevalence of fitness peaks, as well as the existence of accessible (i.e. fitness-increasing) paths to the global fitness optimum. Recent numerical work found that such accessible paths commonly exist in fitness landscapes based on biophysical models of genotype-phenotype (GP) maps, even when fitness values are randomly assigned to phenotypes [1]. Here, we examine such landscapes with random phenotype-fitness assignment more thoroughly to investigate, how their topography depends on the characteristics of the underlying GP map. By simplifying the GP map to a "neutral component" (NC) graph, we can compute the expected prevalence of fitness peaks based only on two GP map characteristics: the evolvabilities and sizes of NCs. Evolvabilities are also important for peak heights and for the existence of accessible paths to global optima. [1] S. F. Greenbury, A. A. Louis, S. E. Ahnert, Nat Ecol Evol. 6, 1742-1752 (2022).

BP 27: Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Thursday 15:00–17:30 Location: H24

Invited Talk BP 27.1 Thu 15:00 H24

Infrared Nanoscopy and Tomography of Intracellular Structures — Joachim Heberle[1], Katerina Kanevche[1], •Emmanuel Pfitzner[1], David Burr[2], Janina Drauschke[2], Andreas Elsaesser[2], and Jacek Kozuch[1] — [1]Freie Universität Berlin, Department of Physics, Experimental Molecular Biophysics, — [2]Experimental Biophysics and Space Sciences, Arnimallee 14, 14195, Berlin, Germany

Although techniques such as fluorescence-based super-resolution imaging or confocal microscopy simultaneously gather morphological and chemical data, these techniques often rely on localized and chemically specific markers. To eliminate this flaw, we have developed a method of examining cellular cross-sections using the imaging power of scattering-type scanning near-field optical microscopy (sSNOM) and Fourier-transform infrared spectroscopy at a spatial resolution far beyond the diffraction limit (nanoFTIR). Herewith, nanoscale surface and volumetric chemical imaging are performed using the intrinsic contrast generated by the characteristic absorption of mid-infrared radiation by the covalent bonds. We employ infrared nanoscopy to study the subcellular structures of eukaryotic (C. reinhardtii) and prokaryotic (E. coli) species, revealing chemically distinct regions within each cell. Serial 100 nm-thick cellular cross-sections were compiled into a tomogram, yielding a three-dimensional infrared image of subcellular structure distribution at 20 nm spatial resolution. The presented methodology can image biological samples with less interference due to the low energy of infrared radiation and the absence of labeling.

Invited Talk BP 27.2 Thu 15:30 H24

Coherent Raman Imaging — •Michael Schmitt[1] and Juergen Popp[1,2] — [1]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Albert-Einstein-Straße 9, 07745 Jena, Germany

Raman-based technologies have profoundly impacted life sciences and biomedical research. Despite their unmatched molecular specificity, traditional Raman spectroscopy suffers from limited sensitivity, making it less suitable for rapid imaging. This limitation is addressed by coherent Raman scattering (CRS) microscopy, primarily through coherent anti-Stokes Raman scattering (CARS) and stimulated Raman scattering (SRS). This talk examines the potential of CARS and SRS imaging for biological and biomedical analysis, offering detailed insights into the molecular composition of biomedical specimens, such as cells or tissue. The presentation will focus on the applications of these techniques in molecular and functional diagnostics in the fields of medicine and life sciences. Furthermore, recent developments in translating CRS into compact, clinically viable systems, such as handheld probes, will be presented, focusing on intraoperative tumour diagnostics for early detection and improved improved therapeutic outcomes.

Acknowledgement: Financial support of the EU, the *Thüringer Ministerium für Wirtschaft, Wissenschaft und Digitale Gesellschaft*, the *Thüringer Aufbaubank*, the BMBF, the DFG, and the Carl Zeiss Stiftung is acknowledged.

Invited Talk BP 27.3 Thu 16:00 H24

Sum Frequency Generation Microscopy of Electrochemical Interfaces — •Steven Baldelli — University of Houston, Houston, Texas

Sum frequency generation spectroscopy (SFG) is a valuable technique to study the molecular properties of surfaces. As a second-order technique, it is uniquely sensitive to the average organization of molecules at the surface. However, as most surfaces are spatially heterogeneous, it isn't easy to interpret the spectrum as a single domain. The development of SFG into microscopy has allowed a more detailed and accurate analysis of the spatio-spectro-temporal evolution of surface chemistry. The SFG microscope development will be presented, and compressive sensing and the application toward electrocatalysis will be used.

BP 27.4 Thu 16:30 H24

Elucidating the Composition, Order, and 3D Molecular Orientation of Thin Films with Phase-Resolved Sum-Frequency Generation Microscopy — •Alexander Fellows, Ben John, Martin Wolf, and Martin Thämer — Fritz-Haber-Institute, Berlin, Germany

The vast majority of molecular interfaces have highly heterogeneous structures, ranging across all length-scales. These manifest as variations in density, composition, and molecular packing structure, all of which are critical in controlling the macroscopic properties and functional behaviour of the films. While various chemical imaging techniques can access many of these important structural details, characterising their relative order and specific packing arrangements represents a formidable challenge.

Here, we present a chemical imaging approach based on phase-resolved sum-frequency generation (SFG) microscopy. By probing molecular vibrations, this technique achieves molecular recognition and thus is sensitive to the local composition and density. Furthermore, through its symmetry selection rules, output SFG signals are dependent on absolute molecular orientations. This hence allows it to distinguish different molecular conformations and characterise the amount of orientational order in the system. Finally, with an azimuthal-scanning approach, the in-plane and out-of-plane signal contributions can be separated, allowing the 3D molecular orientations to be elucidated. By applying SFG imaging to model lipid monolayers, we gain an unprecedented overview of their hierarchical packing structures.

BP 27.5 Thu 16:45 H24

Low temperature multimode atomic force microscopy using an active MEMS cantilever — Michael G. Ruppert[1], Miguel Wiche[2], André Schirmeisen[2], and •Daniel Ebeling[2] — [1]University of Technology Sydney, Australia — [2]Justus Liebig University Giessen, Germany

Low-temperature atomic force microscopy (AFM) is one of the most powerful tools in surface science. With the chemical bond imaging technique, i.e., by using CO functionalized AFM tips, it became possible to visualize the chemical structure of individual organic molecules, which is essential for studying on-surface reactions and molecular manipulation processes. Routinely, such measurements are performed with qPlus sensors. Here, we present a proof of concept for an active microelectromechanical systems (MEMS) microcantilever with integrated piezoelectric sensing and demonstrate its capability to obtain scanning tunneling microscopy as well as high-resolution non-contact atomic force microscopy images on an atomically flat Au(111) surface. Equipped with a focused ion beam deposited tungsten tip, the active MEMS cantilever is able to obtain high contrast scanning tunneling and frequency shift images at the fundamental and a higher eigenmode of the cantilever. This is interesting for the application of multifrequency AFM operation modes that could enhance the capabilities of the bond imaging technique.

BP 27.6 Thu 17:00 H24

Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD) — •Lukas Eriksson[1], Tim Esser[1,2], and Stephan Rauschenbach[1] — [1]University of Oxford, Oxford, UK — [2]Thermo Fisher Scientific, Eindhoven, Netherlands

Direct imaging of (bio-)molecules with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for elucidating molecular structure. However, sample preparation can be a major challenge: either very time- and resource-intensive or incompatible with the vacuum environment required by the imaging method.

Here, we explore preparative mass spectrometry as an alternative workflow towards structural elucidation of biomolecules. A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Scientific Orbitrap UHMR) allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules (m = 100 to 10^6 Da) onto various surfaces, including cryo-EM grids and metal crystals for SPM. Successful deposition and subsequent imaging requires extensive control over conditions such as pressure, temperature, ion trajectories, sample surfaces, and sample transfer to obtain clean, chemically pure samples of the desired species in the right (i.e. native) configuration. The sample holder also enables controlled growth of ice layers for embedding deposited molecules, allowing high-resolution reconstructions of proteins from cryo-EM.

BP 27.7 Thu 17:15 H24

LFM study of copper oxide — •Sophia Schweiss, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Regensburg, Deutschland

Small-amplitude FM-AFM is a method to study surfaces and adsorbates with atomic resolution. At low temperature, the tip apex can be prepared so that it ends in a single O-atom, making the tip inert and enhancing imaging [1, 2]. With a laterally oscillating tip, i.e. lateral force microscopy (LFM), the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction can also be independently measured. Here too, inert tip apices are commonly used. One measurement of E_{diss} relies on the cocking and snapping of the tip over a single chemical bond, for which the current state of the art utilizes CO-terminated tips. In this work, a CO-terminated tip [1] is used to investigate the (2×1)O reconstruction of Cu(110) with LFM. Simulations are performed to guide interpretation. In this larger ongoing study, these LFM measurements will be repeated for a CuOx tip [2] to evaluate it as a tool for measuring E_{diss}.

[1] Gross et al., Science, **325**, 1110 (2009)
[2] Mönig et al., Nat. Nano., **13**, 371 (2018)

BP 28: Microswimmers and Microfluidics (joint session DY/BP/CPP)

Time: Thursday 15:00–17:45 Location: H37

Invited Talk BP 28.1 Thu 15:00 H37

Light-Driven Manipulation of Passive and Active Microparticles — •Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Germany

Chemical gradient near a solid/liquid can result in lateral long-range fluid transport termed diffusioosmotic (DO) flow. For instance, when photosensitive surfactant is irradiated with light converting the majority of the molecules in one of the possible isomers, emerging concentration gradient of isomers generates an osmotic pressure gradient tangent to the wall actuating the surrounding liquid to flow. [1-3] In my talk I will show how one can manipulate microparticles and even induce their self-propulsion by light urtilizing light driven diffusioosmotic (LDDO) phenomenon. Depending on the applied wave length one can either disperse/remove or gather particles. We will discuss how to establish light-driven hydrodynamics as a useful and versatile tool for investigating collective motion of self-propelled particles and aggregation

[1] Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S. Scientific Reports, 6 (2016) 36443. [2] Santer, S. J. Phys. D: Applied Physics, 51 (2017) 013002. [3] Arya, P.; Umlandt, M.; Jelken, J.; Feldmann, D.; Lomadze, N.; Asmolov , E. S.; Vinogradova, O. I.; Santer, S. A. The European Physical Journal E, 44(50) (2021), 1-10.

BP 28.2 Thu 15:30 H37

Regulated polarization of active particles in local osmotic flow fields — •Lisa Rohde, Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Regulation in living systems is a fundamental principle for achieving robust functionality and maintaining specific non-equilibrium states. The control of certain properties and functionalities of systems on the microscale presents particular challenge since thermal fluctuations and environmental perturbations dominate. While synthetic active matter has demonstrated remarkable self-organization capabilities, examples of autonomous regulation processes at the single-particle level remain scarce. Here, we show experimentally that the interplay of two non-equilibrium processes leads to a regulated polarization state of active particles in local osmotic flow fields. Based on thermophoretic repulsive and attractive forces that are generated by a single heat source at the boundary, the active particles encircle the heat source at a stable distance depending on the heat source temperature. The balance of these temperature-induced processes causes a polarization of the active particles that is independent of the heat source temperature. The individual control of heat source and active particles in the experiment allows detailed investigation of the self-regulated polarization effect in which we find hydrodynamic interactions to dominate. As the effects rely on osmotic flows and phoretic interactions, we expect that the observed phenomena can be generalized to other active systems and flow fields.

BP 28.3 Thu 15:45 H37

Active particle steering in three dimensions — •Gordei Anchutkin and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Synthetic active particles serve as a model system that mimic the self-propulsion of living matter to explore fundamental aspects of non-equilibrium physics. Various collective phenomena of active agents have been studied, but mostly in the presence of hydrodynamic and physicochemical boundary effects. While theoretical works predict different collective dynamics in 3D, experimental investigations remain limited due the lack of experimental control over active swimmers in three dimensions.

Here we introduce three-dimensional control to the study of synthetic active matter. We demonstrate simultaneous control of thermophoretic microswimmers in 3D using single-particle tracking through digital holography and dark-field pattern tracking, with real-time wavefront shaping for steering. With the help of these experiments, we explore the interplay of thermophoretic propulsion, gravity, and optical forces for the active particles. By creating a three-dimensional active ensemble, we reveal how bulk interactions and boundary effects shape the collective behavior of active particles.

BP 28.4 Thu 16:00 H37

***Trypanosoma brucei* in microchannels: the role of constrictions** — •Zihan Tan, Julian I. U. Peters, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Trypanosoma brucei (*T. brucei*), a single-celled parasite and natural microswimmer, is responsible for the fatal sleeping sickness in infected mammals, including humans. Understanding how *T. brucei* interacts with fluid environments and navigates through confinements is crucial for elucidating its movement through blood vessels and tissues, and across the blood-brain barrier.

Using a hybrid multiparticle collision dynamics (MPCD)–molecular dynamics (MD) approach, we investigate the locomotion of an in-silico *T. brucei* in three types of fluid environments: bulk fluid, straight cylindrical microchannels, and microchannels with constrictions. We observe that the helical swimming trajectory of the in-silico *T. brucei* becomes rectified in straight cylindrical channels compared to bulk fluid. The swimming speed for different channel widths is governed by the diameter of the helical trajectory. The speed first slightly increases as the channel narrows and then decreases when the helix diameter is compressed. An optimal swimming speed is achieved when the channel width is approximately twice the bulk helix diameter. Furthermore, *T. brucei* notably slows down when entering the narrow constriction in a microchannel and strongly speeds up upon exiting due to a release of deformation energy of the straightened cell body.

BP 28.5 Thu 16:15 H37

Helical motion of microorganisms can be more persistent than straight motion — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[2], Freddy Frischknecht[2], and Ulrich S. Schwarz[1] — [1]BioQuant & Institute for Theoretical Physics, Heidelberg University — [2]Center for Integrative Infectious Disease Research, Heidelberg University

The movement of microorganisms has been extensively modeled by stochastic active particle models. In three dimensions, both swimming microorganisms, like sperm cells and some bacteria, and gliding microorganisms, like malaria sporozoites in the skin, often exhibit helical trajectories. If the internal driving force is the primary source of noise in the system, it induces random, yet time-correlated variations in the torque. To investigate this effect, we introduce a three-dimensional active rotational Ornstein-Uhlenbeck particle model. We find that the presence of a rotational component and the resulting helical path can mitigate the effect of intrinsic noise in the drive, allowing for larger long-time mean square displacements than straight movement at the same speed. The model not only provides qualitative insights into the constraints faced by microbes that may have led to the evolutionary selection of certain motility patterns, but also presents an analytical, quantitative tool for extracting information from these movements. We present and analyze corresponding data for malaria parasites gliding through hydrogels.

15 min. break

BP 28.6 Thu 16:45 H37

Corrugated channels can filter ciliated microorganisms based on the metachronal wavelength — •Gonçalo Antunes and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Many microorganisms (e.g. Paramecium) move by a carpet of cyclically beating cilia that cover their surface. These cilia often beat in an organized fashion, such that the beating phases form a traveling wave, referred to as a metachronal wave. In this study, we investigate the swimming of such microorganisms in corrugated microchannels. We model the motion of the cilia via a time-varying effective slip velocity applied on the microorganism's surface, which we approximate as an infinite slab. By employing the lubrication approximation, we show analytically that the swimming speed of ciliated microorganisms placed inside a corrugated channel is sensitive to the corrugation height, provided that the wavelength of the corrugation matches that of the metachronal wave. Indeed, the direction of motion itself may invert with respect to swimming in bulk fluid, with the channel acting as a virtual barrier which blocks microorganisms under specific conditions for corrugation and slip-velocity modulations, but allow others to pass through. We also show that the interplay between the corrugation and the slip velocity profile allows for the swimming of microorganisms with zero time-averaged slip velocity, which thus cannot swim in bulk fluid. Finally, we complement our theory with preliminary results from hydrodynamic simulations for radially-symmetric microorganisms of finite length in radially-symmetric corrugated channels.

BP 28.7 Thu 17:00 H37

Motion of a single particle partially exposed in a simple shear flow — •Dominik Geyer[1,2], Aouane Othmane[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), FZ Jülich — [2]Department of Physcis, FAU Erlangen-Nürnberg

Sand immersed in the water can be imagined as a wet granular matter. Besides sedimentation, friction, and surface roughness are two relevant physical phonemes within this system. Many body systems in a turbulent regime have been studied using discrete elements methods for a long time, but a single particle in the Stokes flow regime is particularly interesting for biological systems and microfluidic devices.

A layer of quadratic-arranged spheres models the rough surface. The question arises of how to describe the motion of a single traveling particle over this substrate.

We choose a combined numerical and analytical approach. The Stokes equation is solved analytically for the sphere near a rough wall. Lattice Boltzmann simulations with momentum-exchange particle coupling are performed for different wall roughness and friction coefficients.

Although, the Stokes equation assumes that the particle Reynolds number is zero. Surprisingly, the numerical results match our theoretical description until a particle Reynolds number of two. In this regime, friction between the moving particle and the substrate significantly influences the angular velocity but has a minor influence on the traveling velocity in the flow direction.

BP 28.8 Thu 17:15 H37

Rational Design of Smart Microfluidics in Responsive Channels — •Arwin Marbini — Albert-Ludwigs Universität Freiburg

Responsive microfluidics offers exciting potential for self-regulating biomimetic systems. This study explores bifurcating microchannel networks with pressure-sensitive resistances, combining experiments with simulations based on the Hagen-Poiseuille equation and a linear model. These methods extract critical, experimentally inaccessible parameters under steady-state and dynamic conditions. Our findings enable the design of adaptable microfluidic networks, unlocking precise flow control for future applications in biology, soft robotics, and advanced material systems.

BP 28.9 Thu 17:30 H37

Blue Water: A passive, reusable microfiltration device for water purification — •Tim R. Baumann, Ioannis Gkekas, Martina Viefhues, and Dario Anselmetti — Experimental Biophysics, Bielefeld University

Water is the most vital resource for life on Earth. Due to pollution of freshwater and oceans, this valuable resource has become globally endangered. The effects of microplastic pollution are widely discussed in scientific, political, and socioeconomic contexts. Despite regulations on single-use plastics and microplastic output, efforts should also focus on reintegrating microplastics to achieve a sustainable circular economy. Furthermore, microplastic-sized particles can migrate through organic tissue and can therefore be classified as contaminants of emerging concern. However, filtering plastics of this size is a challenging task.

Thus, this work examines and extends the findings of Divi et al. regarding the suspension feeding mechanisms of various ray species. We studied the filtration performance and efficiency for different geometric ratios of channel widths in simulations and laboratory environments. First, we have the main inner channel connected to the pressure inlet. From this, two rows of tilted lamellae structures branch off laterally to the outer secondary channels.

By applying sufficiently high pressure ($> 6 \cdot 10^5\ Pa$) to the inlet and achieving flow and particle velocities of $> 35\ \frac{m}{s}$, we can purify 82 % of half of the initial fluid. To prevent rupturing of our microfluidic chip under this pressure, we further investigated using glass fiber reinforced PDMS and lowering the operating pressure.

BP 29: Focus Session: Innovations in Research Software Engineering (joint session BP/DY)

Research software engineering (RSE) is an emerging field in science, with practitioners spanning a continuous spectrum from "researchers who code" to "software engineers developing for science". In Germany, a growing movement supported by deRSE e.V. is gaining recognition, and more institutions are acknowledging the increasing demand across various disciplines. This focus session will provide a platform to highlight recent advances in applications, tooling, and software in the fields of biophysics, dynamics, and statistical physics, as well as developments in the recognition and proliferation of RSE as a profession within our field and academia in general.

Organized by Simon Christ and Sophia Rudorf (Hannover).

Time: Thursday 15:00–18:00 Location: H44

Invited Talk BP 29.1 Thu 15:00 H44

Community-driven software and data training for computational biology — •Toby Hodges — The Carpentries, Oakland, CA, USA

The Carpentries is a global community teaching essential software and data skills for research. Certified Instructors teach hundreds of workshops to thousands of learners all over the world every year, introducing them to essential skills for computational research such as programming, version control, and data organisation. In recent years, the community has also begun to develop and deliver lessons that build on these foundations, teaching more intermediate and advanced Research Software Engineering skills such as HPC, parallel programming, and containerised computing. This talk will explore how open source, collaborative training efforts can build capacity for computational research, discuss what makes this model work and some lessons learned along the way, and finish with a look at what the community plans to do next.

BP 29.2 Thu 15:30 H44

Python-based interface to micromagnetic simulation software: Ubermag — •Hans Fangohr[1,2,3], Martin Lang[1,2], Samuel J.R. Holt[1,2], Swapneel Amit Pathak[1,2], Kauser Zulfiqar[1,2,4], and Marijan Beg[5] — [1]MPSD, Hamburg, Germany — [2]CFEL, Hamburg, Germany — [3]Univ. Southampton, UK — [4]Univ. Hamburg, Germany — [5]Imperial College London, UK

We describe the Python-based user environment "Ubermag" to help scientists use well-established (micromagnetic) simulation packages.

Within Ubermag [1], researchers can express the physics problem they want to simulate in a scientist-friendly but machine readable problem definition based on Python syntax [2]. Ubermag translates this problem into the configuration files needed for micromagnetic simulation packages such as OOMMF or mumax3. On completion of the simulation, the computed data is presented back to the user at the Python level. Ubermag is often used in Jupyter Notebooks, and supports rich media to provide figures and equations within the notebook.

We report on the motivation for Ubermag, the design and implementation process, and our experiences made both from the perspective of science users and from the research software engineers. We touch on a range of topics, including interface design, domain specific languages, testing, packaging, Jupyter, and reproducibility.

This work was supported by EPSRC UK Skyrmion Grant EP/N032128/1, and the European research projects OpenDreamKit (676541) and MaMMoS (101135546).

[1] DOI 10.1109/tmag.2021.3078896; [2] DOI 10.1063/1.4977225

BP 29.3 Thu 15:45 H44

OCTOPOS.jl: A Julia-based tool for synonymous codon optimization — Simon Christ[1], Jan-Hendrik Trösemeier[2], and •Sophia Rudorf[1] — [1]Institute of Cell Biology and Biophysics, Leibniz University Hannover, Germany — [2]independent researcher

OCTOPOS.jl is a research software designed to optimize synonymous mRNA sequences for improved heterologous gene expression in various host organisms. Combining a detailed mechanistic model of in-vivo protein synthesis with machine learning, OCTOPOS.jl predicts protein expression based on codon choice. Originally developed as a Java desktop application, the software has been reimplemented in the Julia programming language to enhance performance, modularity, and scalability. The new implementation serves as the foundation for a graphical user interface and a web application, accessible at https://octopos.cell.uni-hannover.de/. These updates improve accessibility and usability, broadening its appeal to both computational and experimental biologists. OCTOPOS.jl supports organism-specific genetic sequence engineering and detailed analysis of translation dynamics, thus providing a valuable resource for the synthetic biology and biotechnology communities.

BP 29.4 Thu 16:00 H44

Invert pattern forming systems with BayesFlow to bridge the gap from simulation to experimental observation — •Hans Olischläger — Interdisciplinary Center for Scientific Computing (IWR) — Heidelberg University

The description of experimental systems by complex spatial models, be it with (stochastic) partial differential equations, agent-based simulation or otherwise, is often the condensation of all the central scientific hypotheses regarding a particular object of study.

I argue, that making progress in this kind of modelling is currently hindered by the lack of a tool that enables solving the following inverse problem: Given an observation, determine all the model configurations that are able to produce it. In other words, what is the posterior probability of all model configurations given some (set of) experimental data.

Instead of just preaching that in theory a Bayesian treatment would be nice, I will then continue to present such a tool: amortized Bayesian inference (as implemented in the software package BayesFlow). I will give examples on the classical Gierer-Meinhardt pattern forming PDE and a biophysical model, the Min system, which is used by E. coli to control cell division.

I will also take a step back to give a broader picture of the newly available statistical methods that support complex spatial modelling and their limitations. The aim is to provide some guidance on what you can and cannot infer from your state-of-the-art scientific simulator given observations, and how to do it.

BP 29.5 Thu 16:15 H44

FAIR Data Management for Soft Matter Simulations using NOMAD — •Bernadette Mohr[1], Esma Boydas[1], Nathan Daelman[1], José M. Pizarro[1], Tristan Bereau[3], Claudia Draxl[1], Luca M. Ghiringhelli[4], Martin Girard[2], Denis Usvyat[6], Roser Valentí[7], Silvana Botti[5], and Joseph F. Rudzinski[1,2] — [1]CSMB, HU Berlin — [2]MPIP Mainz — [3]ITP, Heidelberg Uni. — [4]Dept. of Mater. Sci. and Eng., FAU Erlangen — [5]RC-FEMS and Faculty of Physics, RUB Bochum — [6]Inst. für Chem., HU Berlin — [7]ITP, GU FfM

NOMAD [nomad-lab.eu][1, 2] is an open-source, community-driven data infrastructure designed to facilitate FAIR data management in materials science. Currently, it supports over 60 computational codes and encompasses DFT, classical MD, and many-body methods. This contribution will focus on recent developments, following modern software practices, to enhance NOMAD's applicability to soft matter and biological systems, including support for coarse-grained representations and advanced workflows such as free energy calculations. Combined with a schema for representing force fields, molecular topologies, and hierarchical system structures, NOMAD tracks data provenance and streamlines data analysis and the creation of AI-ready datasets. The NOMAD framework meets the classical simulation community's needs for improved data management standards and provides a foundation for building a cohesive, interconnected scientific data ecosystem. [1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

BP 29.6 Thu 16:30 H44

Estimation of kinetic rates by constrained optimization — •Federico Marotta[1], Maria Zimmermann-Kogadeeva[1], Peer Bork[1], Julia Mahamid[1], and Sophia Rudorf[2] — [1]European Molecular Biology Laboratory — [2]Leibniz Universität Hannover

Biological systems often rely on molecular motors to perform useful work. The kinetics of the reactions in a motor's cycle can be easily investigated *in vitro* or in model organisms, but it is difficult to generalize them to a different system. We present a method to estimate the transition kinetics in an uncharacterized system, where minimal data are available, by leveraging a reference system where the kinetics have been elucidated. The motor's activity is represented as a continuous-time Markov chain, characterized by an infinitesimal generator matrix Q whose entries are functions of the transition rates of the cycle (the vector ω) and possibly of the concentrations of external molecules. In the uncharacterized system, the available data induce a constraint on the admissible rates. By employing an extremum principle, we estimate the rates ω_{unc} that minimize the kinetic distance with respect to the reference rates ω_{ref} while respecting such constraint. As an application of this strategy, we describe a model of the translation elongation cycle, where reference data are available for *E. coli in vitro*, and estimate the rates either *in vivo* or in a different organism, under constraints on the total elongation time or the steady-state occupancies, respectively.

BP 29.7 Thu 16:45 H44

Software provisioning for HPC and RSE — •Martin Lang[1,2], Henning Glawe[1,2], Jehferson Mello[1,2], and Hans Fangohr[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Free-Electron Laser Science, Hamburg, Germany — [3]University of Southampton, Southampton, UK

All research software relies on existing libraries for various functionalities such as low-level math operations, FFTs, IO, or other domain-specific operations. Installing these dependencies, potentially based on different compilers or in multiple versions, with all inter-dependencies fulfilled is notoriously difficult.

In the first part of this talk we introduce the open-source package manager Spack, which has a strong focus on HPC and research software. Spack can install software in multiple versions and variants, and supports optimised compilation for the underlying hardware, including compiling on exotic hardware. It comes with a large, community-provided collection of commonly used packages. Spack's packaging files make it easy to specify required dependencies, provide optional features of a software, and ensure compatibility with other libraries.

In the second part we present the concrete setup at our institute. We use Spack to provide the software stack on the local HPC, including pre-compiled packages and toolchains (sets of compilers and libraries) for users to compile their own software. We report on requirements and challenges, and how we address these with Spack. We also touch on scripting the Spack-based installation process including the option to recreate the HPC software environment on a scientist's laptop.

BP 29.8 Thu 17:00 H44

Small scale Research Software Engineering — •Simon Christ — Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Computational Biology

While we are in dire need of research software organizations on a faculty level or larger, small scale software engineering, that is one research software engineer in a group or institute, is something that can be achieved in a short time frame and is probably the most common form today. A field report from Computational Biology where research software engineers are involved in modeling, developing solutions, teaching and maintenance.

BP 29.9 Thu 17:15 H44

Estimation of pKa values in membrane bound proteins — •Jesse Jones[1], Nereu Montserrat i Busquets[1,2], Ana Gamiz Hernandez[3], Ville Kaila[3], and Maria Andrea Mroginski[1] — [1]Technische Universität Berlin, Berlin — [2]Freie Universität Berlin, Berlin — [3]Stockholm Universität, Stockholm

Many key bioenergetic processes involving electron and proton reactions take place in membrane bound protein complexes, generating a proton motive force. Yet the ionizable groups which facilitate these reactions are often buried in hydrophobic pockets in the membrane. These processes are mainly described through pK_a values, which continue to be poorly understood and difficult to obtain despite structural, biochemical and computational advances. Hence, estimating pK_a values of these residues without the need for weeks of work in a laboratory, is important to describe the dynamics of the system, providing information on possible proton pathways. In this work we preview Karlsberg3, a software which uses a Poisson Boltzmann Equation solver (APBS) for proteins and calculates pKa values. Karlsberg3 is, in contrast to its predecessor Karlsberg2+, parallelized, running in modern software environments, and able to take membranes into consideration.

BP 29.10 Thu 17:30 H44

The teachingRSE project - Towards a professionalization of RSE education. — •Florian Goth[1] and Simon Christ[2] — [1]Universität Würzburg, Institut für theoretische Physik und Astrophysik, Am Hubland, 97074 Würzburg — [2]Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Herrenhäuser Str. 2 30419 Hannover

At the deRSE23, the second conference for research software engineering(RSE) in Germany, a group of people came together for a small workshop to discuss how to deal with questions revolving around RSE education. Overwhelmed by the immense resonance to that workshop we took home a tremendous amount of feedback that made obvious that a short blog post will not suffice to adequately represent it. Now it is two years later, and the project produced its first output, the second position paper https://arxiv.org/abs/2311.11457 of de-RSE e.V. and it has sprawled out into a multitude of follow-up projects. In this talk, I will give an overview over the original ideas that we tried to convey in the position paper, and go into more detail on how domain sciences like physics need to change in light of this new specialization.

BP 29.11 Thu 17:45 H44

Python-Based Analysis Pipeline for the Quantification of Mechanics in Neural Organoids — •Michael Frischmann[1,2], Elijah R. Shelton[1], Achim T. Brinkop[1,2], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Ulm, Germany — [3]SyNergy & GSN, Munich, Germany

Neuronal tissues form under the influence of mechanical forces guiding cellular movements. In the mammalian retina, neuronal translocations occur over hours. However, mechanical probing at those timescales in situ have posed experimental challenges. We employed magnetic ferrofluid droplets in mouse stem cell-derived retinal organoids to probe tissue mechanics from seconds to hours. To quantify tissue strain we have developed a Python-based analysis pipeline featuring an accessible graphical user interface (GUI). This pipeline automates strain quantification, image segmentation, and fitting procedures, enabling high-fidelity creep compliance measurements over extended durations. Our measurements reveal power-law scaling of dynamic compliance as well as tensile loss and storage modulus, consistent with soft glassy rheology just above the glass transition. These results demonstrate that neuronal tissues remodel in a scale-free manner while maintaining solid-like properties. This discovery provides a framework for understanding how mechanical signals may govern connectivity in the central nervous system. Integrating neural organoid models, mechanical probing, and computational methods, prepares us to investigate the interplay between biomechanics and neurodevelopment.

BP 30: Protein Structure and Dynamics

Time: Thursday 15:00–18:00 Location: H46

BP 30.1 Thu 15:00 H46

A protein sensor for plasma membrane lipid composition – insights from coarse-grained simulations — Saara Lautala and •Sebastian Thallmair — Frankfurt Institute for Advanced Studies, Frankfurt a.M., Germany

Extended synaptotagmins (E-Syts) are tethering proteins, which keep the plasma membrane (PM) and the endoplasmic reticulum (ER) membrane in close proximity at ER-PM contact sites. C2 domains are responsible for the binding of E-Syts to the PM. After depletion of phosphatidylinositol 4,5-bisphosphate $PI(4,5)P_2$, resynthesis of $PI(4,5)P_2$ takes place at ER-PM contact sites and thus, requires their integrity. The terminal C2C domain of E-Syt3 is known to bind $PI(4,5)P_2$. This results in an apparent paradox as the membrane binding and thus the tethered ER-PM contact site potentially become instable upon $PI(4,5)P_2$ depletion.

Here, we applied coarse-grained molecular dynamics simulations with the Martini 3 force field to investigate the membrane binding of the E-Syt3 C2C domain. Our simulations show that the C2C domain not only exhibits a binding hotspot for $PI(4,5)P_2$, but an additional binding hotspot for phosphatidylserine (PS) as well as a region binding to the membrane core. We will discuss that binding to PS results in a reorientation of the protein on the membrane surface and compare the different binding strengths. Overall, the PS binding site not only contributes to the ER-PM contact site integrity upon $PI(4,5)P_2$ depletion, but might also play a role in sensing low $PI(4,5)P_2$ levels.

BP 30.2 Thu 15:15 H46

Cross correlations in the Fluctuation-Dissipation Relation Reveal Solvent Friction in Hydrophobic Folding Transition — •Niklas Wolf, Viktor Klippenstein, Madhusmita Tripathy, and Nico F. A. van der Vegt — TU Darmstadt, Darmstadt, Germany

The Generalized Langevin Equation is a powerful tool for modeling and understanding the conformational dynamics of molecules in solution. However, recent works[1] have demonstrated that for these kinds of applications, the usual fluctuation-dissipation relation connecting the statistics of the random force to the memory kernel could contain a cross-correlation term. This raises the question of how the memory kernel should be extracted from simulation data and if a naive approach via the Volterra equations even gives a kernel related to a Markovian friction coefficient. We propose an approximation[2] to account for the cross-correlation term and show in a systematic study[3] that this approximation leads to an improved description of long-time dynamics and transition rates. Finally, we show that cross-correlations play an important role in the coil-to-globule transition of a hydrophobic polymer under various solvent conditions, where a naive approach would predict a significant violation of the Stokes-Einstein relation and give a poor description of barrier crossing times with rate theories.

[1] H. Vroylandt 2022 EPL 140 62003
[2] V. Klippenstein N. F. A. van der Vegt 2021 J. Chem. Phys. 154 191102
[3] N. Wolf et al. J. Chem. Phys. (under Review)

BP 30.3 Thu 15:30 H46

Multiscale simulation of protein phase separation — •Supriyo Naskar, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, Mainz, Germany

The post-translational modifiers such as mono and poly ubiquitins and SUMOs are known for their ability to modulate protein-protein interactions by becoming covalently attached to other target proteins. Despite the high similarity in the tertiary structure and sequence, they differentially influence the target protein properties. In this work, we employed a multiscale simulation approach that encompasses atomistic to different level coarse-grained modelling techniques with data-driven machine-learning methods to explore the structural differences and multidimensional energy landscape of ubiquitin and SUMO and their conjugates. We finally study the influence of distinct features of the targets and modifiers on protein phase separation and aggregation, providing molecular-level insight into the corresponding in vitro measurements and instructing further experiments through adjustment of relevant parameters.

BP 30.4 Thu 15:45 H46

Sequence specificity and polymer physics — •Martin Girard — Max-Planck Institute for Polymer Research, Mainz, Germany

Sequence properties of disordered proteins in the context of phase separation has led to development of molecular grammar. So far, this has led to the development of empirical parameters tied to protein sequences.

Using surrogate models for low-complexity sequences, I will show that sequence-property relations are tied to the polymer collapse transition. I will further discuss implications for biological systems.

Invited Talk BP 30.5 Thu 16:00 H46

Topology in biological matter - are there double knots in proteins or maybe even more complicated knots? Prediction and in vitro verification. — •Joanna I Sulkowska — University of Warsaw, Banacha 2C, 02-097, Poland

We have been aware of the existence of knotted proteins for over 30 years-but it is challenging to predict what is the most complicated not that can be formed in proteins. Recently, based on AlphaFold (AF) method we predicted new and the most complex knotted topologies recorded to date - double trefoil knots (see AlphaKnot database). We found five domain arrangements that result in a doubly knotted structure in almost a thousand proteins. The double knot topology is found in knotted membrane proteins from the CaCA family, that functions as ion transporters, in the group of carbonic anhydrases that catalyze the hydration of carbon dioxide, and in the proteins from the SPOUT superfamily that gathers 31 knotted methyltransferases with the active site-forming knot.

Herein, I will present the first crystal structure of a double knotted protein TrmD-Tm1570 from Calditerrivibrio nitroreducens from SPOUT superfamily. The protein consists of two domains TrmD and Tm1570, each embedding a single trefoil knot, which can function on their own. We show that it folds in vitro and is biologically active.

I will also explain how AF and AI methods can be used to design artificially knotted proteins that can be obtained in vitro. This shows that AF, while predicting structure, also takes into account folding and overcoming a non-trivial looping pathway.

15 min. break

BP 30.6 Thu 16:45 H46

Single molecule FRET studies on folding properties of multidomain protein fragments — •Alida Meyer[1], Alexandros Katranidis[2], Nuno Bustorff[2], and Jörg Fitter[1,2] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), AG Biophysik, Aachen, Germany — [2]Forschungszentrum Jülich, ER-C-3 Structural Biology, Jülich, Germany

Protein folding and unfolding are crucial for cellular function and stability. This study emloys single-molecule Förster resonance energy transfer (smFRET) to investigate structural transitions in yeast phosphoglycerate kinase (yPGK). We focus on its two-domain structure and the relationship between the Rossmann-fold topology and folding intermediates. Earlier studies with full-length yPGK labelled with fluorescent dyes at multiple different positions allowed to map several different intra-molecular distances during unfolding transitions [1,2]. To mimic co-translational folding properties, we performed smFRET measurements with truncated yPGK fragments. The results are compared with those of full-length proteins, including whether the same type of unfolding transition occurs as in the full-length protein (e.g., two state transitions or compact intermediates). In addition, the results from truncated fragments are also compared with nascent-chain folding in ribosome-nascent chain complexes (RNCs), analyzed via cryo-electron microscopy. These methods provide insights into how domain topol-

ogy and neighboring structural elements influence multidomain protein folding.

[1] Cerminara et al., Biophysical Journal, 2020, 118, 688
[2] Bustorff et al., Biomolecules, 2023, 13, 1280

BP 30.7 Thu 17:00 H46

Probing the dynamics of small unilamellar vesicles inside Synapsin pools using X-ray photon correlation spectroscopy — •Titus Czajka[1], András Major[1], Hendrik Bruns[1], Christian Hoffmann[2], Dragomir Milovanovic[2], and Tim Salditt[1] — [1]Georg-August-Universität Göttingen — [2]Deutsches Zentrum für Neurodegenerative Erkrankungen, Berlin

The dynamics of many subcellular biological processes are difficult to access directly with microscopic techniques due to the resolution limit. Length and time scales beyond those accessible by conventional light microscopy can be probed via X-ray photon correlation spectroscopy (XPCS), even in dense media, by analysing the intensity autocorrelation function at different scattering vectors. However, the low scattering cross section of dilute biological samples and the sensitivity to radiation damage complicate the application of XPCS to biological systems. We have coated silica nanoparticles with a lipid bilayer to improve the scattering strength and overcome these challenges. Using such colloid-supported lipid bilayers (CSLBs), we have studied the dynamics of small unilamellar vesicles within synapsin protein pools, a system that exhibits evidence of both liquid-like and network-like phases. Our results show distinct diffusion constants at varying protein concentrations and provide evidence for non-diffusive behaviour within the pools.

BP 30.8 Thu 17:15 H46

Novel sample delivery for small nanoparticles and biomolecules for cryo-em — •Kevin Janson[1], Armando D. Estillore[1], Jiri Wald[4,5,6], Madeline Memovich[1], Thomas Marlovits[4,5,6], Amit K. Samanta[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Hamburg, Germany — [3]Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany — [4]Centre for Structural Systems Biology, Hamburg, Germany — [5]Institute of Structural and Systems Biology, University Medical Centre Hamburg-Eppendorf, Hamburg, Germany — [6]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Cryo-electron microscopy (Cryo-EM) is one of the key techniques in the field of structural biology. Recent years brought considerable improvements both on the software and hardware of the microscopes, and resolving high-resolution structures of proteins has become a standard procedure. However, most cryo-EM grids are still prepared by plunge freezing, a technique developed about ~40 years ago. During this process, proteins can be exposed to the air-water interface, possibly causing a preferential orientation or damaging their structure. We present the novel freeze-and-deposit sample delivery approach to deposit particles for cryo-EM using cryogenic shockfreezing technology. The cooling process produces cold high-density beams of nanoparticles. In this process, nanoparticles and macromolecules are aerosolized and rapidly cooled in the gas phase using a cryogenic buffer-gas cell.

BP 30.9 Thu 17:30 H46

Laser flash melting restores native protein conformation after cryoEM preparation by soft-landing, native electrospray ion beam deposition. — Sarah V. Barrass[1], Tim K. Esser[2], Nathan J. Mowry[1], Lukas Eriksson[2], Jakub Hruby[1], Laurence Seeley[3], Marcel Drabbels[1], Lindsay Baker[3], •Stephan Rauschenbach[2], and Ulrich J. Lorenz[1] — [1]EPFL Lausanne — [2]Univ. of Oxford, Dept. of Chem.. — [3]Univ. of Oxford, Dept. of Biochem.

Electron cryo microscopy (cryoEM) is today the dominating method for protein structure determination. Samples for cryoEM consist of thin, freestanding layers of amorphous ice in which proteins are embedded. Conventionally, these samples are prepared by shock-freezing of thin water films held in grid holes.

Alternative sample preparation methods are being developed, as the plunge-freezing method is not compatible with all types of protein sample. One of these methods is electrospray ion beam deposition (ESIBD) where mass-selected proteins from the gas-phase are landed on a thin amorphous carbon film in vacuum and embedded in ice grown from the gas phase for imaging. Recently it was shown that this method yields atomically resolved protein structures characterised by small changes in ternary structure due to dehydration.

Here we show that the dehydration can be reversed by irradiating the sample with short laser pulses, effectively melting the ice for a short time, allowing the protein to recover the native conformation, before the ice rapidly re-vitrifies.

BP 30.10 Thu 17:45 H46

Native Electrospray Ion Beam Deposition for Atomic-level Structure Analysis of Membrane Protein — •Jingjin Fan, Tim Esser, Clare De'Ath, Lukas Eriksson, Abdul Aziz Qureshi, Abraham Abraham, Laurence Seeley, Lindsay Baker, Carol Robinson, and Stephan Rauschenbach — The Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford OX1 3QU, United Kingdom

Membrane proteins play vital roles in cellular physiology, but their structural analysis remains challenging due to heterogeneity, flexible conformations, and demanding native conditions. To address these challenges, we established electrospray ion beam deposition (ESIBD) to directly couple native mass spectrometry (MS) with cryogenic electron microscopy (cryo-EM) for studying membrane protein structures.

Standard membrane proteins, including aquaporin Z (AqpZ) and ammonium transporter B (AmtB), were selected as testing models. By optimizing surfactant, the ion transfer in vacuum and the embedding of the proteins after landing we successfully manipulated membrane protein particles and achieved soft-landing on grids, evidenced by high-resolution imaging in cryoEM.

Our results demonstrate that the membrane structures can be preserved even in the absence of visible micelle.This molecular-level structural analysis captured by ESIBD in vacuum provides new insights into the correct folding of membrane proteins and understanding fundamental questions in structural biology.

BP 31: Active Matter IV (joint session BP/CPP/DY)

Time: Friday 9:30–13:00 Location: H44

Invited Talk BP 31.1 Fri 9:30 H44

Wave propagation in systems of active filaments — •Kirsty Y. Wan — Living Systems Institute, University of Exeter, UK

Active hair-like protrusions called cilia are found in many eukaryotes where they produce physiological flows for a variety of functions. Cilia assume a myriad of configurations both external to an organism for the purposes of feeding or swimming motility, but also internally where they mediate mucociliary clearance in vertebrate tissues. Single cilia can propagate large-amplitude non-decaying bending waves, even in the absence of a cell body. These waves assume a variety of stereotyped forms and frequencies, depending on the species. Multiple cilia also interact to produce different types of local and global coordination patterns, including robust metachronal waves. Do these dynamic states of coordination arise spontaneously, or do they require some form of internal control by the cell or animal? We propose new and emerging organisms to address these questions.

BP 31.2 Fri 10:00 H44

Metabolic activity controls the emergence of coherent flows in microbial suspensions — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to the spatio-temporal variations of environmental parameters within their habitat. In the absence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment may be deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we study the effect of motility and cell density of *C. reinhardtii* in a confined system, on the emergence of bioconvection [2]. This collective phenomenon can be reversibly switched by light and arises due to the natural tendency of the bottom-heavy cells to move against gravity. We show that the rate at which the system evolves, as well as the dominant wavelength of the instability can both be directly controlled by the number density of cells. Further, we provide insights on the internal flow fields and density profiles of single bioconvection plumes for different parameters.

[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).
[2] A.A. Fragkopoulos et al., *arXiv*:2407.09884 (2024)

BP 31.3 Fri 10:15 H44

Tumbling *E.coli* in bulk and close to surfaces — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian institute of science education and research (IISER), Tirupati, India

Escherichia coli (*E. coli*) swims by rotating multiple flagella which are connected to the cell body forming a thick bundle. To change direction, *E. coli* performs tumble events by reversing the rotation of one or more flagella. The involved filaments undergo a series of polymorphic transformations, altering both their helicity and handedness. This complex phenomenon involves the interplay of semiflexible filaments and hydrodynamic flow fields.

Here, we have developed a detailed numerical framework to simulate *E. coli*, capturing the full dynamics of flexible flagella, including their polymorphism and their hydrodynamic interactions. The filaments and the cell body are embedded in a viscous fluid, which we model using multi-particle collision dynamics. We analyzed a large number of tumble events, with fixed tumble time or taken from a gamma distribution, exploring the roles of hook and flagellar flexibility as well as flagellar polymorphism. We find that they strongly influence the distribution of tumble angles. Finally, we also show that close to a flat surface the mean tumble angle is strongly shifted to smaller values. This indicates that tumble events may not be recognized, which could give the impression of suppressed tumbling near surfaces.

BP 31.4 Fri 10:30 H44

***Trypanosoma brucei* (un)chained - effects of confinement on a parasitic microswimmer** — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth — [2]Laboratory of Molecular Parasitology, University of Bayreuth

Trypanosoma brucei is a parasitic unicellular microswimmer that causes the African sleeping sickness. An active spiral movement of the parasite, mediated by a microtubule-driven flagellum that wraps around the cell body, is mandatory to evade the host's immune system while exploring tissues and blood vessels. In addition, the nematic subpellicular micotubule array plays a pivotal role in the elasticity, propulsion, and navigation of the parasite. To study the features and mechanisms behind the cell's motion in such complex environments, we have mimicked spatial confinement in microfluidic devices with different geometries. Our data show that spatial constraints in narrow channels and channel networks can improve cell locomotion of wild-type trypanosomes, supposedly due to the interaction of the elastic cell body and nearby walls. The addition of microtubule-disrupting drugs or the use of mutant strains with altered post-translational modifications of microtubules resulted in significantly altered swimming velocities and marked changes in the intermittent switching between run and tumble phases. Shape analyses of individual cells suggest that microtubules in the sub-pellicular array, the corset that keeps trypanosomes in their native spindle-like shape, are most affected in these cases.

BP 31.5 Fri 10:45 H44

Micro-swimmer motility in presence of signaling factors — Agniva Datta, Robert Grossmann, and •Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

The navigation of bacteria through aqueous environments, driven by the rotation of helical flagella, has been a significant region of interest in the biophysics community for the last few decades. In this study, we focus on the motility of our model organism, Pseudomonas putida, which exhibits persistent mobile episodes (Active Brownian motion) interrupted by stochastic reorientation events (turns), driven by flagellar self-propulsion, thereby leading to a run-and-turn motility.

Key motility parameters including tumbling rates, run lengths, trajectory persistence (rotational diffusion coefficient), and the characteristics of the self-propulsion force*are hypothesized to depend on the density of quorum-sensing autoinducer molecules, produced by the bacteria themselves as signaling factors. To test this hypothesis, we expose swimming bacteria to aqueous environments with controlled autoinducer concentrations and analyze the resulting changes in motility patterns. Through a combination of experimental data and theoretical modeling, we aim to elucidate the principles of micro-swimmer motility in presence of signaling molecules.

BP 31.6 Fri 11:00 H44

Collective dynamics of active dumbbells near a circular obstacle — •Chandranshu Tiwari[1] and Sunil Singh[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India. — [2]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

We present the collective dynamics of active dumbbells in the presence of a static circular obstacle using Brownian dynamics simulation. The active dumbbells aggregate on the surface of a circular obstacle beyond a critical radius, and the aggregate size increases with the activity and the curvature radius. The dense aggregate of active dumbbells displays persistent rotational motion with a certain angular speed, which linearly increases with activity. Furthermore, we show a strong polar ordering of the active dumbbells within the aggregate. The polar ordering exhibits long-range correlation, with the correlation length corresponding to the aggregate size. Additionally, we show that the residence time of an active dumbbell on the obstacle surface increases rapidly with area fraction due to many-body interactions that lead to a slowdown of the rotational diffusion. This article further considers the dynamical behavior of a tracer particle in the solution of active dumbbells. Interestingly, the speed of the passive tracer particle displays a crossover from monotonically decreasing to increasing with the size of the tracer particle upon increasing the dumbbells' speed. Furthermore, the effective diffusion of the tracer particle displays non-monotonic behavior with the area fraction; the initial increase in diffusivity is followed by a decrease for a larger area fraction.

BP 31.7 Fri 11:15 H44

Free growth under tension — •Chenyun Yao and Jens Elgeti — Forschungszentrum Jülich GmbH, Jülich, Germany

Ever since the ground breaking work of Trepat et al. in 2009, we know that cell colonies growing on a substrate can be under tensile mechanical stress. The origin of tension has so far been attributed to cellular motility forces being oriented outward of the colony. Works in the field mainly revolve around how this orientation of the forces can be explained, ranging from velocity alignment, self-sorting due to self-propulsion, to kenotaxis.

In this work, we demonstrate that tension in growing colonies can also be explained without cellular motility forces! Using a combination of well established tissue growth simulation technique and analytical modelling, we show how tension can arise as a consequence of simple mechanics of growing tissues. Combining these models with a minimalistic motility model shows how colonies can expand while under even larger tension. Furthermore, our results and analytical models provide novel analysis procedures to identify the underlying mechanics.

15 min. break

BP 31.8 Fri 11:45 H44

A route to active turbulence in circular activity spots — •Arghavan Partovifard and Holger Stark — Institute of Theoretical Physics, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany.

Active nematics exhibit distinctive behavior such as active turbulence and regular flow patterns under spatially varying activity [1]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investigate active nematics confined to a circular spot by switching off activity outside the spot. The open boundary allows topological defects to enter and leave the spot.

We calculate the total topological defect charge inside the spot using three approaches: counting all defects, measuring the rotation of the director field along the rim of the spot, and integrating the diffusive charge density. All methods agree that for spot radii just larger than the nematic coherence length, the system has a total topological charge of +1, where two +1/2 defects perform a regular swirling motion. As the radius increases, more defects enter and their motion becomes more and more chaotic. Ultimately, the charge per unit area saturates at the value characteristic of bulk active turbulence. For the range of radii where the total charge in the spot is +1, the nematic director exhibits shear-induced anchoring at an angle of 45° with respect to the tangent at the spot rim. With increasing radius, when more defects enter, the anchoring angle deviates from 45° but its distribution still peaks around this value.

[1] A. Partovifard *et. al.*, Soft Matter **20**, 1800 (2024)

BP 31.9 Fri 12:00 H44

Cognitive flocks: order-disorder transitions and threat evasion — •Priyanka Iyer[1], Cecilia Soroco[2], and Gerhard Gompper[1] — [1]Forschungszentrum Jülich — [2]University of British Columbia, Canada

Directed self-propulsion is ubiquitous in living organisms. From E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379.

[2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

BP 31.10 Fri 12:15 H44

Myosin-independent amoeboid cell motility — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell motility is essential for many physiological and pathological processes, such as the immune system, embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode which allows them to move rapidly in a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. We introduce a model for an amoeboid cell where the cortex is described as a thin shell along the cell surface. The cell shape evolves due to polymerization of actin filaments and the forces acting on the cortex. We find analytically and numerically that the state of a resting, non-polarized cell can become unstable for

sufficiently large actin polymerization velocities, resulting in the spontaneous onset of cell polarity, migration, and dynamical shape changes. Notably, this transition only relies on actin polymerization and does not necessitate molecular motors, such as myosin. These findings yield a deeper understanding of the fundamental mechanisms of cell movement and simultaneously provide a simple mechanism for cell motility in diverse configurations.

BP 31.11 Fri 12:30 H44

Active membrane deformations of a synthetic cell-mimicking system — Alfredo Sciortino[1], •Dmitry Fedosov[2], Gerhard Gompper[2], and Andreas Bausch[1] — [1]Physik Department, Technische Universität München, Garching bei München, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

BP 31.12 Fri 12:45 H44

Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles — Eike Eberhard, •Ludwig Burger, Cesar Pastrana, Giovanni Giunta, and Ulrich Gerland — Physik komplexer Biosysteme, Technische Universität München, Deutschland

Recent experiments show that the diffusion coefficient of some metabolic enzymes increases with the concentration of their cognate substrate, a phenomenon known as enhanced diffusion. In the presence of substrate gradients, enhanced diffusion induces enzymatic drift, resulting in a non-homogeneous enzyme distribution. In this work, we study the behavior of enzyme-loaded vesicles exposed to external substrate gradients using a combination of computer simulations and analytical modeling. We observe that the spatially inhomogeneous enzyme profiles generated by enhanced diffusion result in a pressure gradient across the vesicle, which leads to macroscopically observable effects, such as deformation and self-propulsion of the vesicle. Our analytical model allows us to characterize dependence of the velocity of propulsion on experimentally tunable parameters. The effects predicted by our work provide an avenue for further validation of enhanced diffusion, and might be leveraged for the design of novel synthetic cargo transporters, such as targeted drug delivery systems.

BP 32: Computational Biophysics II

Time: Friday 9:30–13:00 Location: H46

BP 32.1 Fri 9:30 H46

From slabs to cubes: finite size effects in biomolecular simulations — •Rodrigo F. Dillenburg and Martin Girard — Max Planck Institute for Polymer Research, Mainz, Germany

Coarse-grained simulations of intrinsically disordered proteins have become essential to the study of biomolecular condensates. Multiple choices of force fields, simulations techniques and box geometries have been employed in such studies, assuming that results will converge due to the law of large numbers. This assumption is, however, not automatically valid for all systems and needs to be carefully examined to assure the validity of the results. In our work we focused on the choice of box geometry (cubic or slab) and statistical ensemble (canonical or grand-canonical) and its effect on the phase behavior of systems undergoing liquid-liquid phase separation. Our results allow us to estimate if a system can be approximated by the thermodynamic limit or if finite size effects have to be taken into consideration. We are able to derive expressions for these corrections depending on the choice of system and are also able to relate it to condensate properties such as surface tension. Our results provide a rational approach to selecting the most appropriate simulation methods for a given system.

BP 32.2 Fri 9:45 H46

Interactions of Imidazolium with Elastin-Like Polypeptides: A Molecular Dynamics Study — •Julia Keil and Nico F. A. van der Vegt — Technische Universität Darmstadt, Germany

Biological buffers are commonly used to adjust the pH value of protein solutions and are typically assumed not to affect other properties of the system.[1] However, a series of experimental observations suggest buffer-specific effects on protein stability.[2] Despite these findings, studies on these effects remain limited, and the underlying mechanisms are still poorly understood.[2-4]

We performed molecular dynamics simulations at constant pH[4] to investigate the interactions between the buffer imidazolium (IMI) and elastin-like polypeptides (ELPs) that contain chemically different amino acids at their variable positions. Our analyses revealed a local accumulation of imidazole (IMI^{o}) around the ELPs and its hydrogen bonding to the ELP backbone, regardless of the ELP composition. In contrast, interactions with imidazolium (IMI^{+}) were found to depend on the ELP composition. A strong local accumulation of IMI^{+} was observed around ELPs containing negatively charged groups, accompanied by hydrogen bonding to their side chains. Conversely, local depletion of IMI^{+} occurred around ELPs with positively charged groups. As a result, the interactions of ELPs with IMI are determined by the specific composition of the ELPs.

[1] *Nat. Chem.* 2021, 13, 1023-1024 [2] *Curr. Opin. Colloid Interface Sci.* 2016, 23, 1-9 [3] *J. Pharm. Sci.* 2017, 106, 3, 713-733 [4] *J. Chem. Theory Comput.* 2022, 18, 10, 6148-6160

BP 32.3 Fri 10:00 H46

Graphite-based Bio-mimetic Nanopores for Protein Sequencing and Beyond — •Chandan K. Das and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Aachen, Germany

Protein sequencing via nanopores offers a transformative approach to bioanalytics, but challenges remain, particularly in linearizing unfolded proteins and controlling translocation speed through solid-state nanopores. This study introduces a novel solution: biomimetic graphite-based nanopores designed with nanometer-sized pores featuring a constriction zone inspired by the alpha-hemolysin protein pore. All-atom molecular dynamics simulations demonstrate the nanopores' ability to achieve ion selectivity and generate electro-osmotic flow (EOF) within the pore lumen due to tailored surface charges. This innovation enables the detection of peptides at the single amino acid level by analyzing ionic current fluctuations during peptide translocation. A critical feature of this design is its capacity to balance hydrodynamic drag, induced by EOF, with electrophoretic force (EPF), facilitating peptide linearization and extending amino acid residence time within the constriction zone. These advancements significantly enhance sequencing resolution and accuracy. Beyond protein sequencing, this technology holds potential for diverse applications, including seawater desalination via electrodialysis and renewable energy generation through salinity gradient-driven ion separation. By providing a robust computational foundation, this study advances the development of graphite-based biomimetic nanopores, offering versatile solutions for bio/nanotechnological challenges and sustainable energy innovations.

BP 32.4 Fri 10:15 H46

Helical transition of protein chain: An in silico study — •tika ram bhandari and martin girard — Max Planck Institute for Polymer Research, Mainz, Germany

Structural transformations in biomolecular systems are critical for physiological functions, with folding and unfolding transitions governing numerous cellular activities. Misfolding of proteins, however, is a key factor in the onset of severe diseases, emphasizing the need for comprehensive studies to understand and control these processes. Computational simulations provide valuable insights into such mechanisms. Here, we employed coarse-grained molecular simulations coupled with Hamiltonian Replica Exchange method to investigate the disordered-to-helical transition of IM30, the bacterial counterpart of the ESCRT-III. By systematically varying the strength of hydrogen bonds, we simulated an in-silico denaturation process, enabling a detailed analysis of the structural properties underlying this transition. Furthermore, we explore the impact of point mutations on the protein's helical propensity using free energy calculations. These approaches provide a deeper understanding of the molecular mechanisms influencing folding behavior and highlights the role of specific mutations in modulating protein structure.

BP 32.5 Fri 10:30 H46

Towards modeling cellular environments from cryo-electron tomography by high-confidence 3D template matching — •Sergio Cruz-León, Jan Philipp Kreysing, Maziar Heidari, Beata Turoňová, Martin Beck, and Gerhard Hummer — Max Planck Institute of Biophysics, Max-von-Laue-Str. 3, 60438, Frankfurt am Main, Germany

The simulation of biologically realistic systems requires precise knowledge of the composition and spatial arrangement of biomolecules in situ. This informa-

tion can be obtained from cryo-electron tomography (cryoET), which images the interior of intact cells in 3D. However, feature identification is limited by the low signal-to-noise ratio and anisotropic resolution of the tomographic data. In this talk, I will present our recent advances in high-confidence 3D template matching (hcTM) for cryoET [1] and how we use hcTM to generate simulation-ready molecular models directly from cells [1,2]. hcTM enables the automated and comprehensive detection of a wide variety of macromolecular complexes within crowded eukaryotic cells. The high-confidence molecular assignments have driven both technical advances [3] and biological discoveries [1,2], fostering robust connections between molecular functionality, spatial localization, and cellular context. Thus, hcTM paves the way for modeling and simulating the dynamics of biomolecules in their native environment.

[1] Cruz-León, et al., Nat. Comm., 2024 [2] Kreysing*, Heidari*, Zila*, et al., BioRxiv, 2024 [3] Tuijtel, et al., Sci. Adv., 2024

BP 32.6 Fri 10:45 H46

Membrane insertion and channel formation of alpha-latrotoxins — •Andreas Heuer[1], Azadeh Alavizargar[1], Björn U. Klink[2,3], and Cristos Gatsogiannis[2,3] — [1]Institute for Physical Chemistry, University of Münster, Germany — [2]Center for Soft Nanoscience (SoN), University of Münster — [3]Institute for Medical Physics and Biophysics

Latrotoxins are the main toxic component of the venom of black widow spiders. It is known that the they provide ion channels in the plasma membrane, allowing, e.g., for a strong influx of Ca2+ ions which may induce a burst of neurotransmitters. Despite its importance, microscopic information about the microscopic structure of latroxin pore formation remained elusive.

In this presentation it is shown how detailed information can be gained by a combination of cryoEM, AlphaFold and Molecular Dynamics (MD) simulations [1]. From this analysis we can identify a unique mechanism of membrane insertion and channel formation for the example of Na+ and Ca2+ transport. From the MD simulations it is possible, e.g., to elucidate the efficiency and the time-scales of the transport processes and to show why the channel is efficient in transporting mono- and divalent ions but not trivalent ions.

[1] Klink, B.U., Alavizargar, A., Kalyankumar KS, Chen M, Heuer A, Gatsogiannis C (2024) Nature Communications 15, 8551

BP 32.7 Fri 11:00 H46

Understanding the impact of functionalized gold nanoparticles (AuNPs) on the lipid bilayer and interfacial water through atomistic molecular dynamics simulations — •Haifa Al Mamari, Srinivasa Varanasi, and Issam Ali — Sultan Qaboos University, Department of Physics

Functionalized gold nanoparticles (AuNPs) show promise as drug delivery systems due to their customizable size, shape, biocompatibility, and surface modifications. However, crossing cell membrane barriers is a challenge, requiring efficient penetration for effective drug delivery. Interfacial water and ions play a crucial role in the interaction between AuNPs and bilayers, making it essential to understand the structural and orientational effects on lipid bilayers. This study explores how nanoparticle surface charge and lipid chemistry impact AuNP-lipid bilayer interactions, focusing on anionic (carboxylate) and cationic (quaternary ammonium) AuNPs with zwitterionic (DPPC), anionic (DPPG), and cationic (DPTAP) bilayers using molecular dynamics simulations.Our analysis shows that AuNPs significantly alter bilayer properties, impacting the area per lipid, membrane thickness, acyl chain order, electrostatic potential, dipole alignment, and head and tail tilt angles. These changes enhance water dipole alignment and modify electrostatic potentials, depending on the nanoparticles surface charge. These insights emphasize AuNPs' potential to reshape membrane properties, providing valuable guidance for nanoparticle-based therapeutic development.

15 min. break

BP 32.8 Fri 11:30 H46

Swimming by spinning: spinning-top type rotations regularize sperm swimming into persistently progressive paths in 3D — •Xiaomeng Ren and Hermes Bloomfield-Gadêlha — School of Engineering Mathematics & Bristol Robotics Laboratory, University of Bristol, BS8 1UB Bristol, UK

Sperm swimming is essential for reproduction, with movement strategies adapted to specific environments. Sperm navigate by modulating the symmetry of their flagellar beating, but how they swim forward with asymmetrical beats remains unclear. Current methods lack the ability to robustly detect the flagellar symmetry state in free-swimming spermatozoa, despite its importance in understanding sperm motility. This study uses numerical simulations to investigate the fluid mechanics of sperm swimming with asymmetrical flagellar beats. Results show that sperm rotation regularizes the swimming motion, allowing persistently progressive swimming even with asymmetrical flagellar beats. Crucially, 3D sperm head orientation, rather than the swimming path, provides critical insight into the flagellar symmetry state. Sperm rotations during swimming closely resemble spinning-top dynamics, with sperm head precession driven by the helical beating of the flagellum. These results may prove essential in future studies on the role of symmetry in microorganisms and artificial swimmers, as body orientation detection has been largely overlooked in favor of swimming path analysis. Altogether, this rotational mechanism provides a reliable solution for forward propulsion and navigation in nature, which would otherwise be challenging for flagella with broken symmetry.

BP 32.9 Fri 11:45 H46

Simulating Trypanosome Motility — •Florian Overberg, Gerhard Gompper, and Dmitry Fedosov — Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

We investigate motility of the protozoan Trypanosoma brucei via numerical simulations, in which a trypanosome model is informed by experimental observations. The cell body is represented by a set of vertices distributed homogeneously on a pre-defined elongated surface, forming a triangulated elastic network of springs. This network model incorporates bending rigidity, area conservation, and volume conservation constraints. For the generation of propulsion, a flagellum is attached to the cell body. The flagellum consists of four parallel filaments, two of which are embedded in the body and used for generating a propagating bending wave. We examine the parasite behavior for various conditions, including different flagellum and body stiffnesses, beating frequencies, actuation wavelengths, and amplitudes. Our simulations yield swimming velocities and rotation frequencies around the swimming axis that are in a good agreement with experimental measurements. Additionally, we investigate the importance of various actuation characteristics, such as orientation of the beating plane and the stress-free conformation of the flagellum. We have also started to study parasite motility in a stationary blood suspension, which serves as a first step to understand trypanosome behavior in one of its natural environments such as blood vasculature.

BP 32.10 Fri 12:00 H46

Leveraging quantum data to advance machine-learning in (bio)molecular simulations — •Leonardo Medrano Sandonas[1], Mirela Puleva[2], Gianaurelio Cuniberti[1], and Alexandre Tkatchenko[2] — [1]TUD Dresden University of Technology, Germany. — [2]University of Luxembourg, Luxembourg.

The rapid advancement of machine learning (ML) applications in chemistry and physics has been driven by the increasing availability of comprehensive quantum-mechanical (QM) datasets. Recently, we introduced high-fidelity property data at the PBE0+MBD level of theory for both small [Sci. Data 8, 43, (2021)] and large [Sci. Data 11, 742, (2024)] drug-like molecules in equilibrium and non-equilibrium states. These datasets have been instrumental in advancing QM-based ML interatomic potentials [10.26434/chemrxiv-2024-bdfr0, (2024)] and enhancing semi-empirical (SE) methods [J. Phys. Chem. Lett., 11, 6835 (2020)], enabling accurate (bio)molecular simulations. In this presentation, we will discuss our recent efforts to improve the transferability and generalizability of the ML-corrected density functional tight-binding method. We demonstrate that equivariant neural networks significantly enhance the accuracy and scalability of ML-based many-body repulsive potentials trained on energies and forces of small organic systems. This approach facilitates the investigation of the energetic and structural properties of large drug-like molecules and molecular dimers. Hence, our findings indicate that combining ML with SE methods achieves both high accuracy and computational efficiency, paving the way for diverse applications in (bio)molecular simulations.

BP 32.11 Fri 12:15 H46

Calibrating 1D-0D Coupled Blood Flow Models: the potential of Neural Network based Surrogates — •Benedikt Hoock[1,2] and Tobias Köppl[3] — [1]Technische Universität München, School of Computation, Information and Technology — [2]Support by Computing Facilities of Leibniz-Rechenzentrum München — [3]Fraunhofer-Institut FOKUS, Berlin

Hydrodynamic models of the human arterial network can simulate the blood flow in parts or the whole body. The calculations can be simplified by solving the incompressible one-dimensional Navier-Stokes equations only for a set of larger vessels and coupling those at their outlets to a Windkessel model (*1D-0D approach*). Here, the right parametrization of the Windkessel parameters, i.e., the resistances and capacities, is crucial to obtaining realistic simulations. This can be done by calibrating the model parameters to match the model predictions with in-vivo blood pressure measurements. Since this requires many computationally expensive model evaluations, we test the potential of surrogates based on neural networks (NN). Once set up in an appropriate architecture, already ordinary fully connected NNs of moderate depth and width two can reproduce the simulations with high accuracy, advancing over e. g. the PINN approach due to their better trainability. We use these in an optimization algorithm to identify the target resistance and capacity with high precision in several test cases. Our efficient calibration scheme is an essential building block for an instantaneous visualization of the organ perfusion in a digital twin of a patient under different motion conditions on a digital treadmill.

BP 32.12 Fri 12:30 H46

MolecuTas: an ML platform for refining quantum properties and bioactivity of complex molecules — •Vicente Domínguez Arca[1,2], Jannis Krüger[2], Álvaro Vallejo Bay[3], Thomas Hellweg[2], and Luis Taboada Antelo[1] — [1]Biosystem and Bioprocesses Engineering, IIM-CSIC, Spain — [2]Physical and Biophysical Chemistry, Bielefeld University, Germany — [3]Applied Physics, University of Santiago de Compostela, Spain

The integration of machine learning (ML) and computational chemistry enables efficient prediction of quantum properties for complex molecules, crucial for advancing drug discovery and materials science. Our ML platform leverages Graph Convolutional Neural Networks (GCNNs) and the "sliding window" methodology to predict quantum mechanical parameters like partial atomic charges, overcoming traditional ab initio constraints. This approach scales to larger, biologically relevant molecules, enhancing molecular dynamics simulations and rational drug design.

Focusing on marine saponins -complex thalassochemicals with unique sulfated glycoside structures- our platform improves charge distribution predictions, enabling precise simulations of bioactive interactions. These advances highlight the therapeutic potential of marine saponins in oncology, lipid metabolism, and immune modulation. By applying our platform to marine saponins, this research bridges computational and experimental workflows, fostering the discovery of novel thalassochemicals for applications in functional foods, pharmaceuticals, and sustainability.

BP 32.13 Fri 12:45 H46

Ab-initio optimization and AI-powered inference for parametrizing complex biological models under low data availability — •Thomas R. Sokolowski — Frankfurt Institute for Advanced Studies (FIAS), Ruth-Moufang-Str. 1, 60438 Frankfurt am Main, Germany

Early development unfolds under diverse circumstances and time scales, but always facing the impacts of inevitable biological noise. To cope with this, various developmental mechanisms evolved, with their differences shaped by physical and environmental constraints. In spite of decades of research, we still lack theories that explain these processes truly mechanistically. Increasing computational power allows for constructing developmental models with increasing complexity, but since corresponding experimental data is scarce, the parametrization of such models becomes a key problem itself. I will contrast two strategies for parametrizing biophysical models in development and beyond: optimization of normative theories, and Bayesian inference. I will present a framework that unifies both strategies in a mathematically rigorous fashion and enables quantitative transition between them. I will then present our results combining both strategies for understanding embryogenesis in two organisms: (1.) optimization of a spatial-stochastic model of the gap gene system in Drosophila, and (2.) elucidation of robust cell-fate assignment in early mouse embryogenesis via AI-powered simulation-based inference (SBI). Our results highlight distinct developmental strategies that emerged under the different circumstances faced by the two organisms.

BP 33: Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by
Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Friday 10:30–12:45 Location: H24

Invited Talk BP 33.1 Fri 10:30 H24

Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things — •Steven Lee — University of Cambridge

The talk will outline two single-molecule fluorescence approaches that can be used to determine orthogonal metrics about a single emitter.

The first half introduces "POLCAM," a simplified single-molecule orientation localization microscopy (SMOLM) method based on polarised detection using a polarisation camera. POLCAM's fast algorithm operates over 1000 times faster than the current state-of-the-art, allowing near-instant determination of molecular anisotropy. To aid adoption, open-source image analysis software and visualization tools were developed. POLCAM's potential was demonstrated in studying alpha-synuclein fibrils and the actin cytoskeleton of mammalian cells. (Nature Methods 2024). The second approach focuses on "Single-Molecule Light Field Microscopy" (SMLFM), encoding 3D positions into 2D images for volumetric super-resolution microscopy. SMLFM shows an order-of-magnitude speed improvement over other 3D PSFs, resolving overlapping emitters through parallax. Experimental results reveal high accuracy and sensitivity in point detection, enabling whole-cell imaging of single membrane proteins in live primary B cells and high-density volumetric imaging in dense cytosolic tubulin datasets. (Nature Comms 2024)

Invited Talk BP 33.2 Fri 11:00 H24

MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research — •Andreas Römpp — Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

Mass spectrometry imaging is an analytical technique that provides spatially-resolved molecular information for a wide range of compound classes. In contrast to many histological methods, it does not require labeling. The capabilities and limitations of MS imaging will be discussed on the basis of several application areas with a focus on food analysis and pharmaceutical research. In our study 'MALDI mass spectrometry imaging: from constituents in fresh food to ingredients, contaminants and additives in processed food' (https://doi.org/10.1016/j.foodchem.2022.132529) we analyzed a range of plant-based and meat-based food. The analysis of natamycin in cheese and acrylamide in gingerbread constitute the first mass spectrometry imaging measurements of a food additive and a food contaminant, respectively. MS imaging is the only method that can analyze the distribution of drug compounds in animal models or human tissue (without labeling). This is exemplified on the detection of antituberculosis drugs in mouse model tissue including our most recent study on the clinical stage antibiotic BTZ-043 which has just been accepted for publication in Nature Communications (https://doi.org/10.1038/s41467-025-56146-9).

BP 33.3 Fri 11:30 H24

On-Surface Synthesis and Characterization of a Nitrogen-Containing Heterocycle — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Matthias Zeilerbauer[1], Shadi Fatayer[2], and Laerte Patera[1] — [1]University of Innsbruck, Austria — [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Nitrogen-containing heterocycles are fundamental building blocks in nature, forming the core of essential biomolecules and pharmaceuticals. This study demonstrates the on-surface formation of an N-heterocyclic organic compound via thermal activation of a tailored precursor. High-resolution non-contact atomic force microscopy (nc-AFM) provides bond-level resolution of the synthesized structures. Complementary scanning tunneling spectroscopy visualizes changes in the electronic structure resulting from the formation of the heterocycle. Density functional theory calculations (DFT) reveal the most probable reaction mechanism, highlighting the critical role of hydrogen release as the driving force of the reaction. These findings emphasize the versatility of on-surface synthesis as a powerful tool for creating complex organic compounds.

BP 33.4 Fri 11:45 H24

Elasticity Mapping of Nonahelicene with Submolecular Resolution by NC-AFM — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 NishigoNaka, Myo-daiji, Okazaki 444-8585, Japan

Controlled modification of atomic configurations of molecules and materials is an exciting goal for non-contact atomic force microscopy (NC-AFM). Certain changes like shifts of the electronic energy gaps may be expected, but are not well explored and not established on the molecular scale. Here we report quantitative measurement of atomic-scale deformation in single molecules with NC-AFM. Individual molecules of nonahelicene ([9]H) and coronene (Cor) were studied on a Ag(110) surface under ultrahigh vacuum and cryogenic conditions by the measurement of frequency-shift distance curves for this. The molecular responses can be replicated with an empirical Lennard-Jones model, but for [9]H an elastic contribution is required to account for its elastic nature. Furthermore, a 3D-force mapping technique, termed molecular deformation mapping (MDM), allows to study the lateral position dependence of the elastic response. The MDM of [9]H reveals a spatially strongly anisotropic behaviour for the elasticity, interaction forces, elongation and binding energy of the tip to the molecule. The result is rationalized in terms of an aromaticity model.

BP 33.5 Fri 12:00 H24

Detection and control of quantum proton ordering in hydrogen bonds at the atomic scale — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Directly probing the spatial arrangements and quantum nature of protons in hydrogen-bonded (H-bonded) materials and biosystems is the key to understand their macroscopic properties and functions. Here, exploiting bond-resolved atomic force spectroscopy (BR-AFS) combined with path-integral molecular dynamics method, we demonstrate for the first time that BR-AFS measurements along the apparent H-bond between proton donor and acceptor atoms allows the identification of both classical H-bonds with inherent directionality and non-classical H-bonds with quantum proton delocalization in self-assembled imidazole derivatives on surfaces. Unlike the conventional unidirectional H-bonding in linear chains, chiral cyclic hexamers exhibit unique quantum proton ordering in their ground states, which contain a mix of classical and non-classical H-bonds, breaking rotational symmetry. Furthermore, we show the capability to switch the quantum-proton-ordering state on and off by altering the adsorption registry coupled with a collective transfer of six protons within the cyclic H-bonds. These findings open new pathways for detecting and controlling complex proton orders and for engineering proton-based quantum states with atomic-level precision.

BP 33.6 Fri 12:15 H24

Imaging of the conformations of individual β-cyclodextrins with non-contact AFM — Marko Grabarics[1], •Benjamin Mallada[1,2,3], Shayan Edalatmanesh[2,3], Stephan Rauschenbach[1], Pavel Jelinek[2,3], and Bruno de la Torre[2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]CATRIN, Palacký University Olomouc, CZ — [3]Institute of Physics, Czech Academy of Sciences, CZ

Glycans, biopolymers essential to biology and materials science, are highly complex due to their structural diversity, conformational flexibility, and numerous possible isomers. Conventional methods often struggle to resolve these structures with atomic precision, especially under solvent-free conditions. We employ nc-AFM under UHV to determine the atomic structure of β-cyclodextrin (β-CD), a cyclic glucose molecule.

Our results reveal the adsorption geometries, hydroxy group positions, and stabilizing hydrogen bonds on a Au(111) surface. The primary face forms a closed hydrogen-bond network, while the secondary face exhibits pairwise interactions between OH groups of the same glucose monomer. DFT calculations validate these findings, enabling precise structural assignment and capturing subtle conformational differences.

This work highlights nc-AFM's capability to overcome the limitations of conventional sequencing techniques and represents the first application of nc-AFM to glycans. Future integration with ion deposition techniques could extend its utility to more complex glycans.

BP 33.7 Fri 12:30 H24

Domain size effects in the spectra of micro-heterogeneous samples — •Thomas Mayerhöfer[1,2] and Jürgen Popp[1,2] — [1]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Helmholtzweg 4, 07743 Jena, Germany

Samples are often not composed of a single pure compound but are instead mixtures of different substances. Under the Bouguer-Beer-Lambert approximation, the absorbance spectra of such mixtures can be simply derived by summing the spectra of the individual components, with each spectrum weighted by the molar fraction of the corresponding compound.

In the context of wave optics, the resolving power of light at a given wavelength becomes crucial. If a microscope using light at this wavelength can distinguish structural details within the sample, the sample is classified as micro-heterogeneous. In this case, spatial averaging occurs at the intensity level, involving reflectance and transmittance rather than absorbance.

The shift from micro-heterogeneity to macro-heterogeneity is gradual and cannot be described by an analytical formula due to the wave nature of light. This has significant implications for spectrum interpretation, as it can lead to substantial variations in peak shapes, positions, and intensities, e.g., during mitosis.

BP 34: Statistical Physics in Biological Systems II (joint session DY/BP)

Time: Friday 11:30–13:00 Location: H43

Invited Talk BP 34.1 Fri 11:30 H43

Equilibrium and non-equilibrium dynamics of biological systems with memory — •Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin

Biological systems are many-body systems. Thus, their dynamics, when described in terms of a low-dimensional reaction coordinate, is governed by the generalized Langevin equation (GLE), an integro-differential equation of motion which contains friction memory [1]. Two examples will be discussed:

Protein-folding kinetics is standardly described as Markovian (i.e., memoryless) diffusion in a one-dimensional free-energy landscape. By analysis of molecular-dynamics simulation trajectories of fast-folding proteins the friction is demonstrated to exhibit significant memory with a decay time of the same order as the folding and unfolding times [2,3,4]. Memory friction leads to anomalous and drastically modified protein kinetics: the folding and unfolding times are not dominated by free-energy barriers but rather by non-Markovian friction.

Active motion of organisms obviously is far from equilibrium. The parameters of an appropriate non-equilibrium GLE are extracted from trajectories. It is demonstrated that the motion of single-cellular algae is characterized by pronounced memory friction, which allows to classify and sort individual cells.

[1] Memory and Friction: From the Nanoscale to the Macroscale, BA Dalton, A Klimek, H Kiefer, F N Brünig, H Colinet, L Tepper, A Abbasi, RR Netz, https://arxiv.org/pdf/2410.22588

BP 34.2 Fri 12:00 H43

Mean transient drift of synaptic weights in feed-forward spiking neural networks with spike-timing-dependent plasticity — •Jakob Stubenrauch and Benjamin Lindner — BCCN Berlin and Physics Department HU Berlin, Germany

Spike-timing dependent plasticity (STDP) [1] is a phenomenological model for the dynamics of single synaptic weights. This concise microscopic (single-synapse) description allows for the derivation of macroscopic network theories, capturing for instance learning, forgetting, and representational drift.

For the development of such theories it is important to characterize the stochastic process of synaptic weights. Early attempts capture this process for Poissonian presynaptic spikes and conditionally Poissonian postsynaptic spikes [2]. However, since STDP depends on fine spike-timing differences below 20 ms [1], it is important to characterize the synaptic dynamics for neuron models that describe the fast response mechanistically.

Leveraging a recent theory [3] as well as established results for the leaky integrate-and-fire neuron [4,5], we analytically compute the drift and diffusion of feed-forward synapses in a setup where a layer of presynaptic Poisson processes feeds into a recurrent network of leaky integrate-and-fire neurons.

[1] Bi and Poo, J. Neurisci. (1998) [2] Kempter et al., Phys. Rev. E (1999) [3] Stubenrauch and Lindner, Phys. Rev. X (2024) [4] Brunel et al., Phys. Rev. Lett. (2001) [5] Lindner and Schimansky-Geier, Phys. Rev. Lett. (2001)

BP 34.3 Fri 12:15 H43

A Biophysical Model for Temperature-Sensitivity of Neurons — •Julian Voits[1], Wojciech Ambroziak[2,3], Jan Siemens[2,4], and Ulrich S. Schwarz[1,5] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]Department of Pharmacology, University of Heidelberg, Germany — [3]Department of Translational Disease Understanding, Grünenthal GmbH, Aachen, Germany — [4]Molecular Medicine Partnership Unit (MMPU), European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [5]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

Control of body temperature is essential for our well-being and especially important during periods of fever or heat acclimation, e.g. due to traveling or climate change. An essential element of body temperature control are temperature-sensitive neurons, particularly warm-sensitive ones in the preoptic area of the hypothalamus. Since the discovery of temperature-sensitive ion channels, it has become clear that the underlying molecular mechanisms are rather diverse. In this work, we introduce a mathematical model based on a reduced version of the Hodgkin-Huxley model that can predict the frequently observed linear dependence of spiking rates on temperature in warm-sensitive neurons. Additionally, we present data showing how neurons adapt to varying temperatures over time, along with evidence of hysteresis in many temperature-sensitive neurons.

BP 34.4 Fri 12:30 H43

Position-Dependent Non-Markovian Effects Improve Protein Folding Simulations — •Lucas Tepper, Cihan Ayaz, Benjamin Dalton, and Roland Nezt — Freie Universität Berlin

It's common to project a protein's full atomic resolution onto a one-dimensional reaction coordinate to capture key aspects of its folding process. As a direct consequence of this dimensionality reduction, non-Markovian memory effects emerge. Accounting for memory effects in the framework of the generalized Langevin equation (GLE) with linear friction has proven efficient, accurate and insightful. However, recent advances in deriving GLEs with non-linear, position-dependent friction kernels raise questions about their applicability to protein folding simulations. We derive a novel method to extract position-dependent friction kernels from time series data via conditional Volterra equations. When applied to two protein test systems, the position- and time-dependent friction is strongest for long memory times in the folded states, where atoms are tightly packed. Additionally, we propose a novel and numerically efficient GLE simulation setup, confirming the accuracy of the extracted kernels. Compared to linear friction GLE simulations, our results show that position-dependent non-Markovian effects are critical for accurately reproducing protein folding kinetics when using low-dimensional reaction coordinates.

BP 34.5 Fri 12:45 H43

Multicomponent mixtures exhibit a vast nucleation-and-growth regime — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Phase coexistence is crucial for understanding how cells regulate biomolecular condensates. Despite of the multicomponent and multiphase nature of such condensates, the direct study of coexisting phases is limited to only few components since the parameter space is high-dimensional. So far, no theory provides a direct and concrete estimation of the phase coexistence behavior of multicomponent mixtures. As a first-level description of multicomponent phase behavior, we derive scaling relations for the number of coexisting phases in typical multicomponent mixtures in equilibrium. The scaling relations reveal that the interactions required to have many coexisting phases only scales very weakly with the number of components, whereas the stability analysis of the homogeneous state suggests a much stronger scaling. This discrepancy implies that large parts of the phase diagram of multicomponent mixture are in the nucleation-and-growth regime, where the homogeneous state is locally stable while multiple coexisting phases are preferred energetically. This suggests that multicomponent mixtures can achieve versatility and controllability in phase behavior with moderate interactions, which might be utilized by cells to create or destroy biomolecular condensates.

BP 35: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H2

Invited Talk BP 35.1 Fri 13:15 H2

Active control of forces, movement and shape: from biological to non-living systems — •Ulrich S. Schwarz — Heidelberg University, Heidelberg, Germany

Animal cells are highly dynamic and continuously generate force, for example for division, migration and mechanosensing. Their main force generators are myosin II molecular motors, whose activity is precisely controlled by biochemical circuitry. We first discuss how this system can be hijacked by optogenetics, thus that cellular force generation can be controlled in time and space using light. Next, we use active gel theory combined with van der Waals theory for myosin II molecules to demonstrate that cell contractility is sufficient to explain cell migration and that optogenetics can be used to initiate and revert migration. For two myosin II species, we predict the possibility of oscillations. We then move up in scale and analyze force generation in intestinal organoids, which are epithelia with the topology of a sphere. Combining experimental data, image processing and the bubbly vertex model, we show how apico-basal asymmetries can lead to cell extrusion and budding. We finally discuss how force generation and shape changes can be achieved in non-living systems, in particular for nematic elastomers, in which the direction of contraction is imprinted during polymerization and actuation is achieved by temperature control.

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Overview of Invited Talks and Sessions

(Lecture halls H34, H38, and H46; Poster P3 and P4)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H34	**Impact of smallest loops and composition fluctuations on the structure of end-linked polymer model networks** — •Michael Lang, Reinhard Scholz, Toni Müller
CPP 5.1	Mon	11:30–12:00	H38	**Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via *ab initio* spectroscopy simulations** — •Daniel Sebastiani, Pouya Partovi-Azar
CPP 8.1	Mon	15:00–15:30	H38	**The Nanoscale Photovoltaics Laboratory on a Tip** — •Stefan Weber
CPP 16.1	Tue	9:30–10:00	H34	**Multifunctional structural batteries** — •Göran Lindbergh
CPP 17.1	Tue	9:30–10:00	H38	**Continuum models for water's peculiar behavior on the nanoscale** — •Alexander Schlaich
CPP 18.1	Tue	9:30–10:00	H46	**Hybrid materials from colloidally stable nanocellulose and nanoparticles - scattering techniques are needed for characterization** — •Eva Malmström, Åsa Jerlhagen, Benedikt Sochor, Korneliya Gordeyeva, Stephan Roth
CPP 20.1	Tue	11:30–12:00	H38	**Tailored polymer thin films enabled by initiated chemical vapor deposition (iCVD): From fundamentals to functional applications** — •Stefan Schröder
CPP 23.1	Wed	9:30–10:00	H34	**Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties** — •Manfred Wilhelm
CPP 26.1	Wed	11:30–12:00	H34	**Polyelectrolytes in the confined space of mesopores for transport regulation** — •Annette Andrieu-Brunsen
CPP 30.1	Wed	16:15–16:45	H34	**Challenges and Opportunities in Bringing Machine Learning to a Synchrotron** — •Alexander Hexemer, Tanny Chavez, Wiebke Köpp, Dylan McReynolds, Stephan Roth, Tim Snow, Sharif Ahmed
CPP 31.1	Wed	16:15–16:45	H38	**Moving with minimum effort – Optimal work protocols for systems with memory** — •Sarah Loos, Samuel Monter, Felix Ginot, Clemens Bechinger
CPP 34.1	Thu	15:00–15:30	H34	**Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials** — •Valentina Guccini
CPP 37.1	Thu	16:15–16:45	H34	**Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level** — Marie Hartwig-Nair, Sara Florisson, Kristofer Gamstedt, •Malin Wohlert
CPP 38.1	Thu	16:15–16:45	H38	**Adsorption and Interaction of Amino Acids on Titanium Oxide Photocatalyst** — Miguel Blanco-Garcia, Mona Kohantorabi, Benedikt Socher, Ulrike Protzer, Stephan V. Roth, Cristiana Di Valentin, Andreas Stierle, •Heshmat Noei
CPP 41.1	Fri	9:30–10:00	H38	**Simulations of reaction equilibria in macromolecular systems** — •Peter Košovan

Invited Talks of the joint Symposium Physics of Embryonic Development Across Scales: From DNA to Organisms (SYED)

See SYED for the full program of the symposium.

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher
SYED 1.2	Mon	10:00–10:30	H1	**A tissue rigidity phase transition shapes morphogen gradients** — Camilla Autorino, Diana Khoromskaia, Bernat Corominas-Murtra, Zena Hadjivasiliou, •Nicoletta Petridou

SYED 1.3	Mon	10:30–11:00	H1	**Building quantitative dynamical landscapes of developmental cell fate decisions** — •David Rand
SYED 1.4	Mon	11:15–11:45	H1	**Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate** — •Anne Grapin-Botton, Byung Ho Lee, Masaki Sano, Daniel Riveline, Kana Fuji, Tetsuya Hiraiwa
SYED 1.5	Mon	11:45–12:15	H1	**Chromosomes as active communication and memory machines** — •Leonid A. Mirny

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

CPP 1.1–1.6	Mon	9:30–11:15	H34	**Gels, Polymers Networks and Elastomers I**
CPP 2.1–2.11	Mon	9:30–12:45	H37	**Active Matter I (joint session DY/BP/CPP)**
CPP 3.1–3.7	Mon	9:30–11:15	H38	**Organic Electronics and Photovoltaics I**
CPP 4.1–4.6	Mon	11:30–13:00	H34	**Crystallization, Nucleation and Self-Assembly I**
CPP 5.1–5.5	Mon	11:30–13:00	H38	**Composites and Functional Polymer Hybrids**
CPP 6.1–6.4	Mon	15:00–16:00	H34	**Gels, Polymers Networks and Elastomers II**
CPP 7.1–7.7	Mon	15:00–17:00	H37	**Active Matter II (joint session BP/CPP/DY)**
CPP 8.1–8.3	Mon	15:00–16:00	H38	**Hybrid and Perovskite Photovoltaics I**
CPP 9.1–9.6	Mon	15:00–16:45	H46	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 10.1–10.4	Mon	16:15–17:15	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
CPP 11.1–11.3	Mon	16:15–17:00	H38	**Hybrid and Perovskite Photovoltaics II**

CPP 12.1–12.4	Mon	17:00–18:00	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session CPP/BP)**
CPP 13.1–13.5	Mon	17:15–18:30	H38	**Molecular Electronics and Excited State Properties I**
CPP 14.1–14.4	Mon	17:30–18:30	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
CPP 15.1–15.74	Mon	19:00–21:00	P4	**Poster Session I**
CPP 16.1–16.6	Tue	9:30–11:15	H34	**Energy Storage and Batteries I**
CPP 17.1–17.6	Tue	9:30–11:15	H38	**Modeling and Simulation of Soft Matter I**
CPP 18.1–18.6	Tue	9:30–11:15	H46	**Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)**
CPP 19.1–19.11	Tue	9:30–13:00	H47	**Active Matter III (joint session DY/BP/CPP)**
CPP 20.1–20.5	Tue	11:30–13:00	H38	**Interfaces and Thin Films I**
CPP 21.1–21.6	Tue	14:00–15:30	H34	**Modeling and Simulation of Soft Matter II**
CPP 22.1–22.5	Tue	14:00–15:15	H38	**Organic Electronics and Photovoltaics II**
CPP 23.1–23.6	Wed	9:30–11:15	H34	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 24.1–24.7	Wed	9:30–11:15	H38	**Hybrid and Perovskite Photovoltaics III**
CPP 25.1–25.20	Wed	10:00–12:00	P3	**Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)**
CPP 26.1–26.5	Wed	11:30–13:00	H34	**Nanostructures, Nanostructuring and Nanosized Soft Matter I**
CPP 27.1–27.6	Wed	11:30–13:00	H38	**Molecular Electronics and Excited State Properties II**
CPP 28.1–28.4	Wed	15:00–16:00	H34	**Modeling and Simulation of Soft Matter III**
CPP 29.1–29.4	Wed	15:00–16:00	H38	**Organic Electronics and Photovoltaics III**
CPP 30.1–30.8	Wed	16:15–18:30	H34	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I**
CPP 31.1–31.6	Wed	16:15–18:00	H38	**Responsive and Adaptive Polymers**
CPP 32.1–32.45	Thu	9:30–12:00	P3	**Poster Session II**
CPP 33.1–33.5	Thu	11:45–13:00	H34	**Modeling and Simulation of Soft Matter IV**
CPP 34.1–34.3	Thu	15:00–16:00	H34	**Focus Session: Interactions Between Water and Cellulose I**
CPP 35.1–35.9	Thu	15:00–17:45	H37	**Microswimmers and Microfluidics (joint session DY/BP/CPP)**
CPP 36.1–36.4	Thu	15:00–16:00	H38	**Organic Electronics and Photovoltaics IV**
CPP 37.1–37.3	Thu	16:15–17:15	H34	**Focus Session: Interactions Between Water and Cellulose II**
CPP 38.1–38.5	Thu	16:15–17:45	H38	**Interfaces and Thin Films II**
CPP 39	Thu	18:00–19:00	H38	**Members' Assembly**
CPP 40.1–40.7	Fri	9:30–11:15	H34	**Energy Storage and Batteries II**
CPP 41.1–41.6	Fri	9:30–11:15	H38	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids I**
CPP 42.1–42.12	Fri	9:30–13:00	H44	**Active Matter IV (joint session BP/CPP/DY)**
CPP 43.1–43.11	Fri	9:30–12:45	H47	**Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)**
CPP 44.1–44.4	Fri	11:30–12:30	H34	**2D Materials**
CPP 45.1–45.5	Fri	11:30–12:45	H38	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids II**
CPP 46.1–46.1	Fri	13:15–14:00	H2	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 H38

Sessions

– Invited Talks, Contributed Talks, and Posters –

CPP 1: Gels, Polymers Networks and Elastomers I

Time: Monday 9:30–11:15 Location: H34

Invited Talk CPP 1.1 Mon 9:30 H34

Impact of smallest loops and composition fluctuations on the structure of end-linked polymer model networks — •Michael Lang, Reinhard Scholz, and Toni Müller — Leibniz-Institut für Polymerforschung, Dresden, Germany

A self-consistent scheme of differential equations is developed for predicting the frequency of the two smallest loop defects within polymer model networks. Without any adjustable parameter, we obtain excellent agreement with Monte Carlo simulations that sample loop formation only up to the given maximum loop size. The formation of loops of second generation leads to correlations between connected junctions that cannot be treated exactly by considering statistical arguments alone, which is in contrast to reversible networks where equilibrium statistics are sufficient. These correlations and the statistics of the junctions are provided by our model. Comparison with more realistic simulation data in three dimensions indicates that composition fluctuations of cross-links and chains clearly impact network formation. The differences between the statistics of the network junctions and our mean field predictions provide insight into the size of the domains with a predominance of chains or junctions and thus, regarding the quality of the mixture. Our results are highly relevant for an accurate modeling of network structure, improved estimates of the elastic properties of polymer networks, and for advanced analysis techniques of the network structure like network disassembly spectrometry or multiple quantum nuclear magnetic resonance.

CPP 1.2 Mon 10:00 H34

Hybrid PNIPAM Films for Green Hydrogen Production — •Morgan P. Le Dû[1], David P. Kosbahn[1], Thomas Baier[1], Qi Zhong[2], Apostolos Vagias[3], Robert Cubitt[3], Narendra Chaulagain[4], Karthik Shankar[4], Hagen Übele[5], Katharina Krischer[5], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Zhejiang Sci-Tech University, Hangzhou, China — [3]Institut Laue-Langevin (ILL), Grenoble, France — [4]University of Alberta, Department of Electrical and Computer Engineering, Edmonton, Canada — [5]TUM School of Natural Sciences, Nonequilibrium Chemical Physics, 85748 Garching, Germany

Platinum (Pt) doped carbon nitride (CN) is a promising photocatalyst under visible light for green hydrogen (H2) production. We develop this system in a thin polymer film to make it industrially scalable. The poly(N-isopropylacrylamide) (PNIPAM) hydrogel is used as a host matrix and water storage medium to facilitate homogeneous dispersion of the catalytic centers. The hybrid film's vertical distribution and inner microstructure are studied under in situ conditions with time-of-flight neutron reflectometry (ToF NR) and grazing incidence small angle neutron scattering (GISANS). The resulting H2 produced is measured by gas chromatography.

CPP 1.3 Mon 10:15 H34

Effect of different network topologies on swelling and mechanical properties of polyelectrolyte hydrogels — •Somesh Kurahatti, Mariano Brito, David Beyer, and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

We investigate the properties of polyelectrolyte hydrogels with various network heterogeneities, particularly their swelling capacity, elastic modulus and salt partitioning. We benchmark the scaling predictions for elastic modulus and equilibrium swelling ratio of the hydrogels under various salinity conditions, verifying the theoretically predicted behavior. Decoupling the elastic modulus from the swelling behavior is beneficial for applications such as super absorbers. Here, for example, now wants to increase the swelling ratio while maintaining a reasonable mechanical strength. We therefore explore mechanical and structural properties of the hydrogels with varying topologies, namely gels with dangling ends, gels with floating chains, and bottle-brush gels in counterpart to a reference regular gel. We observe that incorporating dangling ends changed swelling ratio and bulk modulus inline with the scaling predictions, whereas bottle-brush and floating-chain gels deviate from the predictions. Specifically, floating chains resulted in higher moduli and higher swelling ratio, while bottle-brush gels resulted in lower moduli and lower swelling ratios than the regular counterpart, each maintaining the same swelling ratio and modulus. The new swelling-mechanical relations allow us to treat them in a decoupled manner via the topology variation, which turns out to be of paramount relevance in the optimization and on-demand design of hydrogels.

CPP 1.4 Mon 10:30 H34

Aqueous foams stabilized by PNIPAM microgels: A multi-scale investigation — •Joanne Zimmer, Luca Mirau, Gaëtan Barth, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

Foams possess several structural motifs on different length scales with the smallest building blocks being the foam films or even the liquid/air interface. In this work, PNIPAM microgels (MG) are used as foam stabilizers as they are highly interfacial active and temperature responsive. In addition, the MG stiffness and by this their interfacial activity can be tuned by variation of the crosslinker content. We present a multi-scale approach towards understanding how the MG properties are related to the macroscopic foam and foam film stability. Spatially resolved disjoining pressure isotherms are measured with a Thin Film Pressure Balance (TFPB). The isotherms provide information about the film thickness, surface mobility and film stability. These properties are correlated with macroscopic foam characteristics such as foamability, stability and drainage dynamics. Indeed, the results are in good agreement on all length scales: A lower crosslinker content supports foam formation due to a faster surface coverage and results in an increased foam stability, as a more rigid surface layer is formed. Increasing the amount of crosslinker in the MG induces a transition from Poiseuille flow to plug flow in the foam during drainage which coincides with an increasing mobility of the surface of a single foam film measured in a TFPB.

CPP 1.5 Mon 10:45 H34

Phase separation in elastic polymer networks — •Takahiro Yokoyama[1,2], Yicheng Qiang[3], Chengjie Luo[3], Oliver Paulin[3], David Zwicker[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

Phase separation in polymer networks, from synthetic gels to biopolymer networks, significantly influences their structural and mechanical properties. While previous studies suggest that network mechanics regulate phase separation of the network itself and the embedded (complex) liquid, the fundamental principles governing this interaction remain poorly understood. To address this knowledge gap, we used molecular dynamics (MD) simulations to explore the phase behavior of elastic polymer networks. We systematically changed the quality of the (implicit) solvent, polymer chain length, and polymer flexibility. Our simulations identified two distinct phase separation behaviors depending on the polymer flexibility: macrophase separation into a polymer-rich and polymer-poor region for flexible polymer chains, and microphase separation with finite-sized pores for networks formed by semi-flexible chains. For the latter systems, we found that the pore size decreased with increasing chain stiffness. Furthermore, the network elasticity increased with decreasing pore size, following a power law as recently proposed by field theory. This study highlights the importance of polymer stiffness in shaping the size and distribution of (biomolecular) droplets within elastic networks.

CPP 1.6 Mon 11:00 H34

Nanoscopic measurements of the water content in microgels using fluorescence lifetime imaging — •Dominik Wöll[1], Alexandre Fürstenberg[2], Jörg Enderlein[3], Oleksii Nevskyi[3], Sankar Jana[1], Hannah Höche[1], and Leon Trottenberg[1] — [1]RWTH Aachen University, Institute of Physical Chemistry, Germany — [2]University of Geneva, Department of Physical Chemistry and Department of Inorganic and Analytical Chemistry, Genf, Switzerland — [3]Georg August UniversityGöttingen, 3rd Institute of Physics - Biophysics, Germany

The role of water molecules in the structure, function, and dynamics of (bio-)materials is significant, and thus, an estimation of the number of water molecules within different compartments is crucial. It has been demonstrated that the fluorescence of red emissive dyes is quenched in the presence of H_2O, with the excited energy transferred to surrounding H_2O molecules. Fluorescence lifetime imaging (FLIM) can thus be used to quantify the number of water molecules in proximity to the probing dye Atto 655, which was covalently embedded into microgels in the present study. Microgels represent an intriguing class of nanoparticles with considerable potential for applications in drug delivery and medicinal chemistry. We recorded FLIM images at varying H_2O:D_2O ratios, in both the swollen and collapsed states of the microgels at 22 °C and 40 °C, respectively. Stern-Volmer analysis enabled the calculation of the number of water molecules in the immediate vicinity of the dye molecule within the microgels at varying temperatures.

CPP 2: Active Matter I (joint session DY/BP/CPP)

Time: Monday 9:30–12:45 Location: H37

CPP 2.1 Mon 9:30 H37

Odd dynamics and pattern formation in mixtures of magnetic spinners and passive colloids — •Dennis Schorn[1], Stijn van der Ham[2], Hanumantha Rao Vutukuri[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

Starfish embryos aggregate into chiral crystals exhibiting odd elasticity (Tan *et al.* Nature **607**, 287 (2022)). Similar structures have been recently observed in externally driven magnetic colloids. In this talk, I present experiments and simulations of binary mixtures of magnetic spinners and passive colloids. We develop a model to predict the phase diagram of the system, which comprises four distinct phases that can be systematically reproduced in experiments. In particular, our simulations and experiments show a phase where the passive particles form a gel-like network featuring significant holes filled with self-organized rotating chiral clusters made of spinners. This phase can be reversed by changing the system's composition and magnetic field strength, featuring a system spanning spinner phase with embedded counter-rotating chiral clusters made of passive colloids. Our system may open the route towards a new type of viscoelastic active chiral matter involving nonreciprocal interactions between both species.

CPP 2.2 Mon 9:45 H37

Symmetry breaking in active non-reciprocal systems — •Kim L. Kreienkamp and Sabine H. L. Klapp — TU Berlin, Germany

Non-reciprocity significantly impacts the dynamical behavior in mixtures. One of its particularly striking consequences is the spontaneous emergence of time-dependent phases that break parity-time symmetry [1-3]. Here, we study a paradigmatic model of a non-reciprocal polar active mixture with completely symmetric repulsion [4,5]. Using a combination of field theory and particle-based simulations, we identify two qualitatively distinct regimes of non-reciprocity-induced dynamics. In the regime of weak intra-species alignment, non-reciprocity leads to asymmetric clustering in which only one of the two species forms clusters. Notably, the asymmetric density dynamics is driven alone by non-reciprocal orientational couplings [4,5]. In contrast, in the strongly coupled regime, the corresponding field theory exhibits exceptional points that have been associated with the emergence of chiral phases where the polarization direction rotates over time [2]. Our simulations confirm that spontaneous chirality arises at the particle level. In particular, we observe chimera-like states with coexisting locally synchronized and disordered regions. At the coupling strengths associated with exceptional points, the spontaneous chirality peaks.

[1] Z. You et al., PNAS 117, 19767 (2020).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] K. L. Kreienkamp and S. H. L. Klapp, NJP 24, 123009 (2022).
[4] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRE (2024).
[5] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRL (2024).

CPP 2.3 Mon 10:00 H37

Emergent phases in a discrete flocking model with non-reciprocal interaction — •Swarnajit Chatterjee, Matthieu Mangeat, and Heiko Rieger — Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Non-reciprocal interactions arise in systems that seemingly violate Newton's third law "actio=reactio". They are ubiquitous in active and living systems that break detailed balance at the microscale, from social forces to antagonistic inter-species interactions in bacteria. Non-reciprocity affects non-equilibrium phase transitions and pattern formation in active matter and represents a rapidly growing research focus in the field. In this work, we have undertaken a comprehensive study of the non-reciprocal two-species active Ising model (NRTSAIM), a non-reciprocal discrete-symmetry flocking model. Our study uncovers a distinctive *run-and-chase* dynamical state that emerges under significant non-reciprocal frustration. In this state, A-particles chase B-particles to align with them, while B-particles avoid A-particles, resulting in B-particle accumulation at the opposite end of the advancing A-band. This run-and-chase state represents a non-reciprocal discrete-symmetry analog of the chiral phase seen in the non-reciprocal Vicsek model. Additionally, we find that self-propulsion destroys the oscillatory state obtained for the non-motile case, and all the NRTSAIM steady-states are metastable due to spontaneous droplet excitation and exhibit motility-induced interface pinning. A hydrodynamic theory supports our simulations and confirms the reported phase diagrams.

CPP 2.4 Mon 10:15 H37

Emergent phases in a discrete flocking model with reciprocal interaction — •Matthieu Mangeat[1], Swarnajit Chatterjee[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We have undertaken a comprehensive study of the two-species active Ising model (TSAIM), a discrete-symmetry counterpart of the continuous-symmetry two-species Vicsek model, motivated by recent interest in the impact of complex and heterogeneous interactions on active matter systems. In the TSAIM, two species of self-propelled particles undergo biased diffusion in two dimensions, interacting via local intraspecies alignment and reciprocal interspecies anti-alignment, along with the possibility of species interconversion. We observe a liquid-gas phase transition, exhibiting macrophase-separated bands, and the emergence of a high-density parallel flocking state, a feature not seen in previous flocking models. With species interconversion (species-flip dynamics), the TSAIM corresponds to an active extension of the Ashkin-Teller model and exhibits a broader range of steady-state phases, including microphase-separated bands that further enrich the coexistence region. We also find that the system is metastable due to droplet excitation and exhibits spontaneous motility-induced interface pinning, preventing the system from reaching long-range order at sufficiently low noise. A hydrodynamic theory complements our computer simulations of the microscopic model and confirms the reported phase diagrams.

CPP 2.5 Mon 10:30 H37

Emergent collective behavior from cohesion and alignment — •Jeanine Shea and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany.

Collective behavior is all around us, from flocks of birds to schools of fish. These systems are immensely complex. To explore their basic characteristics, we introduce a minimal model for cohesive and aligning self-propelled particles in which group cohesion is established through additive, non-reciprocal torques [1]. These torques cause constituents to effectively turn towards one another, while an additional alignment torque competes in the same spatial range. By changing the strength and range of these torque interactions, we uncover six states which we distinguish via their static and dynamic properties. These states range from disperse particles to closely packed worm-like formations. A number of the states generated by this model exhibit collective dynamics which are reminiscent of those seen in nature.

[1] Knežević, M., Welker, T. and Stark, H. Collective motion of active particles exhibiting non-reciprocal orientational interactions. Sci Rep 12, 19437 (2022).

Invited Talk CPP 2.6 Mon 10:45 H37

Collective behavior of photoactive macroscopic particles — •Iker Zuriguel — University of Navarra, Pamplona, Spain

Active matter refers to systems of interacting, self-propelled agents that convert energy into mechanical motion, representing a nice example of out-of-equilibrium systems. In this work, a novel type of active particles is introduced. These are active granular (i.e. they interact solely through physical contacts) and photoactive, meaning that they self-propel using energy from light. Therefore, by means of a programmable LED panel, we are able to change the illumination pattern and, consequently, the particle activity in space and time, allowing a precise exploration of a variety of scenarios related to collective behavior. This possibility has been exploited in microscopic systems but is genuinely new in macroscopic ones.

First, we will present the clustering behavior of these agents under homogeneous illumination. By varying the illumination intensities and changing the population size, we observed a power-law-like distribution for both the cluster sizes and durations. We identified a transition from unstable to stable clusters, as indicated by the divergence of average cluster durations. Higher particle activities and smaller populations led to the creation of small unstable clusters, while lower particle activities and larger populations result in big, stable clusters that persist over time. This transition is explained with the help of a simple model capturing the most important processes involved in cluster dynamics. In the last part of the talk, the collective behavior under inhomogeneous illumination patterns will be introduced.

15 min. break

CPP 2.7 Mon 11:30 H37

Swarming model with minority interaction exhibits temporal and spatial scale-free correlations — •Simon Syga[1], Chandraniva Guha Ray[2,3,4], Josué Manik Nava Sedeño[5], Fernando Peruani[6,7], and Andreas Deutsch[1] — [1]Technische Universität Dresden — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Center for Systems Biology Dresden — [5]Universidad Nacional Autónoma de México — [6]Université Côte d'Azur, Nice — [7]CY Cergy Paris Université

Collective motion is a widespread phenomenon in social organisms, from bird flocks and fish schools to human crowds and cell groups. Swarms of birds and fish are particularly fascinating for their coordinated behavior and rapid escape

maneuvers during predator attacks. Critical motion is hypothesized as an optimal trade-off between cohesive group behavior and responsiveness to well-informed individuals. However, traditional models only show criticality at the phase transition between ordered and unordered motion. Here, we extend the Vicsek model with a minority interaction, where individuals primarily follow neighbors but can switch to follow a defector moving against a well-aligned group. This triggers cascades of defections, leading to rich dynamics, including large-scale fluctuations, scale-free velocity distributions, and a scale-free return time distribution of the order parameter. Our model underscores the biological importance of minority interactions in swarming and their role in critical behavior.

CPP 2.8 Mon 11:45 H37

'Predator-prey' driven swarmalator systems — •Ginger E. Lau, Mario U. Gaimann, and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Swarmalators are an active matter system of oscillators which exhibit swarming and collective motion in physical space, as well as synchronization behavior in an additional phase variable space, originally introduced by O'Keeffe *et al.* (*Nat. Commun.* 8(1), 1504, 2017). Such systems with bidirectional couplings in space and phase can be observed in nature, such as in the chorusing behavior of Japanese tree frogs characterized by Aihara *et al.* (*Sci. Rep.* 4(1), 3891, 2014). The interplay between attraction, repulsion, and phase synchronization provides several distinct regimes of self-organizational behavior. Akin to biological swarm systems responding to predator interactions, swarmalators can respond collectively to external perturbations by a repulsive driver. In previous work, driving was realized with a mobile 'pacemaker' by Xu *et al.* (*Chaos* 34(11), 113103, 2024). The present study introduces a new 'predator-prey' driven swarmalator model showing rich adaptive behavior. This could have a wide variety of potential future applications, from biological physics to swarm robotics to nature-inspired learning algorithms and methods of inference.

CPP 2.9 Mon 12:00 H37

Inertial active matter governed by Coulomb friction — •Alexander Antonov[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]University of Rome La Sapenzia, Rome, Italy

Coulomb, or dry friction, is a common phenomenon that can be encountered in various systems, such as granular matter or Brownian motors. The Coulomb friction force resists the motion and, unlike the friction in wet systems, is almost independent of the relative velocity. We show that this characteristic feature of Coulomb friction leads to emergence of dynamical states when subjected to active, or self-propelled motion [1]. At low activity levels, the dynamics resembles Brownian motion, while at greater activity, a dynamic Stop & Go regime emerges, marked by continuous switching between diffusion and accelerated motion. At even higher activity levels, a super-mobile regime arises, characterized by fully accelerated motion and an anomalous scaling of the diffusion coefficient with activity. Near the transition between the Stop & Go and super-mobile regimes, we reveal a novel activity-induced phase separation in collective behavior [2]. Our theoretical findings have been also demonstrated in experiments, where vibrobots on a horizontal surface are activated by vertical oscillations generated using an electromagnetic shaker.

[1] A.P. Antonov, L. Caprini, A. Ldov, C. Scholz, and H. Löwen, Phys. Rev. Lett. 133, 198301 (2024)

[2] A.P. Antonov et al., in preparation.

CPP 2.10 Mon 12:15 H37

Active nematic turbulence with substrate friction — •Peter A. E. Hampshire[1,2] and Ricard Alert[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, Dresden, Germany

Active nematics with high activity exhibit turbulent-like flows, characterized by vortices, spatio-temporal chaos and power laws in the energy spectra [1-3]. Continuum models have been successfully used to predict the scaling of the energy spectra with the wavevector. Most theoretical work has focused on free-standing, active nematic films. However, in several experimental realisations, such as bacterial colonies and epithelial monolayers, the active nematic is in contact with a solid substrate. We generalised a 2D, incompressible active nematic model to include substrate friction, and studied its impact on the transition to turbulence and the energy spectra of the turbulent-like flows. We find a variety of dynamic states including flow in lanes, stable vortices and both isotropic and anisotropic turbulence. At high activity and moderate friction, we found a power-law scaling in the kinetic energy spectrum $E(q) \sim q^3$, where q is the wavevector, at low wavevectors. The exponent of 3 can be justified with a power-counting argument. Overall, we have developed a model for active nematic turbulence on a substrate that can be compared to biological systems. [1] L. Giomi, *Phys. Rev. X* **5**, 031003 (2015). [2] R. Alert, J.-F. Joanny, J. Casademunt, *Nat. Phys.* **16**, 682-688 (2020). [3] B. Martínez-Prat*, R. Alert*, et al., *Phys. Rev. X* **11**, 031065 (2021).

CPP 2.11 Mon 12:30 H37

Self-sustained patchy turbulence in shear-thinning active fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg

Bacterial suspensions and other active fluids are known to develop highly dynamical vortex states, denoted as active or mesoscale turbulence. We reveal the pronounced effect of non-Newtonian rheology of the carrier fluid on these turbulent states, concentrating on shear thinning. As a consequence, a self-sustained heterogeneous state of coexisting turbulent and quiescent areas develops, which results in anomalous velocity statistics. The heterogeneous state emerges in a hysteretic transition under varying activity. We provide an extensive numerical analysis and find indirect evidence for a directed percolation transition. Our results are important, for instance, when addressing active objects in biological media with complex rheological properties.

CPP 3: Organic Electronics and Photovoltaics I

Time: Monday 9:30–11:15 Location: H38

CPP 3.1 Mon 9:30 H38

Demonstration of flexible organic solar cells in space — •Lukas V. Spanier[1], Lennart K. Reb[2], Michael Böhmer[3], Zerui Li[1], Christoph Dreissigacker[4], Thomas Voigtmann[4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Zentrales Technologielabor, Garching, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]DLR Institut für Materialphysik im Weltraum, Köln, Germany

The deployment of flexible organic solar cells (OSCs) in space presents a transformative opportunity for exceptionally lightweight power generation on satellites and deep space research probes, promising record-breaking gravimetric power densities. In this study, we report the successfull launch, operation and recovery of flexible PEN-based OSCs on a suborbital rocket launch, assessing their performance in the harsh conditions of space. Flexible OSC modules were integrated into the payload and exposed to vacuum, microgravity, and cosmic radiation during the flight. Post-flight analysis of the recovered cells further confirmed the cells' operational viability. The experiment demonstrates the potential of OSCs for reducing launch mass and enabling novel satellite architectures, paving the way for their adoption in future space missions.

CPP 3.2 Mon 9:45 H38

Evaluate the energy losses in non-fullerene based organic photovoltaic — •Maryam Alqurashi[1], Shahidul Alam[2], Jose Jurado[1], Julien Gorenflot[1], and Frederic Laquai[1,2] — [1]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia — [2]Physical Chemistry and Spectroscopy of Energy Materials, Department of Chemistry, Ludwig Maximilian University of Munich, D-81377 Munich, Germany

Organic photovoltaics that use non-fullerene acceptors are gaining popularity because they can potentially increase power conversion efficiency. However, they suffer from significantly higher total energy losses than inorganic photovoltaics, primarily due to non-radiative recombination, a process in which electron-hole pairs recombine without generating current. Electroluminescence spectroscopy helps evaluate charge transfer state energy, which is crucial in charge recombination. This study focused on three systems: PM6:Y6, PM6:IT-4F, and PM6:ITIC. The PM6:Y6-based device showed higher radiative recombination, while the PM6:IT-4F system exhibited the highest order of non-radiative recombination. The total open circuit voltage losses were 0.64 eV, 0.67 eV, and 0.56 eV for PM6:Y6, PM6:IT-4F, and PM6:ITIC, respectively. Despite PM6:Y6 achieving a higher power conversion efficiency, its open circuit voltage losses were comparable to that of the other two systems.

CPP 3.3 Mon 10:00 H38

Towards printing of organic solar cells out of green solvents — •Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Despite big achievements in terms of power conversion efficiencies in the last years, with champion efficiencies above the 20% limit, it remains an unresolved challenge to fabricate large-area organic solar cells without sacrificing efficiencies. Large-area deposition of the conjugated polymer donor and small molecule acceptor blends via printing is key in the device upscaling. Another issue calling the attention is the fabrication of environmentally friendly organic solar cells. To become environmental-friendly, the used solvents are a key factor. Today, still the most used solvents are harmful and can cause environmental pollution during the device fabrication process and waste solvent treatment. Accordingly, we investigate the printing of donor-acceptor blend films out of different solvents for use as active layers in organic solar cells with advanced in-situ scattering methods. We use grazing incidence small and wide-angle X-ray scattering (GISAXS and GIWAXS) in-situ during printing to gain a fundamental understanding of the underlying film formation processes. Different examples of polymer donors and small molecule acceptors are presented, and the resulting morphologies are correlated with solar cell device performance. A special emphasis is put on the shift towards more environmentally friendly solvents, which will also be a prerequisite to promote the large-scale production of organic solar cells.

CPP 3.4 Mon 10:15 H38

The Role of Oxygen Insertion on Performance of A-D-A-type Non-Fullerene Acceptors (NFA) in Organic Solar Cells — •Wejdan Althobaiti[1], Yakun He[1], Julien Gorenflot[1], Wisnu Hadmojo[1], Sandeep Sharma[1], Filip Aniés[1], Weimin Zhang[1], Shahidul Alam[1], George Harrison[1], Anirudh Sharma[1], Shadi Fatayer[1], Derya Baran[1], Iain McCulloch[2], Thomas Anthopoulos[1], Martin Heeney[1], and Frédéric Laquai[1] — [1]King Abdullah University of Science and Technology (KAUST), Saudi Arabia — [2]University of Oxford, UK

Charge transfer in OSCs can occur through two pathways: photo-induced electron transfer from the donor to the acceptor, controlled by the electron affinity (EA) offset, and photo-induced hole transfer from the acceptor to the donor, governed by the ionization energy (IE) offset. Here, we report the synthesis of a novel NFA coded TPTI-BT, whose properties were first predicted by computational chemistry before the material was synthesized. Despite the favorable properties for high device performance, TPTI-BT exhibited moderate device performance, in particular when compared with the structurally-related and efficient acceptor O-IDTBCN. In fact, the chemical structure of TPTI-BT is very similar to that of O-IDTBCN, it contains only two additional oxygen atoms in the donor core of the A-D-A-type acceptor backbone structure. Interestingly, this causes TPTI-BT to exhibit overall lower device performance. We present a comparative study of these two NFAs and elucidate the origin of the lower performance of the TPTI-BT caused by two additional oxygen atoms.

CPP 3.5 Mon 10:30 H38

Revealing the effect of solvent additive selectivity on morphology and formation kinetics in printed non-fullerene organic solar cells at ambient conditions — •Jinsheng Zhang and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Solvent additives have received tremendous attention in organic solar cells as an effective way to optimize morphology and phase separation. However, most research primarily focuses on solvent additives with superior solvation for non-fullerene acceptors (NFA) over polymer donors, such as the 1-chloronaphthalen (1-CN) and 1, 8-diiodooctane (1,8-DIO). Few researches are related to solvent additives characterized by better solubility for polymer donors than NFA. Furthermore, the impact of solvent additives is mainly investigated through spin coating rather than slot-die coating, which exhibits distinct kinetics in film formation. Hence, the influence of solvent additive selectivity on the kinetics of active layer formation in the printed active layer remains unknown. In this study, we use PBDB-T-2F as the donor and BTP-C3-4F as the acceptor and introduce two distinct solvent additives one with superior solubility for PBDB-T-2F compared to BTP-C3-4F, and the other with inferior solubility for PBDB-T-2F. The drying process of the slot die coated active layers with different solvent additives is studied by in situ UV-vis absorption spectra and in situ grazing incidence wide angle X-Ray scattering (GIWAXS).

CPP 3.6 Mon 10:45 H38

Locally Resolved Thermally Induced Degradation on PM6:Y6-based Organic Solar Cells — •Shahidul Alam[1,2], José P. Jurado[2], Biwajit Pal[2], Zhuo Xu[3,4], Aurelien D. Sokeng[3,4], Harald Hoppe[3,4], and Frédéric Laquai[1,2] — [1]Physical Chemistry and Spectroscopy of Energy Materials, Department of Chemistry, LMU Munich, Germany — [2]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Kingdom of Saudi Arabia — [3]Laboratory of Organic and Macromolecular Chemistry (IOMC), FSU Jena, Germany — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), FSU Jena, Germany

The commercialization of new photovoltaic technology is impeded by the degradation of organic photovoltaic devices caused by thermal factors. Therefore, it is crucial to have an in-depth awareness of the underlying causes of thermal device instability and to develop effective approaches to reduce its negative impacts. This study examines the thermal degradation of PM6:Y6 bulk heterojunction solar cells, which are currently considered at the forefront of organic solar cell technology. The investigation focuses on the effects of varying temperatures on the performance and locally resolved thermally induced impact of these solar cells. We report a comprehensive study probing the influence of thermal annealing of solar cells by the use of several advanced optoelectrical and imaging characterization techniques.

CPP 3.7 Mon 11:00 H38

Thermal degradation behavior of BTP-4F-12 based green-solvent organic solar cells — •Zerui Li[1], Jinsheng Zhang[1], Simon Wegener[1], Yingying Yan[1], Xiongzhuo Jiang[1], Kun Sun[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [3]Applied Sciences Cluster, University of Petroleum and Energy Studies UPES, Dehradun, Uttarakhand, 248007, India

Thermal degradation is inevitable for organic solar cells in real application conditions. The common research of thermal stability could only observe ex-situ conditions before and after heating and the device behavior during heating is missing, which is insufficient to the understanding of degradation mechanisms. Herein, a new observation aspect is realized to analyze the thermal degradation of BTP-4F-12 based green-solvent organic solar cells with the application of operando GIWAXS/GISAXS, which provides a deep learning of thermal degradation. The OSC devices show a harsh Voc loss with temperature increase, which would recover mostly after getting cooled down to low temperature, while the loss of FF and Jsc during aging is irreversible. Thus, polymer donors play a crucial role in the device performance as well as thermal behavior. In addition, such thermal degradation is driven by the evolution of the molecular stacking and aggregation and thermal expansion/contraction during aging.

CPP 4: Crystallization, Nucleation and Self-Assembly I

Time: Monday 11:30–13:00 Location: H34

CPP 4.1 Mon 11:30 H34

Confined crystallization for studying kinetics and crystal orientation of interface-induced polymer crystallization — •Marthinus van Niekerk, Thomas Thurn-Albrecht, and Oleksandr Dolynchuk — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Understanding interfacial interactions is essential to understanding the mechanisms and kinetics of interface-induced crystallization (IIC), namely heterogeneous nucleation or prefreezing, and resultant material properties. While heterogeneous nucleation is an activated process occurring below T_m, prefreezing is an equilibrium process producing a stable crystalline layer above T_m that thickens upon cooling. Quantifying the influence of interfacial interactions on the kinetics of IIC and crystal morphology has long been elusive and is addressed in this work. We present a systematic study of confined crystallization in micrometer-sized dewetted droplets of poly(ϵ-caprolactone) (PCL) on a range of substrates, allowing numerical analysis of isolated nucleation events and kinetics. Our results show that prefreezing significantly enhances crystallization kinetics compared to nucleation, resulting in simultaneous crystallization of PCL droplets close to T_m. X-ray scattering reveals the preferred crystal orientation in PCL droplets crystallized by IIC, which is strongest for prefreezing and is supported by striking differences in lamellar morphologies observed in AFM. Thus, we present both quantified nucleation kinetics and crystal orientation for different cases of IIC and show that prefreezing enhances crystallization kinetics and anisotropic crystal orientation most effectively.

CPP 4.2 Mon 11:45 H34

Liquid crystalline ordering of conjugated polymers at the vacuum interface — Anton Sinner, Alexander Johannes Much, and •Oleksandr Dolynchuk — Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany

Structure formation in films of conjugated polymers (CPs) strongly affects their optoelectronic properties and is of fundamental interest in the context of sanidic liquid crystalline (SLC) phases discovered in board-like polymers. Recent experimental results on films of the model CP poly(3-hexylthiophene) (P3HT) revealed the edge-on crystal orientation in the top film layer and suggested that the vacuum interface induces it. Here, we use grazing-incidence wide-angle X-ray scattering to study in situ the crystallization and melting in films of P3HT and polydiketopyrrolopyrrole (PDPP), another board-like CP, at the vacuum interface. Upon cooling from the melt, the ordering of both P3HT and PDPP indeed starts at the vacuum interface as an edge-on oriented disordered SLC phase and undergoes multiple SLC transitions with decreasing temperature. The same thermal hierarchy of SLC phases is observed for both CPs during melting, demonstrating that the vacuum interface stabilizes the edge-on disordered SLC phase above its bulk transition temperature, similar to the surface freezing of short alkanes. Notably, the observed effects are much stronger for PDPP, also resulting in a thicker edge-on oriented layer of more than 100 nm. Thus, we show that surface-induced SLC ordering is a general phenomenon of CPs, presumably due to their board-like architecture, and it significantly influences the molecular orientation in CP films.

CPP 4.3 Mon 12:00 H34

How Aqueous Solutions of Low-end Mono-alcohols Crystallize? — •Vasileios Moschos[1] and George Floudas[1,2] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Aqueous solutions of low-end aliphatic mono-alcohols, such as ethanol and 1-propanol, display several peculiar features originating from hydrogen bonding, and in particular, antagonistic hydrophilic/hydrophobic interactions of the head/tail that give rise to local nano-heterogeneity. By combining structural (XRD), thermodynamic (Differential Scanning Calorimetry, DSC) and dynamical (Dielectric Spectroscopy, DS) probes, the pertinent phase diagrams of the two binary mixtures are established, comprising of liquid 1-propanol/ethanol, liquid water, hexagonal ice and different hydrates. The two phase diagrams are discussed in terms of up to five different Regimes (Regime I-V), all sharing a droplet arrangement of the minority component, with the exception of Regime I in ethanol/water binary system, where molecular mixing of the two components occurs. By probing the dynamics of the mixtures over an extended frequency and temperature range, different relaxation processes are identified, either associated with with the dynamics of pure alcohol (Debye-like and α-process) or alcohol/water mixtures.

CPP 4.4 Mon 12:15 H34

Intra-crystalline chain diffusion, semicrystalline morphology and mechanical modulus of selected aliphatic polyesters — •Qiang Yu, Albrecht Pezold, and Thomas Thurn-Albrecht — Martin-Luther-University Halle-Wittenberg

Aliphatic polyesters are good candidates to replace commodity plastics in many applications due to their similar mechanical and thermal properties, and superior degradability. However, their intra-crystalline chain diffusion (ICD, the mobility of polymer chains in the crystalline phase) and semicrystalline morphology have not been widely studied. From our recent studies, based on model polymers, semicrystalline polymers exhibit different morphological features depending on the timescale of ICD ($\langle\tau_c\rangle$) relative to the kinetics of crystal growth (τ_{lc}). To check the generality of the findings, our study is expanded into a series of A-B aliphatic polyesters. $\langle\tau_c\rangle$ and τ_{lc} of the polyesters were investigated by nuclear magnetic resonance (NMR) and polarized optical microscope, respectively. The semicrystalline morphology was monitored by small angle X-ray scattering (SAXS) during isothermal crystallization. Long $\langle\tau_c\rangle$ (not measurable by NMR) was qualitatively differentiated by different crystal thickening slopes (SAXS measurement). The results show that our findings are also valid for the investigated polyesters. The different crystal thickening slopes show that the ICD of polymers slows down due to the formation of layers of ester groups in the crystal. At last, we report on the exponential dependence of shear modulus of the polyesters with long $\langle\tau_c\rangle$ on their crystallinity.

CPP 4.5 Mon 12:30 H34

Self-assembled Peptides Structure Mediated by Solid Interfaces — •Leila Sahebmohammadi[1], Pol Besenius[2], Markus Mezger[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Germany — [2]Department of Chemistry, Johannes Gutenberg-Universität Mainz, Germany — [3]Faculty of Physics, Universität Wien, Austria

The self-assembly of amphiphilic, C3-symmetric dendritic peptides is driven by non-covalent interactions and steric limitations. This study focuses on peptides with a thermosensitive moiety. In phosphate buffer, oppositely charged peptide amphiphiles form 1D nanorod-like patterns, confirmed by circular dichroism spectroscopy to follow a ß-sheet structure. Atomic Force Microscopy (AFM) revealed temperature-dependent helical filaments, where higher temperatures increased filament length and pitch due to the hydrophobic thermosensitive moiety, while reducing filament height. Quartz Crystal Microbalance with Dissipation (QCM-D) showed a temperature-responsive, layer-by-layer adsorption process forming stable multilayers. Lysine-based cationic comonomers improved adsorption and coating uniformity on gold (Au) and silicon (Si) surfaces. Extreme pH conditions (2 or 12) caused multilayer removal, revealing a pH-responsive mechanism from weakened electrostatic interactions. This study demonstrates how self-assembly and surface confinement adapt peptide assembly, offering insights for modifying surface properties for diverse applications.

CPP 4.6 Mon 12:45 H34

Crystallization and Pseudo-Isodimorphism in Statistical Co-Polythiophenes — •Alexander Johannes Much[1], Jakob Boris Günther Danziger[1], Qian Wang[2], Michael Sommer[2], and Oleksandr Dolynchuk[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Technische Universität Chemnitz

Statistical copolymerization is a powerful and widely used way to tailor material properties like solubility or mechanical properties. The copolymer properties depend largely on their co-crystallization and the crystal structure formed, which has been studied for polyesters, polyamides, and polycarbonates. The results suggest three co-crystallization scenarios: (1) total exclusion of comonomers, (2) total inclusion of comonomers (isomorphism), and (3) partial inclusion of comonomers into two crystal lattices (isodimorphism).

Here we study the co-crystallization and crystal structure of poly-(3-hexylthiophene)-stat-poly-[3-(6-cyanohexyl)thiophene] statistical copolymers using differential scanning calorimetry (DSC) and wide-angle X-ray scattering (WAXS). The composition-dependent melting temperatures and enthalpies obtained from DSC show minima, which is typical of isodimorphic co-crystallization. However, WAXS clearly indicates single crystal lattices in all copolymers, with a monotonic dependence of lattice constants on composition. This finding is inconsistent with isodimorphism, making the co-crystallization of these statistical copolythiophenes only pseudo-isodimorphic. Hence, our results suggest that the current classification of statistical copolymer crystallization is incomplete and needs to be extended.

CPP 5: Composites and Functional Polymer Hybrids

Time: Monday 11:30–13:00 Location: H38

Invited Talk CPP 5.1 Mon 11:30 H38

Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via *ab initio* spectroscopy simulations — •Daniel Sebastiani and Pouya Partovi-Azar — Martin Luther University Halle-Wittenberg, Halle (Saale), Germany

The remarkable theoretical specific capacity of elemental sulfur (~1675 mAh/g) and its abundance make lithium-sulfur (Li-S) batteries an attractive alternative to current lithium-ion technology. Nevertheless, their cycle life has so far been limited due to an irreversible capacity fade. To tackle this issue, numerous studies have focused on structural optimization of sulfur cathodes including utilization of sulfur/carbon copolymers. Among others, sulfur-*n*-1,3-diisopropenylbenzene (S/DIB) copolymer, a 3D network of DIB molecules interconnected via sulfur chains, has shown a promising performance as an active cathode material.

In this talk, we will present our recent works employing a quantum-chemical approach for the characterization of S/DIB copolymer cathodes through simulation of their Raman fingerprints during discharge. Theoretically predicted Raman responses, calculated at density-functional theory (DFT) level along with DFT-based *ab initio* molecular dynamics simulations, hint at activities at certain frequencies which can be exploited to experimentally distinguish between the underlying structures involving short or those having longer sulfur chains. These predictions are all proven plausible by experimental Raman measurements on Li-S coin cells.

CPP 5.2 Mon 12:00 H38

Unveiling the Kinetics of Block Copolymer Micelles Close Packing by In Situ GISAXS — •Guangjiu Pan[1], Jinsheng Zhang[1], Altantulga Buyan-Arivjikh[1], Zhuijun Xu[1], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden

Packing spheres has long been a key topic in science. While hard spheres often form dense, close-packed structures like face-centered cubic (FCC) lattices, soft spheres, such as block copolymers in selective solvents, tend to arrange into

less dense structures. However, when using block copolymer templates in the sol-gel method, these soft spheres can achieve close-packed structures. In this study, in situ grazing-incidence small-angle X-ray scattering (GISAXS) is used to examine the self-assembly and co-assembly processes during the formation of close-packing structures. The results reveal that the hybrid films preferentially develop an FCC structure with cluster nuclei. After the polymer template is removed, a superlattice-like mesoporous metal oxide film is obtained, showcasing the potential for advanced applications due to its well-organized nanostructures.

CPP 5.3 Mon 12:15 H38

Optimizing the internal structure of soft elastic composite materials — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We study magnetic gels and elastomers, soft materials composed of magnetic or magnetizable particles embedded in a soft polymeric matrix material. These materials can be controlled by external magnetic fields, which induce deformations (magnetostriction) or changes in the rheological behavior (magnetorheological effect).

In particular, we investigate how these two effects depend on the arrangement of magnetizable particles within the elastic matrix. For the magnetostrictive effect, we consider model systems of spherical shape, for which we can analytically calculate how the volume change and overall elongation or contraction under applied magnetic fields depends on the configuration (within the linear elastic regime) [1]. Based on these formulae, we optimize the structures for maximized deformations, using an adaption of simulated annealing. Additionally, we investigate cubical systems for their magnetorheological effects, also presenting the internal arrangements that maximize these effects. The optimized arrangements are compared to regular lattice configurations.

The method that we present here can be transferred to the investigation of other types of soft elastic composite systems, driving them towards their full potential in light of future applications.

[1] L. Fischer, A. M. Menzel, PNAS Nexus **3**, pgae353 (2024).

CPP 5.4 Mon 12:30 H38

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity — •Lucas P. Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Daniel Söderberg[3], and Stephan Roth[2,3] — [1]Heinz Maier-Leibnitz-Zentrum, Technische Universität München — [2]Deutsches Elektronen Synchrotron DESY — [3]Department of Fibre and Polymer Technlogy, KTH Royal Institute of Technology

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is a conductive polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water (≈50 V%), causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, in humid environments, a minor amount of water is still absorbed, leading to a change in film morphology: the absorbed water induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. QENS also provides information on the diffusive and hydrogen-bonding behavior of water.

CPP 5.5 Mon 12:45 H38

Enhanced Physical Properties and Shape Recovery in Epoxy-Based Shape Memory Polymer Nanocomposites under Gamma Irradiation for Aerospace Applications — •Eman Taha — 1 Ahmed El-Zomor St, 11727, Cairo, Egypt.

This research explores the impact of gamma irradiation on the structural and functional properties of epoxy-based shape memory polymer nanocomposites, specifically engineered for potential satellite deployment mechanisms in space applications. To enhance durability and adaptability in extreme conditions, multi-walled carbon nanotubes (MWCNTs) were incorporated into the epoxy matrix, with surfactants added to improve dispersion. Using a Cobalt-60 gamma irradiation facility, doses ranging from 250 to 1000 kGy were applied, uncovering dose-dependent changes in thermal stability and mechanical properties. Surface tension tests confirmed effective dispersion with nonionic (Tween 80) and anionic (SDS) surfactants, while cationic surfactants had less impact. Thermogravimetric analysis revealed enhanced thermal stability at moderate doses due to increased crosslinking. Dynamic mechanical analysis showed shifts in viscoelastic behavior and higher glass transition temperatures (Tg), critical for thermal stress resistance. Shape memory performance improved at 250 kGy but declined at higher doses, indicating a balance between radiation exposure and functionality. These findings highlight controlled gamma irradiation as a tool to optimize the performance and stability of epoxy-based nanocomposites with MWCNT reinforcement, advancing their suitability for space applications.

CPP 6: Gels, Polymers Networks and Elastomers II

Time: Monday 15:00–16:00 Location: H34

CPP 6.1 Mon 15:00 H34

Scattering data of A_4B_4 model networks reveal structure induced apparent interaction and cross-link repulsion — •Reinhard Scholz and Michael Lang — Leibniz-Institut für Polymerforschung, Hohe Str. 6, 01069 Dresden, Germany

Based on computer simulations, we analyze how different forms of labeling the network components allow to extract complementary structural information from scattering data. The analysis relies upon simulations of hetero-complementary bound four-functional star polymers A_4 and B_4. For optimized contrast between A and B stars, the calculated dynamic scattering intensity resembles A-B block copolymers with an apparent repulsion between both components, accounting for ordering effects due to the complementary coupling scheme. The position of the observed scattering peak is compatible with radius of gyration and end-to-end extension of A-B chains connecting adjacent star centers, providing access to the mesh size of the network. In samples with optimum contrast, the static correlation length Ξ is in the same range but somewhat smaller than the respective correlation length for homogeneously labeled polymers. Choices of the scattering contrast focusing on the star centers or on small regions around these reveal a correlation hole. Accordingly, scattering is suppressed towards small wave vectors, allowing for a decomposition of the observed scattering intensity into a product of the form factor of the labeled star sections and a structure factor describing the distribution of cross-links in space.

CPP 6.2 Mon 15:15 H34

Responsive Microgel Based Membranes — •Thomas Hellweg — Universität Bielefeld, Fak. f. Chemie, Physikalische und Biophysikalische Chemie, Universitätsstr. 25, 33615 Bielefeld

If microgels are made with comonomers which can act as (photo-)crosslinkable secondary crosslinker, they can be deposited in thin layers and subsequently be cross- linked by irradiation [1, 2]. Upon cross-linking freestanding membranes are obtained, which still exhibit the temperature response of the original microgels. The present contribution describes the synthesis and properties of the respective microgels, the membrane formation, and the membrane properties. The thermal response of the obtained 2D materials can be exploited to make gating membranes [3] which modulate ion flow by changing temperature which can be used in electrochemical devices. The resistance is found to steeply increase by up to an order of magnitude at the volume transition of the original microgels. Hence, these freestanding microgel membranes might be useful for building self- regulating fuel cells. Moreover, they can be doped with metal nanoparticles granting them catalytic activity and allowing to use them in flow reactors or microfluidic cells for chemical conversion [4].

[1] M. Dirksen, et al., Langmuir 2022, 38, 638-651.
[2] M. Dirksen, et al., RSC Adv., 2021, 11, 22014.
[3] S. Uredat, et al. , Phys. Chem. Chem. Phys. 2024, 26, 2732-2744
[4] V. Sabadasch, et al., ACS Applied Materials & Interfaces , 2022, 14, 43, 49181.

CPP 6.3 Mon 15:30 H34

Correlation between swelling ability, softness and adhesion of PNIPAM microgels — •Carina Schneider, Kevin Hagmann, Joanne Zimmer, Franziska Braun, and Regine von Klitzing — Departement of Physics, TU Darmstadt, Hochschulstraße 8, 64289, Darmstadt

PNIPAM microgels (poly-N-isopropylacrylamide) are polymeric cross-linked networks with a core-shell structure. Due to their volume phase transition, it is possible to control their swelling and mechanical behavior. However, the concept of softness in these microgels, is highly complex and is not a single, well-defined property. In this study we show that it rather has a multifold characteristic that arises from a combination of several factors, such as their (de-)swelling ability, mechanical properties and adsorption behavior at interfaces. The cross-linker density of the microgels affect their adsorption behavior at interfaces and faceting. For exploring the multifold softness of adsorbed PNIPAM microgels, atomic force microscopy (AFM) is used to directly probe the mechanical and adhesion properties through indentation measurements and related them to their swelling ability. These insights into the microgel behavior could inform the design of next-generation microgels for biomedical applications.

CPP 6.4 Mon 15:45 H34

Deformation and actuation of 3D-printed polymeric microstructures predicted by finite element simulations — •Santiago Gomez Melo and Ulrich Schwarz — Univesität Heidelberg, Heidelberg

Mechanical metamaterials with promising properties can be manufactured via 3D-printing of polymers. Computational modelling, in addition to aiding conceptualization and characterization, opens the gate towards computer rationalized material design. We present two projects to this end. First, we discuss the experimental investigation of 3D-printed tetrahedral polymeric microlattices with X-ray nanotomography. Step-wise loading and image processing allowed us to evaluate the evolution of the displacement fields. Finite element simulations were used to understand the strain accumulation around lattice defects. Second, we demonstrate that the thermomechanical response of printed nematic elastomer microstructures can be controlled via confinement in PDMS-scaffolds. We applied Landau-de Gennes theory combined with nonlinear morphoelasticity to predict the molecular orientation from the scaffold geometry and the actuation upon heating, in excellent agreement with experimental measurements of birefringence patterns.

CPP 7: Active Matter II (joint session BP/CPP/DY)

Time: Monday 15:00–17:00 Location: H37

CPP 7.1 Mon 15:00 H37

Emerging cellular dynamics from turbulent flows steered by active filaments — Mehrana Nejad[1,4], Julia Yeomans[2], and •Sumesh Thampi[2,3] — [1]Department of Physics, Harvard University, Cambridge, MA 02138 — [2]The Rudolf Peierls Centre for Theoretical Physics, Parks Road, Oxford OX1 3PU, UK — [3]Department of Chemical Engineering, Indian Institute of Technology, Madras, Chennai, India 600036 — [4]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Describing the mechanics of cell collectives and tissues within the framework of active matter, without resorting to the details of biology is an exciting area. We develop a continuum theory to describe the dynamics of cellular collectives, discerning the cellular force-generating active filaments from cells shape. The theory shows that active flows and straining part of the active turbulence can elongate isotropic cells, which form nematic domains. This is important as cell morphology is not only an indicator of diseases but it can affect the nucleus morphology, gene expression and other biochemical processes inside the cells. Our theory highlights the importance of distinguishing the roles of active filaments from cell shape and explains outstanding experimental observations such as the origin of cell-filament alignment patches. Further, we reconcile how the contractile forces generated by the cytoskeletal network makes the cells to exhibit flow behaviours similar to that of extensile active systems. Revealing the crucial role of activity and rheology to describe the dynamics of cellular layers, our study is in consonance with a number of experimental observations.

CPP 7.2 Mon 15:15 H37

Defects in active solids: self-propulsion without flow — •Fridtjof Brauns[1], Myles O'Leary[2], Arthur Hernandez[3], Mark Bowick[1], and Cristina Marchetti[4] — [1]Kavli Institute for Theoretical Physics, Santa Barbara, USA — [2]Princeton University, Princeton, USA — [3]Leiden University, Leiden, the Netherlands — [4]University of California Santa Barbara, Santa Barbara, California 93106, USA

Topological defects are a key feature of orientational order and act as organizing centers of orientation fields. Self-propulsion of +1/2 defects has been extensively studied in active nematic fluids, where the defects are advected with the fluid through the flow field they generate. Here, we propose a minimal model for defect self-propulsion in a nematic active solid: a linear elastic medium with an embedded nematic texture that generates active stress and in turn is coupled to elastic strain. We show that such coupling gives rise to self-propelled +1/2 defects that move relative to the elastic medium by local remodeling of the nematic texture. This mechanism is fundamentally different from the fluid case. We show that this mechanism can lead to unbinding of defect pairs and stabilize +1 defects. Our findings might help explain how orientational order, e.g. of muscle fibers, is reconfigured during morphogenesis in solid-like tissues. For instance, motility and merging of +1/2 defects play a crucial role in setting up the body axis during Hydra regeneration.

CPP 7.3 Mon 15:30 H37

Isovolumetric dividing active matter — Samantha R. Lish[1], Lukas Hupe[1], Ramin Golestanian[1,2], and •Philip Bittihn[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We introduce and theoretically investigate a minimal particle-based model for a new class of active matter where particles exhibit directional, volume-conserving division in confinement while interacting sterically, mimicking cells in early embryogenesis. We find that complex motion, synchronized within division cycles, displays strong collective effects and becomes self-similar in the long-time limit. Introducing the method of normalized retraced trajectories, we show that the transgenerational motion caused by cell division can be mapped to a time-inhomogenous random walk with an exponentially decreasing length scale. Analytical predictions for this stochastic process allow us to extract effective parameters, indicating unusual effects of crowding and absence of jamming. Robustness of our findings against desynchronized divisions, cell size dispersity, and variations in confinement hints at universal behavior. Our results establish an understanding of the complex dynamics exhibited by isovolumetric division over long timescales, paving the way for new bioengineering strategies and perspectives on living matter.

CPP 7.4 Mon 15:45 H37

Tracking plankton-to-biofilm transition in phototrophic bacteria — •Anupam Sengupta — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — Institute for Advanced Studies, University of Luxembourg, Luxembourg

Phototrophic bacteria commonly inhabit natural aquatic and marine ecosystems, exhibiting both motile and sessile lifestyles [1]. Yet, how and when they switch between the two states has remained unknown. Using quantitative imaging, AFM and mathematical modeling, we track the conditions and phenotypic changes across multiple generations in Chromatium okenii, a motile phototrophic purple sulfur bacterium [2]. Enhanced cell-surface adhesion together with changes in the cell shape and cellular mass distribution facilitate the motile-to-sessile shift. Our results, supported by cell mechanics model, establish a synergistic link between motility, mass distribution and surface attachment in promoting biofilm lifestyle. [1] T. Sommer et al., Geophys. Res. Lett. 44, 2017. [2] F. Di Nezio,.., & A. Sengupta, Plos one 19, e0310265, 2024.

15 min. break

CPP 7.5 Mon 16:15 H37

How localized active noises influence the conformations and dynamics of semiflexible filaments — •Shashank Ravichandir[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Universität Augsburg, 86159 Augsburg, Germany

The structure and dynamics of active polymers have been recently studied in some detail. In these works all the monomers are considered to be active. However, in most biological systems non-equilibrium fluctuations manifest as activity only at isolated locations within the polymer. There have been only few studies of such polymers, in which the active monomers occur periodically along the polymer contour. We consider arbitrary active-passive copolymers and isolate the effects of the number and locations of active monomers on the conformational and dynamical properties of polymers. We use Langevin dynamics simulations to calculate the end-to-end distance, radius of gyration, and mean-squared displacement of such semiflexible filaments and classify the various states of these polymers based on their conformational properties. We also present preliminary results of polymers in which the location of active monomer moves dynamically along the chain contour. This is an idealized model of biopolymers such as DNA, during DNA transcription, and microtubules, which are driven by kinetic motors that traverse along its length.

CPP 7.6 Mon 16:30 H37

Sequence-specific folding of partially active polymers — •Shibananda Das — Department of Physics, Indian Institute of Science, Bengaluru, India

Biological polymers like actin filaments and microtubules exhibit important physical properties due to their out-of-equilibrium behavior induced by ATP or GTP. In contrast, synthetic polymers rely on energy from their surrounding environment, often using local chemical, electrical, or thermal gradients to remain far from equilibrium. Theoretically, active polymers serve as minimal models for these systems, enabling systematic study of the competition between thermodynamic and active forces while they undergo conformational changes.

Using a combined analytical and numerical approach, we investigate an active polymeric chain composed of multiple self-avoiding units, representing good solvent condition in the absence of active forces. For partially active polymers without orientational constraints, we find that distribution of the active units in distinct sequences along the backbone can induce a significant collapse into folded, globular structures. Detailed analysis shows that this activity-dependent collapse is driven by a reduction in swim pressure of the monomers, linking the

distribution of active forces along the polymer contour to its folded conformations.

CPP 7.7 Mon 16:45 H37

Effect of interactions on the chemotactic response of active-passive chains — •Hossein Vahid[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of Augsburg, Augsburg, Germany

Living organisms, from single cells to populations, exhibit complex behaviors driven by the need to navigate toward favorable environments. These behaviors are often shaped by interactions within clusters or mixed populations, where collective dynamics play a crucial role in the characteristic properties of multicellular systems.

Chemotactic bacteria, found in diverse environments such as the gastrointestinal tract, plant surfaces, and aquatic ecosystems, demonstrate the significance of chemotaxis at the population level. While extensive research has focused on the properties of active polymers in spatially homogeneous activity fields, their behaviors in inhomogeneous fields remain less explored.

This study investigates the behavior of self-propelled polymers in activity gradients, emphasizing the effects of inter- and intra-chain interactions, such as steric and excluded volume effects, on chemotactic responses. These interactions give rise to distinct phases or collective behaviors that influence the stability and persistence of chemotaxis. Additionally, polymer density emerges as a critical factor impacting diffusion and the overall efficiency of chemotaxis. This work aims to study the dynamics of the active polymer populations in non-uniform environments systematically.

CPP 8: Hybrid and Perovskite Photovoltaics I

Time: Monday 15:00–16:00 Location: H38

Invited Talk CPP 8.1 Mon 15:00 H38

The Nanoscale Photovoltaics Laboratory on a Tip — •Stefan Weber — Institute for Photovoltaics, University of Stuttgart — Max Planck Institute for Polymer Research

Electrical scanning probe microscopy (SPM) modes are ideal for nanoscale photovoltaic measurements. I will discuss our recent work on developing specialized SPM techniques to study hybrid perovskite materials. Optimizing perovskite solar cells requires understanding energy losses, instability, and aging processes. These macroscale properties result from the interplay between nanoscale structure and function, including twin domains, grain boundaries, interfaces, and crystal grain orientations. Using static and time-resolved Kelvin probe force microscopy (KPFM), we can map the local surface potential, surface photovoltage (SPV), and cross-sectional potential distributions under operating conditions. With Nano-SPV spectroscopy, we achieve 10-20 nm lateral- and sub-millisecond temporal resolution. Our research aims to address key challenges in perovskite research, such as phase segregation, degradation, and interface heterogeneity, advancing understanding of loss mechanisms and instabilities in MHP solar cells.

CPP 8.2 Mon 15:30 H38

Sputter-Deposited TiOx Thin Film as a Buried Interface Modification Layer for Efficient and Stable Perovskite Solar Cells — •Xiongzhuo Jiang[1], Kun Sun[1], Zerui Li[1], Zhuijun Xu[1], Guangjiu Pan[1], Yusuf Bulut[1,2], Benedikt Sochor[2], Matthias Schwartzkopf[2], Kristian A. Reck[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — [3]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts-Universität zu Kiel, 24143 Kiel, Germany

It is crucial to suppress the non-radiation recombination in the hole-blocking layer (HBL) and at the interface between the HBL and active layer for performance improvement. Herein, TiO_x layers are deposited onto a SnO_2 layer via sputter deposition at room temperature, forming a bilayer HBL. The structure evolution of TiO_x during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering. After sputter deposition of TiO_x with a suitable thickness on the SnO_2 layer, the bilayer HBL shows a suitable transmittance, smoother surface roughness, and fewer surface defects, thus resulting in lower trap-assisted recombination at the interface between the HBL and the active layer. With this SnO_2/TiO_x functional bilayer, the perovskite solar cells exhibit higher power conversion efficiencies than the unmodified SnO_2 monolayer devices.

CPP 8.3 Mon 15:45 H38

Dynamics and kinetics of light-induced phase segregation in $MAPbBr_{1.8}I_{1.2}$ perovskites — •Ivan Zaluzhnyy[1], Linus Pithan[2], Rustam Rysov[2], Frederik Unger[1,2], Jakub Hagara[1], Ekaterina Kneschaurek[1], Paul Zimmermann[1], Sebastian Schwartzkopff[1], Lena Merten[1], Dmitry Lapkin[1], Alexander Hinderhofer[1], Fabian Westermeier[2], Michael Sprung[2], Yana Vaynzof[3,4], Fabian Paulus[5,4], and Frank Schreiber[1] — [1]University of Tübingen — [2]Deutsches Elektronen-Synchrotron DESY — [3]Technical University of Dresden — [4]Center for Advancing Electronics Dresden (cfaed) — [5]IFW Dresden

Hybrid organic-inorganic perovskites tend to undergo several structural transformations that can be caused by temperature, humidity and light. Here we use X-ray photon correlation spectroscopy (XPCS) to study the dynamics of light-induced phase segregation in $MAPbBr_{1.8}I_{1.2}$ and the formation of Br-rich and I-rich domains. We observe that the phase segregation is characterized by three distinct time scales corresponding to the rapid formation of small seeds of the I-rich phase, fluctuations of the ion distribution around the quasi-equilibrium state (dynamics), and a directional drift of the ions within the crystal grains (kinetics). We also observe the influence of defects in the halide sublattice on phase separation and find that samples with interstitial halides exhibit slower phase separation as samples with vacancies in the halide sublattice.

CPP 9: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 15:00–16:45 Location: H46

CPP 9.1 Mon 15:00 H46

Ferroelectric Microelectrodes for Hybrid Neuroelectronic Systems — •Maximilian T. Becker[1,2], Roland Thewes[3], and Günther Zeck[4] — [1]Department of Embedded Systems, Hahn-Schickard, Freiburg, Germany — [2]Faculty of Engineering, University of Freiburg, Freiburg, Germany — [3]Chair of Sensor and Actuator Systems, TU Berlin, Berlin, Germany — [4]Institute of Biomedical Electronics, TU Wien, Vienna, Austria

Direct electrical interfacing of semiconductor chips with individual neurons and neural networks forms the basis for a systematic assembly and investigation of hybrid neuroelectronic systems with future applications in information technology and biomedicine. The neuroelectronic interface is realized via microelectrodes to bidirectionally transmit electrical signals between neurons and the semiconductor chip. Here, we introduce the concept of ferroelectric microelectrodes and discuss the physics of ferroelectric interfaces in neuroelectronic applications. As an example, we present neural recordings from retinal ganglion cells (RGCs) interfaced with a ferroelectric complementary metal-oxide-semiconductor microelectrode array (CMOS-MEA) and discuss the results in detail.

CPP 9.2 Mon 15:15 H46

Highly sensitive, specific and label-free detection of SARS-CoV-2, Influenza A and RSV proteins via surface plasmon resonance technique using the biofunctionalization with 1 nm thick carbon nanomembranes — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Rania Ennaciri[1], Martha Frey[1], Christof Neumann[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany

Accurate and rapid detection of respiratory viruses like SARS-CoV-2, Influenza A and RSV is crucial for improving global health outcomes. We present a novel surface plasmon resonance (SPR) platform using a biofunctionalized 1 nm-thick carbon nanomembrane (CNM) for enhanced viral protein detection. The azide-modified CNM (N3-CNM) enables covalent antibody binding, ensuring selective immobilization of target proteins. Our platform achieves equilibrium dissociation constants (KD) of 570 * 30 pM and 22 * 3 pM for SARS-CoV-2 nucleocapsid and spike proteins, with detection limits (LODs) of ~190 pM and ~10 pM, respectively. For Influenza A and RSV, KD values are 86 * 4 pM and 3 * 0.2 pM, with LODs of ~90 pM and ~2 pM. Multiplexed detection with no cross-

reactivity supports rapid, accurate point-of-care diagnostics. Validation with nasopharyngeal swabs confirms a LOD of ~40 pM for SARS-CoV-2 spike protein, highlighting CNMs' promise in infectious disease diagnostics.

CPP 9.3 Mon 15:30 H46

Superselective multivalent client recruitment in biomolecular condensates — •Xiuyang Xia and Erwin Frey — Ludwig-Maximilians-Universität München

Biomolecular condensates (BMCs) are membraneless organelles formed via liquid-liquid phase separation, playing a crucial role in organizing cellular functions by selectively concentrating specific molecules. In this talk, I will present a new theoretical framework that models multivalent client recruitment in valence-limited, multicomponent systems like BMCs. We uncover how enthalpic and entropic factors interplay under valence constraints to enable switch-like recruitment and precise compositional regulation.

This work advances our understanding of the principles governing BMC composition and highlights the broader significance of multivalency in biological systems, offering insights into cellular organization and potential therapeutic applications.

CPP 9.4 Mon 15:45 H46

What is the structure of a biomolecular condensate? — •Charlotta Lorenz[1,2], Teagan Bate[1], Takumi Matsuzawa[1], Kaarthik Varma[1], Sully Bailey-Darland[1], George Wang[1], Dana Matthias[1], Harsha Koganti[2], Nicola Galvanetto[2], Matti Valdimarsson[2], Aleksander Rebane[3], Etienne Jambon-Puillet[4], Ben Schuler[2], and Eric R. Dufresne[1] — [1]Cornell University, Ithaca, NY, USA — [2]University of Zurich, Zurich, Switzerland — [3]New York University Abu Dhabi, Abu Dhabi, United Arab Emirates — [4]École Polytechnique Paris, Paris, France

Biomolecular condensates are important for a variety of cellular functions, such as biochemical regulation, structural organization, and RNA metabolism. While the properties and physiology of these condensates depend on their structure, this important aspect has received little experimental consideration. On the other hand, recent simulations of disordered proteins with interactions based on the sticker-and-spacer suggest fascinating structures in the bulk and surface of condensates. We aim to reveal the structure of biomolecular condensates using X-ray scattering. Here, we will present results for a simple model system and apply our approach to the structure of condensates made of disordered proteins. We particularly consider the change in condensate structure due to small molecules.

CPP 9.5 Mon 16:00 H46

Encoding how shear stress during gelation boosts the stiffness of collagen networks — •Pavlik Lettinga[1,2], Lens Dedroog[2], Olivier Deschaume[2], Yovan de Coene[2], Carmen Bartic[2], Erin Koos[2], and Mehdi Bouzid[3] — [1]Forschungszentrum Jülich — [2]KU Leuven — [3]Université Grenoble Alpes

Collagen is one of the main building blocks of the mammalian extracellular matrix, due to its ability to form tough structures with a wide variety of non-linear mechanical properties allowing it to support multiple tissue types. However, the mechanical properties of collagen gels have been extensively studied under static conditions, whereas in nature gelation will mostly take place in the presence of flow. Here we show how the elastic modulus of collagen hydrogels can be increased up to an order of magnitude by applying a stress ramp at a well-defined moment during gelation. Where the first stress block induces most of the final strain and alignment, sequential increases in stress cause a dramatic increase of the modulus. This high modulus is preserved by keeping the high stress until the gel is fully matured. Coarse-grained simulations of a model gel system show that that the microscopic mechanism of inducing high stiffness is due to formation of extra cross bridges and could be very generic. Thus, we not only show that the true non-linear capabilities of biomaterials are tenfold higher than previously assessed, but also provide insight into in vivo structure formation of collagen and potentially other (bio-)polymers.

Invited Talk CPP 9.6 Mon 16:15 H46

In situ control of cells and multicellular structures at the microscale by two-photon lithography — •Christine Selhuber-Unkel — Heidelberg University, IMSEAM, Heidelberg, Germany

In vivo, cells and multicellular assemblies often experience strong confinement by their surrounding tissue environment, particularly in cancer. Thus, replicating these confined environments in situ is essential for investigating their impact on cellular systems. Using two-photon lithography, we printed structures directly within and around multicellular assemblies. For example, we fabricated dome-shaped confinements with micrometer-scale openings to encapsulate cancer spheroids. This enabled us to study how confinement influences cancer cell migration and spheroid behavior. Our findings revealed that confinement slows cell migration and alters actin dynamics. In addition, in situ printed structures can also directly interfere with migrating cellular assemblies. Additionally, elastic structures can be created to mechanically stimulate cells, offering further control over cellular behavior. Therefore, two-photon lithography proves to be a powerful tool for manipulating the growth, migration, and morphology of live cells, making it particularly useful for exploring how changing physical microenvironment in situ affect cell responses.

CPP 10: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 16:15–17:15 Location: H34

CPP 10.1 Mon 16:15 H34

Beyond contact angle measurements of aerophilic surfaces — •Alexander Tesler[1], Wolfgang Goldmann[1], Anca Mazare[2], Ben Fabry[1], Stefan Kolle[3], Robin A.H. Ras[4], Heikki Nurmi[4], George Sarau[5], and Silke Christiansen[5] — [1]Biophysics Chair, Erlangen, Germany — [2]WW4-LKO, Erlangen, Germany — [3]UCSD, San Diego, USA — [4]Aalto University, Epsoo, Finland — [5]Fraunhofer Institute, Forchheim, Germany

Aerophilicity can provide surface resilience to the detrimental effects of wetting-related phenomena. However, the development of such superhydrophobic surfaces with a long-lasting entrapped air layer, called plastron, is hampered by the lack of evaluation criteria and methods that can unambiguously distinguish between stable and metastable Cassie-Baxter wetting regimes. The information to evaluate the stability of the wetting regime is missing from the commonly used contact angle goniometry. Therefore, it is necessary to determine which surface features can be used as a signature to identify thermodynamically stable plastron. Here, I describe a methodology for evaluating the thermodynamic underwater stability of the Cassie-Baxter wetting regime of superhydrophobic surfaces by measuring the surface roughness, solid-liquid area fraction, and Young's contact angle. The method allowed the prediction of passive plastron stability for over one year of continuous submersion,[1] impeding mussel and barnacle adhesion,[2] and inhibition of metal corrosion in seawater.[3] [1] Tesler et al., Commun. Mater. 2024, 5, 112. [2] Tesler et al., Nat. Mater. 2023, 22, 1548. [3] Prado et al., Adv. Funct. Mater. 2024, 35, 2407444.

CPP 10.2 Mon 16:30 H34

Fluid flow inside slit-shaped nanopores: the role of molecular surface morphology — •Giorgia Marcelli[1], Tecla Bottinelli Montadon[1], Roya Ebrahimi Viand[1], and Felix Höfling[1,2] — [1]Institute of Mathematics, Freie Universität Berlin, Germany — [2]Zuse Institute Berlin, Germany

The boundary conditions of nanoscale flows near surfaces can deviate from the no-slip condition observed at macroscopic scales, and used in classical fluid mechanics. In this context, we investigate the influence of surface morphology on fluid flow inside slit-shaped nanopores [1]. Using non-equilibrium molecular dynamics (NEMD) simulations, we demonstrate that the surface morphology effectively controls the slip length, which approaches zero when the molecular structures of the pore wall and the fluid are matched. We examine two types of pore walls, mimicking a crystalline and an amorphous material, that exhibit markedly different surface resistances to flow. The resulting flow velocity profiles are consistent with Hagen–Poiseuille theory for incompressible, Newtonian fluids when adjusted for surface slip and effective viscosity; the latter is found to vary substantially with the pore width. Moreover, analysis of the hydrodynamic permeability shows that the simulated flows are in the Darcy regime. We further show that thermal isolation within the pore causes a linear increase in fluid temperature along the flow, which we relate to strong viscous dissipation and heat convection, utilizing the conservation laws of fluid mechanics.

[1] G. Marcelli, T. Bottinelli Montadon, R. Ebrahimi Viand, and F. Höfling, arXiv:2411.04882 [cond-mat.soft].

CPP 10.3 Mon 16:45 H34

How do polymers of different architecture penetrate nanochannels? — •Panagiotis Kardasis[1] and George Floudas[2] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The way that polymers penetrate narrow pores is of both academic and technological importance. Capillary force can drag polymer chains into nanopores, a process called imbibition. Using in situ nanodielectric spectroscopy (nDS), we report the imbibition and following adsorption kinetics of star cis-1,4-polyisoprenes (SPI) and of bottlebrush polymers directly at the chain length scale by monitoring the evolution of the normal modes, during the flow within in alumina nanopores (AAO), as a function of chain architecture (vs linear), pore size, molar mass, and temperature. We demonstrate that the imbibition kinetics of SPIs proceeds via a slow adsorption mechanism, about 2 orders of magnitude

slower than in linear polyisoprenes (PI). We further demonstrate that the bottlebrush topology results in slower adsorption in nanopores in comparison to linear counterpart, albeit, with different dependence. Additionally, bottlebrushes present weaker temperature dependence comparing to both linear and star polymers. Furthermore, we explore how symmetric star / linear and brush / linear blends penetrate the same nanopores and we demonstrate that differences in the imbibition and adsorption kinetics can be used to separate the homogeneous blend to its components, giving rise to *topology sorting*, based on the relative viscosities and pore diameter.

CPP 10.4 Mon 17:00 H34

Removing particles from hydrophobic surfaces by single water drops — •Franziska Sabath, Stefanie Kirschner, and Doris Vollmer — Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The accumulation of dust on surfaces is a well-known phenomenon in everyday life, for example on windows and solar panels. Both manual cleaning and self-cleaning of hydrophobic surfaces with water can restore the properties of soiled surfaces. However, it is not yet understood how particles are removed by a water drop and which forces play a role for successfully removing the particles. We investigated the removal of two or more particles from hydrophobic coatings by a single water drop. For this purpose, we used a confocal microscope with a sliding drop setup. This implies that the particles was moved at constant velocity while the drop is hold in position by a blade. The sliding drop and the way in which the particles are picked up and pulled along by the water drop can be imaged. From the deflection of the blade, we can determine the force required to pull the particles along with the drop. Here, we focus on the removal of spherical model particles and the impact of drop volume, particles size and particle velocity on the particle removal. At low velocities the particles remain attached to the drop. With increasing velocity we observe that the particle detachment becomes more likely. In case of particle detachment, we observe a correlative effect: after the second particle has reached the rear side of the drop, both particles can detach together.

CPP 11: Hybrid and Perovskite Photovoltaics II

Time: Monday 16:15–17:00 Location: H38

CPP 11.1 Mon 16:15 H38

Structure and morphology investigations on slot-die coated perovskite nanocrystal films — •Thomas Baier[1], Altantulga Buyan-Arivjikh[1], Lixing Li[1], Xiaojing Ci[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Applied Sciences Cluster, University of Petroleum and Engergy Studies UPES, Dehradun, Uttarakhand 248007, India

Perovskite quantum nanocrystals hold great potential for contributing to the future renewable energy mix by serving as the active layer in solar cells. This potential arises from quantum confinement effects, which occur when crystal sizes are reduced below the Bohr radius. These nanocrystals achieve high power conversion efficiencies, excellent photoluminescence quantum yield (PLQY), narrow photoluminescence (PL) peaks, and enhanced stability compared to bulk perovskite. Additionally, the choice of X halides (I-, Br-, Cl-) and A-site cations (FA+, MA+, Cs+) within the ABX3 perovskite structure allows precise bandgap tuning. Cesium-formamidinium lead iodide perovskite nanocrystals have been prepared and slot-die coated. These perovskite nanocrystals as active layers are investigated using in-situ grazing incidence small- & wide-angle x-ray scattering (GISAXS & GIWAXS) to better understand the layers formation process.

CPP 11.2 Mon 16:30 H38

Tracking the Crystallization Pathway of Perovskite using Microscopy, Spectroscopy and Machine Learning — •Meike Kuhn[1], Milan Harth[2], Alessio Gagliardi[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Simulation of Nanosystems for Energy Conversion, Technische Universität München, Hans-Piloty-Str. 1, 85748 Garching b. München, Germany

The interest in perovskite materials has grown significantly in recent years due to their diverse applications, with the crystallization process playing a crucial role in determining the final properties of perovskite films. Time-resolved techniques, such as microscopy and spectroscopy, enable detailed analysis of the various stages of perovskite formation.

In this study, we investigated the crystallization of methylammonium lead iodide (MAPbI3) blade coated from dimethylformamide (DMF), using a combined microscopy and spectroscopy approach. This approach allowed us to observe morphological and optical changes during intermediate phase formation and perovskite conversion, influenced by the addition of various additives. By applying a machine learning model to the microscopy data, we developed a predictive framework capable of estimating spectroscopic signals, thus enabling insights into physical properties with time-resolved microscopy.

CPP 11.3 Mon 16:45 H38

Utilizing CsPbBr3 Nanocrystals as Nucleation Seeds for Scalable FAPbI3 Thin Films — •Altantulga Buyan-Arivjikh[1], Jascha Fricker[1], Thomas Baier[1], Xiaojing Ci[1], Lixing Li[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22604 Hamburg, 22607, Germany

Lead-halide perovskites have gained a significant interest in the scientific community owing to their favorable optoelectronic properties combined with their ease of production and abundance of raw materials. In many cases, polycrystalline thin films are fabricated, where the crystallinity and morphology of the thin film are critical factors influencing the properties and performance of perovskites. In this work, we present a novel approach for improving the quality of FAPbI3 thin films by utilizing CsPbBr3 nanocrystals as nucleation seeds. In-situ optical spectroscopy experiments reveal a faster transition of FAPbI3 into the photactive phase in the seeded thin films as well as a reduced defect density. In-situ grazing incidence wide angle X-ray scattering (GIWAXS) measurements confirm the former and additionally show that the seed crystals improve the thin film texture by inducing a preferred crystallite orientation.

CPP 12: Biomaterials, Biopolymers and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Monday 17:00–18:00 Location: H46

CPP 12.1 Mon 17:00 H46

Polymer Assisted Condensation and Heterochromatin — •Jens-Uwe Sommer — Leibniz-Institut für Polymerforschung Dresden (IPF), Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Many biomolecular condensates are formed through the co-condensation of proteins and polynucleotides. In most cases, the proteins that constitute the majority of the condensate exhibit a miscibility gap in aqueous solution at elevated concentrations in vitro. Recently, we published the theory of Polymer-Assisted Condensation (PAC), which predicts the formation of the condensate within the polymer's volume of gyration, where interactions with the three-dimensional conformation of the polymer trigger the phase transition of the protein component [1]. A key feature of these liquid condensates is their robustness against changes in parameters, as well as the dominant role played by the condensation free energy of the protein component. The formation and properties of heterochromatin, a genetically silenced region of eukaryotic chromosomes, can be explained by PAC, which resolves several issues present in previously published theories. Recently, we developed a field-theoretic approach to PAC to better understand the adsorption and desorption scenarios of heterochromatin at the nuclear lamina.

[1] J.-U. Sommer, H. Merlitz, and H. Schießel, Macromolecules 55, 4841 (2022); L. Haugk, H. Merlitz, and J.-U. Sommer, Macromolecules 57, 9476 (2024)

CPP 12.2 Mon 17:15 H46

How specific binding induces sol-gel transitions and liquid-liquid phase separation in RNA/protein solutions: Coarse-grained simulations versus Semenov-Rubinstein Theory — •Xinxiang Chen, Jude Ann Vishnu, Pol Besenius, Julian König, and Friederike Schmid — Johannes Gutenberg-University, Mainz, Germany

Liquid-liquid phase separation plays a central role in cellular organization, including RNA splicing. RNA-protein interactions are crucial to these processes. A key factor in controlling the phase behavior of RNA-protein systems is the sequence of binding and neutral domains. Using molecular dynamics simulations, we investigate phase transitions in RNA-protein solutions that are driven solely by specific binding interactions. The model omits nonspecific interactions including electrostatic interactions. We show that specific binding interactions

induce a percolation transition with double reentrant behavior without phase separation, if the neutral linker size is long. Comparing our results with the two-component Rubinstein-Semenov theory, we find that the theory qualitatively reproduces the phase diagram of the percolation transition and the impact of the neutral domains. Phase separation is observed when reducing the neutral linker size in an asymmetric system, resulting in a closed-loop phase diagram. We also study the effect of modulating the sequence and find that blockiness of sticker sites introduces microstructure in the dense liquid phase. These insights enhance our understanding of how specific binding and domain arrangement regulates condensate formation in RNA-protein systems.

CPP 12.3 Mon 17:30 H46

Model particles to study interaction of microplastic particles — •Kai Gossen, Andreas Fery, and Günter Auernhammer — IPF Dresden, Dresden, Germany

Microplastic in the environment is typically coated by natural organic matter forming an ecocorona. We present an approach to model ecocorona on particles with well-defined polymers, synthetic and derived from natural polymers. Polystyrene particles were coated with fluorescent polyelectrolyte multilayer systems, PS(Chitosan/Hyaluronic acid) and PS(Poly(dimethyldiallylammonium chloride) /Polystyrene sulfonate) by the layer-by-layer method. Systems with 2, 4 and 6 bilayers were synthesized. The second layers were fluorescently labelled with SNARF conjugated dextran.

It was found that zeta potentials of the PS(Chi/HS)2/4/6 systems assume values (-20 mV to -35 mV) that are similar to those of PS-ecocorona particles (-40 mV to -5 mV). The pH-dependent fluorescence of particle suspensions and individual particles were measured at pH values between pH 3 and pH 8. A well measurable pH dependence between pH 4.5 and 8 for the PS(Chi/HS) systems and the PS(PDADMAC/PSS) system could be measured. The system could serve to selectively study effects of surface properties of ecocorona coated particles such as surface stiffness or zeta potential.

CPP 12.4 Mon 17:45 H46

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — •Souraj Mandal[1], Anna Fritschen[2], Alina Filatova[3], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany — [2]BioMedical Printing Technology, Department of Mechanical Engineering, Technical University of Darmstadt, 64289 Darmstadt, Germany — [3]Stem Cell and Developmental Biology, Technical University of Darmstadt, 64287 Darmstadt, Germany

Three-dimensional cellular models hold great promise for drug testing, but their success relies on maintaining a controlled supply of oxygen and nutrients. Artificial vascular networks aim to mimic blood vessel functions, yet ensuring robust endothelial cell (EC) attachment remains a significant challenge. In this study, we designed a mediator between artificial network surfaces and ECs using Poly(N-isopropylacrylamide) (PNIPAM) microgels (MGs) that remain mechanically stable in nutrient solutions. Charged MGs were synthesized and tested for adhesion on plasma-treated model surfaces. The microgel-coated substrates were exposed to cell static culture media and under defined flow. Atomic force microscopy (AFM) confirmed stable adhesion of MG particles before and after exposure. Initial experiments explored EC attachment on positively and negatively charged MG surfaces, followed by mechanical property characterization. The MG coatings were biofunctionalized with integrin-recognized ligands to enhance EC adhesion and proliferation further.

CPP 13: Molecular Electronics and Excited State Properties I

Time: Monday 17:15–18:30 Location: H38

CPP 13.1 Mon 17:15 H38

Revealing the Origin of low-energy Excited State Absorption in the nonlinear Optical Properties of Thiophene — •Mustapha Driouech, Michele Guerrini, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Optical nonlinearities in organic molecules are useful for advanced applications. Among them, optical limiting is particularly relevant to prevent critical damage to the human eyes and artificial sensors from intense radiation. In this ab initio study, we investigate the nonlinear optical properties of thiophene oligomers with a non-perturbative approach based on real-time time dependent density functional theory [1]. We study the optical absorption spectra obtained after applying a broadband instantaneous electric field. For sufficiently high intensities, we observe the appearance of absorption peaks at low energies that are not present in the linear spectra. To investigate in more details the nonlinear mechanisms involved, we perform pump-probe simulations combined with analysis of the population dynamics revealing that the emerging features are due to excited state absorption in the visible region. Our results show that this fully ab initio methodology is able to capture and unravel the fundamental mechanisms of optical nonlinearities in organic molecules.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).

CPP 13.2 Mon 17:30 H38

Theoretical perspectives on ground- and excited state absorption in organic materials: comparing TDDFT, GW/BSE, and post-Hartree-Fock methods — •Narges Taghizade[1], Andreas Windischbacher[1], Andreas W. Hauser[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Experimental Physics, Graz University of Technology, Austria

Ground- and excited-state absorption (ESA) properties of conjugated organic materials are fundamental to the development of advanced optoelectronic devices. In this contribution, we specifically focus on molecules, which pose challenges to traditional theoretical approaches owing to significant electron correlation resulting in complex charge transfer and multi-reference characteristics, particularly when it comes to excited state properties. To address these complexities, we compute the ground and ESA spectra using a number of complementary, advanced theoretical methods. First, we employ time-dependent density functional theory within the linear and quadratic response frameworks, respectively. Second, we present results from a GW/BSE many-body perturbation theory approach thereby addressing the challenge of accurately accounting for charge transfer excitations. Third, we also apply post-Hartree-Fock methods, such as the multi-configurational self-consistent field method in order to tackle the strong electron correlation and multi-reference effects. The comparison of our results highlights the strengths and limitations of various computational approaches and offers a pathway toward improved theoretical models for the design of efficient optoelectronic materials.

CPP 13.3 Mon 17:45 H38

Charge and energy transfer mechanisms in a singlet fission donor-acceptor complex — •Karin S. Thalmann[1], Johan E. Runeson[1], Pedro B. Coto[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Spanish National Research Council (CSIC), Madrid, Spain

Singlet fission is a photophysical process transforming a singlet excited electronic state to two triplet states [1]. Thus, materials exhibiting singlet fission have the potential to increase the efficiency of solar cells. Adding an acceptor to a singlet fission active molecule enables the extraction of charges and excitation energy. In our work, we study a diazadiborine dimer as donor [2] and tetracyanoquinodimethane as acceptor molecule. Using *ab initio* multireference perturbation theory calculations, we build a vibronic model Hamiltonian and further perform quantum dynamical [3] and mixed quantum-classical simulations [4] to analyse the charge and energy transfer dynamics in the complex. With our techniques, we characterise competing charge and energy transfer processes as well as intramolecular and intermolecular singlet fission. The analysis reveals the role of the different electronic states and vibrational modes in the dynamics of the donor-acceptor complex.

[1] M. B. Smith *et al.*, *Chem. Rev.* **110**, 6891-6936 (2010).
[2] T. Zeng, *J. Phys. Chem. Lett.* **7**, 4405-4412 (2016).
[3] S. R. Reddy *et al.*, *J. Phys. Chem. Lett.* **9**, 5979-5986 (2018).
[4] J. E. Runeson *et al.*, *J. Chem. Phys.* **159**, 094115 (2023).

CPP 13.4 Mon 18:00 H38

The Influence of Solvent Nature and Annealing Conditions on the TADF Properties of DMAC-TRZ in Films and Single Crystals — •Anatolii Kuimov[1], Sergey Bagnich[1], Christopher Greve[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Germany — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Germany

We investigated the impact of molecular arrangement and post-processing conditions on the thermally activated delayed fluorescence (TADF) of the donor-acceptor type molecule DMAC-TRZ. Specifically, we studied luminescence at various temperatures and time delays after excitation across different solid-state morphologies, including amorphous films, polycrystals, and single crystals, complemented by X-ray analysis of the single crystal. In single crystals, we observed that emission energy, the singlet-triplet gap, and TADF intensity were influenced by processing conditions, such as aging, thermal and solvent annealing, and the choice of solution for crystal growth. These effects are attributed to changes in the torsion angle between the donor and acceptor moieties. Comparisons with polycrystals and amorphous films reveal that introducing morphological disorder promotes a more orthogonal donor-acceptor arrangement, leading to a smaller singlet-triplet gap and enhanced TADF. Our findings emphasize the pivotal role of molecular conformation in modulating photophysical properties. This study highlights the potential of tailoring material performance through

structural modifications and annealing strategies to optimize TADF efficiency for organic optoelectronic applications.

CPP 13.5 Mon 18:15 H38

Effect of Junction Structure on Quantum Interference in Single-Molecule Junctions — •Aoshi Yamane, Shintaro Fujii, and Tomoaki Nishino — Department of Chemistry, School of Science, Institute of Science Tokyo, 2-12-1 Ookayama, Meguro-ku, Tokyo, Japan

The destructive quantum interference (DQI) effect in single-molecule junctions induces a steep decrease in electron transmission at specific energies, enables high on/off ratios of electrical conductivity, and is expected to be applied to molecular devices such as transistors and switches. Here, we aimed to elucidate the effects of molecular and molecule/metal interface structures on DQI. We focused on disubstituted naphthalene with different types and positions of anchoring groups connecting molecules and electrodes. Break junction measurements of the molecular junctions demonstrated that for naphthalenedithiol (NDT), 2,7-NDT showed significantly lower conductivity compared to 2,6-NDT, indicating the presence of DQI in 2,7-NDT. On the other hand, for naphthalenedicarbonitrile (NDCN), 2,6-NDCN and 2,7-NDCN showed similar conductance. Combined with Flicker noise analysis and DFT-NEGF transmission calculations, we demonstrate that the DQI features in 2,7-NDCN are masked by the contribution of electrode-π coupling, which short-circuit the molecular junctions. The present study provides important insights into the control of unique electron transport properties induced by DQI in single-molecule junctions.

CPP 14: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 17:30–18:30 Location: H34

CPP 14.1 Mon 17:30 H34

Vapor-mediated wetting and imbibition control on micropatterned surfaces — •Ze Xu and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Wetting and evaporation of droplets on micropatterned surfaces are ubiquitous in nature and key to many technological applications, such as water/ice-proof coatings, spray cooling, inkjet printing, and semiconductor surface processing. The wettability of micropatterned surfaces is governed by surface chemistry and topography, and significant effort has been devoted to overcoming this intrinsic behavior, e.g. to dry or coat structures surfaces, by use of external stimuli like electromagnetic fields. However, these methods usually require specific materials, thus limiting their practical use. Here, we show that the spreading behavior of water droplets on hydrophilic surface patterns can be controlled and even temporarily inhibited by the presence of the vapor of a low surface tension liquid. We show that this delayed wicking arises from Marangoni forces due to vapor condensation at the droplet periphery that compete with the capillary wicking force of the surface topography. We further demonstrate how modulating the vapor concentration in space and time can be used to guide droplets across patterns and even extract liquid from fully imbibed films, devising new strategies for coating, cleaning and drying of functional surface designs.

CPP 14.2 Mon 17:45 H34

Gradient dynamics model for volatile binary mixtures including Marangoni flows — •Jan Diekmann und Uwe Thiele — Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster

We present a mesoscopic thin-film model in gradient dynamics form for binary liquid mixtures on solid substrates incorporating interface tension-induced flow, and volatility in a narrow gap. Thereby, we use and expand models established in [1-4] by accounting for the two substances in each of two bulk phases - liquid and gas - and for the enrichment of one component at the liquid-gas interface. We discuss the different contributions to the free energy, thereby employing Flory-Huggins theory of mixing for the condensed phase and assuming ideal gases for the vapor phase. The resulting five-field model is then analyzed with numerical time simulations focusing on the interplay of the drop dynamics with the developing lateral concentration gradients, and the resulting Marangoni flows. The results are compared to experimental findings [5].

[1] Thiele et al. Physical Review Fluids, 2016. doi:10.1103/physrevfluids.1.083903
[2] Xu et al. Journal of Physics: Condensed Matter, 2015. doi:10.1088/0953-8984/27/8/085005
[3] Hartmann et al. Langmuir, 2024. doi: 10.1021/acs.langmuir.3c03313
[4] Thiele et al. Physical Review Letters, 2013. doi: 10.1103/physrevlett.111.117801
[5] Chao et al. Proceedings of the National Academy of Sciences, 2022. doi: 10.1073/pnas.2203510119

CPP 14.3 Mon 18:00 H34

Fast dynamics of PNIPAM microgels at fluid interfaces: insights from droplet bouncing and jetting — Atieh Razavi, Suvendu Mandal, Benno Liebchen, Regine von Klitzing, and •Amin Rahimzadeh — Technische Universität Darmstadt, Hochschulstrasse 8, 64289 Darmstadt, Germany

PNIPAM microgels, as cross-linked polymer networks, are known to adsorb at the air-water interface, reducing surface tension. The kinetics of their adsorption, and thus the dynamic surface tension, depend on their cross-linking density, which determines the stiffness of individual microgels. Under interfacial perturbations such as dilation, softer microgels restore surface tension more rapidly, creating interfaces with higher surface elastic moduli, as shown by interfacial rheology studies using profile analysis tensiometry (1-10 s timescales). However, the behavior of microgels under very rapid interfacial deformations (milliseconds) remains unclear. We address this question through experiments involving droplet bouncing and jetting, processes relevant to applications such as inkjet printing and needle-free drug delivery. Our results demonstrate that microgels rapidly respond to fast interfacial deformations, with softer microgels restoring surface tension more efficiently. This quicker response allows greater interfacial extension in the presence of softer microgels. Molecular dynamics simulations corroborate our experimental findings, providing further insight into the mechanisms at play. This study highlights the critical role of microgel stiffness in determining their interfacial dynamics across a wide range of timescales and deformation rates.

CPP 14.4 Mon 18:15 H34

Soft dynamic wetting transition — •Christopher Henkel[1], Vincent Bertin[2], Jacco Snoeijer[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, Universität Münster, Germany — [2]Physics of Fluids Group, Faculty of Science and Technology, Mesa+ Institute, University of Twente, The Netherlands — [3]Center for Nonlinear Science (CeNoS), Universität Münster, Germany

We investigate the forced receding and advancing dynamics of a three-phase contact line on a viscoelastic substrate, i.e., the wetting transition of a substrate from macroscopically dry to wet or vice versa. Thereby, we use the Landau-Levich (or dip-coating) geometry, where a solid viscoelastic plate is dragged out of or pushed into a liquid bath. We employ a mesoscopic hydrodynamic model in long-wave approximation, i.e. valid at small contact angle and plate inclination. The elastic response of the substrate follows the Winkler foundation with a Kelvin-Voigt relaxation. In particular, we investigate how the shape and stability of the meniscus changes with the plate velocity and the substrate softness. In this we compare numeric results with asymptotic analytic calculations. Finally, we explore whether the occurrence of stick-slip motion in the advancing case can be predicted, using simple scaling arguments.

CPP 15: Poster Session I

Time: Monday 19:00–21:00 Location: P4

CPP 15.1 Mon 19:00 P4

Exploring Green Solvent Additives for Enhanced Solubility in Organic Photovoltaics Processing — •Leonhard Schatt, Fabian Eller, and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Organic Photovoltaic (OPV) devices offer the potential for low-cost production of devices that convert light into electricity. These devices are typically processed from solution, which allows for simple, scalable production methods such as printing. However, the solvents used by most research groups are halogenated aromatic solvents, as green solvents often lack good solubility for the solutes used. We are therefore experimenting with additives in green solvents as a method of tuning solubility. We monitor the solubility with in-situ solubility measurements to study the effects of additive type and volume fraction. This will allow us to map the solubility space of the high performance OPV material PM6. Our aim is to contribute to the replacement of halogenated solvents for OPV processing and to make our organic electronic material processing feasible for industrial applications.

CPP 15.2 Mon 19:00 P4

Comparing Machine Learning Force Fields for Proton Transfer Dynamics in Solid Acids — •Jules Oumard, Aaron Flötotto, and Christian Dressler — Technische Universität Ilmenau, Fakultät für Mathematik und Naturwissenschaften, Institut für Physik, Fachgebiet Theoretische Festkörperphysik, Weimarer Straße 32, 98693, Ilmenau

Solid acids are excellent water-free proton conductors and can be used in fuel cells. [1]. The rarity of long-range proton transfer events in ab initio molecular dynamic simulations makes the calculation of converged diffusion coefficients challenging. This can be overcome by accelerating these simulations with machine learning force fields (MLFF). We compare two MLFF approaches: Gaussian Approximation Potentials (GAP) with on-the-fly learning [2] and equivariant graph neural networks [3]. A protocol for fine-tuning GAP models is presented. We evaluate the calculated diffusion coefficients and explain trends in terms of jump rate functions and anion rotation rates.

[1] Mohammad, N. et al. (2016). Journal of Power Sources, 322, 77-92. doi:10.1016/j.jpowsour.2016.05.021

[2] Jinnouchi, R. et al. (2019). Physical Review B, 100(1), 014105. doi:10.1103/PhysRevB.100.014105

[3] Batatia, I., et al. (2022). Advances in Neural Information Processing Systems. https://openreview.net/forum?id=YPpSngE-ZU

CPP 15.3 Mon 19:00 P4

Towards Theoretical UV/Vis Spectra with Experimental Accuracy. Benchmarks for Spiropyran Photoswitches — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Molecular photoswitches are molecules that undergo an isomerization upon irradiation with specific wavelengths. One key feature for understanding this process are the UV/Vis spectra of the involved species (e.g. the closed and open forms in the case of spiropyran, SP). First-principles methods like density-functional theory (DFT) allow the calculation of UV/Vis spectra within certain approximations. However, the properties of the chosen functional, the description of solvation, as well as the accuracy of conformational and vibrational sampling all contribute to discrepancies between theory and experiment. This motivates us to establish a rigorous theoretical approach to assist in the prediction and analysis of UV/Vis spectra for molecular photoswitches. As a crucial step, we here benchmark different approaches for predicting UV/Vis spectra of SP switches against experimental references. We emphasize the influence of different functional approximations and highlight the role of the conformational ensemble and molecular vibrations sampling (e.g. via by machine learning enhanced molecular dynamics simulations). The importance of these different effects is discussed, with the goal of providing best practice guidelines that enable robust predictions.

CPP 15.4 Mon 19:00 P4

Optical properties of diamondoid organotin sulfur clusters with fluorescent ligands — •Alexander Schauerte[1], Jie Wang[2], Felix Thomas[1], Irán Rojas León[2], Stefanie Dehnen[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-University of Marburg, Renthof 7a, D-35032 Marburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

White light is important in our daily life as well as in technology and research. It has been shown that diamondoid organotin clusters with organic ligands emit a brilliant white light beam when pumped with an infrared laser.

We investigate the fluorescent properties of tin-sulfur/selenium clusters with three phenyl- and one tetraphenylethylene ligands using photoluminescence- and spatially resolved photoluminescenceexcitation- spectroscopy. Through temperature-dependent measurements of compounds prepared as glass and as powder, we conclude that the electron-phonon-coupling and short-range ordering seems to be reduced in a glass state compared to a powder.

Furthermore, we investigate the white light generation (WLG) and second harmonic generation of different cluster compounds, which show a dependence of the WLG-efficiency on the chemical composition. The glass has a lower excitation power threshold for WLG than the powder.

CPP 15.5 Mon 19:00 P4

Electromagnetic Compatibility Measurements of Polymers in the Automotive Industry: Shielding Effectiveness According to ASTM D 4935 — Leopold Handke, Nicola Peranio, and •Verena Cerna — Technische Hochschule Ulm, Ulm, Deutschland

Electromagnetic compatibility (EMC) is a key concern in the automotive industry due to the growing complexity of vehicle electronic systems and the need to prevent electromagnetic interference that could affect their performance and safety. Polymers used in automotive components must meet specific EMC requirements to ensure proper functioning of vehicle electronics. This study investigates the shielding effectiveness (SE) of various polymer materials using standardized measurements according to ASTM D 4935. Shielding effectiveness for both magnetic (B-field) and electric (E-field) fields was measured over a frequency range from 50 kHz to 3 GHz. SE measurements provide valuable insights into the frequency-dependent shielding properties of plastics, offering a basis for selecting appropriate materials for automotive applications to address EMC challenges.

CPP 15.6 Mon 19:00 P4

Time-resolved structure formation in biohybrid coatings revealed by in-situ GISAXS and machine learning — •Julian E. Heger[1], Shachar Dan[2], Yufeng Zhai[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]1TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

Relationships between the structure and property of functional films are at the heart of material science, which makes understanding of how film morphology influences its function essential. Achieving a comprehensive and statistically relevant understanding of the film's characteristics often requires the use of indispensable tools like grazing-incidence small-angle X-ray scattering (GISAXS). GISAXS enables the exploration of the film's characteristic morphology in reciprocal space, such as characteristic size distributions. However, a challenge arises due to the loss of phase information during measurements, which inhibits a direct transformation from reciprocal space to real space via inverse Fourier transform. In addressing this obstacle neural networks (NN) emerge as promising solutions, as they offer potential ways to enable a fast transformation of GISAXS data. Here, we present the results of applying a NN which is trained on synthetic GISAXS data to evaluate the film formation of biohybrid coatings during deposition from in-situ GISAXS synchrotron data.

CPP 15.7 Mon 19:00 P4

Simulation-Based Neural Network with Embedded Prior Knowledge for Predicting Morphological Parameters in GISAXS — •Shachar Dan[1], Eldar Almamedov[2], Matthias Schwartzkopf[1], Sven-Jannik Wöhnert[1], Andre Rothkirch[1], Yufeng Zhai[1], Jose I. Robledo[4], Volker Skwarek[2], and Stephan V. Roth[3] — [1]DESY, Notkestraße 85, D-22607 Hamburg — [2]HAW, Berliner Tor 5, D-20099 Hamburg — [3]KTH, Teknikringen 56 SE-10044 Stockholm — [4]FZ-Jülich, Wilhelm-Johnen- Straße D-52428 Jülich

In-situ grazing-incidence small-angle X-ray scattering (GISAXS) is a powerful technique for analyzing nanoscale structures, yet its interpretation is challenging due to the inverse problem caused by phase information loss. Advances in simulation software and deep learning techniques have opened the door to the idea of using simulations, which can now be generated more efficiently in diverse configurations, to train neural networks (NNs). However, simulations often fail to fully represent experimental data, creating a significant sim-to-real gap. In our work, we tackle this challenge by embedding prior knowledge about the system into the NN training process. By incorporating constraints based on this knowledge, we train models on simulations and apply them to experimental data, enabling reasonable predictions of morphological parameters such as cluster radii, intercluster distances, and grain size distributions. This approach aims to accelerate material characterization at the nanoscale and provide a portable and efficient counterpart to traditional methods.

CPP 15.8 Mon 19:00 P4

Low-Temperature Photoluminescence Characterization of Hybrid Metal Halides — •Anton Krüger[1], Meng Yang[2], Alexander Schauerte[1], Dominik Muth[1], Johanna Heine[2], and Marina Gerhard[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, D-35032 Marburg, Germany

In order to remove the toxic lead component of the otherwise promising perovskite materials, many different approaches have been pursued.

Here, the photoluminescence (PL) and absorption properties of crystalline non-toxic hybrid main group metal halide compounds, $(\alpha\text{-Me-2-NA})_4E_2X_{10}$ (NA=Naphthylmethylammonium, E=Sb/Bi, X=Halide) are investigated by means of time-resolved PL spectroscopy, steady-state PL spectroscopy as well as PL excitation spectroscopy.

It is shown that the absorption and PL properties of these materials depend on the metal/halide composition, giving rise to a variety of absorbers and emitters. Furthermore, temperature dependent spectroscopic experiments reveal a thermochromic behavior of the compounds.

CPP 15.9 Mon 19:00 P4

Effect of fluorinated tail groups on the properties of aromatic self-assembled monolayers — Yangbiao Liu[1], Sonja Katzbach[2], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany. — [2]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Electric transport properties of functional self-assembled monolayers (SAMs) are important for interface engineering in organic electronics and molecular

electronics. As was shown recently, substituting only one terminal hydrogen atom in SAMs with a halogen atom changes their electric conductance noticeably. In this context, we studied the respective effects in a series of non-substituted and methyl-substituted biphenylthiolate (BPT) SAMs on Au(111), exchanging the terminal hydrogen atom/atoms for fluorine/fluorines and testing not only single-component but binary SAMs as well. The gradual variation of the work function with the SAM composition was accompanied by a gradual variation of electrical conductance, decreasing, in particular, by two orders of magnitude at going from CH3-BPT to CF3-BPT SAMs. The observed behavior was tentatively explained by the higher projected density-of-states at the position of the terminal tail groups in the CH3-BPT (H-BPT) case compared to CF3-BPT (F-BPT) and by the appearance of an internal electrostatic field in the SAMs, leading to a change and renormalization of the energy level alignments within the junction upon contact of the SAMs to the top EGaIn electrode.

CPP 15.10 Mon 19:00 P4

Charge separation in a porphyrin-based metal-organic framework incorporating fullerene — •Martin Richter[1], Xiaojing Liu[2], Pavel Kolesnichenko[1], Christof Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Germany

Porphyrin-based materials are attracting great interest due to their wide range of potential applications. They can be embedded into metal-organic frameworks (MOF) to manipulate and investigate the relations between function and structure. In conjunction with an electron acceptor, charge separation can be achieved, which is beneficial for applications such as solar cells or photocatalysis. Experiments on ZnTPP (Zinc 5,15-bis-(3,4,5-trimethoxyphenyl)-10,20-bis-(4-carboxyphenyl)) in a surface-anchored MOF (SURMOF) with fullerene C_{60} loaded into the pores, have demonstrated that photoexcitation can enhance the conductivity by up to two orders of magnitude [1]. Here, we investigate excited states dynamics after optical excitation with transient absorption spectroscopy on the femto- to nanosecond time scale. Charge separated states can be identified, which have a lifetime of 212-360 ps. The charge separation occurs after excitation of both the Soret band and the Q band within only a few hundred femtoseconds.

[1] X. Liu et al., Angew. Chem. Int. Ed. 2019, 58, 9590.

CPP 15.11 Mon 19:00 P4

Structural influences on nonlinear optical activity for supercontinum generation: isolated cubane — •Alexander Kapp and Simone Sanna — Institute for Theoretical Physics, 35392 Gießen, Germany

It has been suggested that adamantane-based molecular clusters can convert a narrowband laser source into a broadband supercontinuum. Unlike thermal emitters, the resulting spectra are coherent and not constrained by Planck's law, making them highly valuable for various applications, such as high-resolution monitoring and spectroscopy.

In order to expand our library of suitable molecules, we investigate the electronic and optical properties of materials with similar symmetry. This involves performing first-principle density functional theory calculations to identify appropriate structures. Here, we focus specifically on isolated cubane (C_8H_8) molecules and their derivatives, analyzing their electronic and structural properties and their correlation with the optical response.

CPP 15.12 Mon 19:00 P4

Impact of Classical and Quantum Light on Donor-Acceptor-Donor Molecules — •Haraprasad Mandal[1,2], Sajal Kumar Giri[3], Sara Jovanovski[1], Oleg Varnavski[1], Malgorzata Zagorska[4], Roman Ganczarczyk[4], Tse-Min Chiang[3], George C. Schatz[3], and Theodore Goodson III[1] — [1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, United States — [2]Department of Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria — [3]Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States — [4]Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Investigations of entangled and classical two-photon absorption have been carried out for six donor (D)-acceptor (A)-donor (D) compounds containing the dithieno pyrrole (DTP) unit as donor and acceptors with systematically varied electronic properties. Comparing ETPA (quantum) and TPA (classical) results reveals that the ETPA cross section decreases with increasing TPA cross section for molecules with highly off-resonant excited states for single-photon excitation. Theory (TDDFT) results are in semiquantitative agreement with this anticorrelated behavior due to the dependence of the ETPA cross section but not TPA on the two-photon excited state lifetime. The largest cross section is found for a DTP derivative that has a single photon excitation energy closest to resonance with half the two-photon excitation energy. These results are important for the possible use of quantum light for low-intensity energy-conversion applications.

CPP 15.13 Mon 19:00 P4

Correlating molecular properties to the SHG response: Prerequisites for white light generation. — •Ferdinand Ziese and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different substituents [1,2]. Systematic investigations further our understanding of the origin of this behavior, we have investigated structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules [3]. Core modifications mostly change the characteristic of the response in a more subtle manner while the exchange of substituents exhibit a greater impact. Distinct changes to the intensity, energy, and characteristic can be observed. The presented results provide a theoretical foundation for the design of tailored nonlinear optical sources.

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[2] N. W. Rosemann, J. P. Eußner, E. Dornsiepen, S. Chatterjee, S. Dehnen, J. Am. Chem. Soc. 2016 138 (50), 16224-16227

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CPP 15.14 Mon 19:00 P4

Effect of Deposition Rates on the Morphology and Efficiency of Blue TADF OLEDs — •Tolga Durmus, Marius Schnapp, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The efficiency and stability of blue thermally activated delayed fluorescence (TADF) OLEDs are strongly influenced by the structural properties of their active layers. In this study, we investigate the impact of varying deposition rates on the morphology of these layers, focusing on their amorphous or crystalline nature. Atomic force microscopy (AFM) is used to analyze the surface morphology of the deposited layers and we aim to establish a correlation between the deposition conditions, the structural properties of the layers, and the efficiency of the OLEDs. These investigations are expected to provide valuable insights into optimizing fabrication parameters for improved blue TADF-OLEDs.

CPP 15.15 Mon 19:00 P4

Temperature-dependent Transient Electroluminescence of Blue TADF OLEDs — •Klara-Maria Bögle, Felix Kübert, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Third generation OLEDs use, in contrast to first and second generation OLEDs, ambient thermal energy to increase fluorescence, so-called Thermally-Activated Delayed Fluorescence (TADF). This is achieved via reverse inter-system crossing (*rISC*), which means that non-radiative triplet excitons are up-converted to radiative singlet excitons. This process significantly increases the internal quantum efficiency, up to 100%. In this study, OLEDs with the multiple resonance blue TADF emitter ν-DABNA embedded in an mCP matrix are investigated. Transient electroluminescence (EL) reveals a strong temperature dependence, which we model with rate equations to better understand the TADF process in an OLED under operating conditions. The rate equations describe the population densities of the triplets, singlets and charge carriers using the different rates of *(r)ISC*, triplet-triplet annihilation (*TTA*), triplet-polaron annihilation (*TPA*) as well as the (non-) radiative singlet/triplet decay rates. Traditionally, such analysis is often based on transient photoluminescence at room temperature, which also lacks charge carrier contributions and is thus inconclusive. We therefore aim to get a full picture of *all* population densities and recombination mechanisms to better understand efficiency limiting processes.

CPP 15.16 Mon 19:00 P4

Porous poly(ethylene glycol) films as a versatile platform for ssDNA immobilization and hybridization — Zhiyong Zhao and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Poly(ethylene glycol) (PEG) films, fabricated by thermally induced crosslinking of amine and epoxy-terminated four-arm STAR-PEG precursors, were used as porous and bioinert matrix for single-stranded DNA (ssDNA) immobilization and hybridization. The immobilization relied on either the reaction between the amine groups in the PEG matrix and N-hydroxy succinimide (NHS) ester groups of the NHS-ester-decorated ssDNA or the reaction between the epoxy groups in the matrix and thiol groups of the respectively substituted ssDNA. The mixing ratio of the precursors was varied to tune the density of the amine and epoxy groups available for the immobilization. Spectroscopic and electrochemical data confirmed the successful immobilization of the ssDNA probes into the PEG matrix as well as the high hybridization efficiency, selectivity, and sensitivity of the resulting DNA sensors. Whereas these sensors were equivalent to the direct ssDNA assembly in terms of efficiency, they exhibited better selectivity and bioinert properties because of the bioinert character of the PEG matrix.

The above findings place PEG films as a promising platform for highly selective ssDNA sensing, leveraging their flexible chemistry, 3D character, and bioinert properties.

CPP 15.17 Mon 19:00 P4

The effect of spherical nanoceria on the anionic polysaccharides and in vitro behavior as a wound dressing — •Alexandra Feraru[1,2], Zsejke-Réka Tóth[2], Klára Magyari[2,3], Monica Baia[4,5], Tamás Gyulavári[6], Emoke Páll[7], Emilia Licarete[8], Codrut Costinas[1,5], Oana Cadar[9], Ionel Papuc[7], and Lucian Baia[2,4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [2]Nanostructured Materials and Bio-Nano-Interfaces Center, Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, T. Laurian 42, 400271 Cluj-Napoca, Romania — [3]INSPIRE Research Platform, Babes Bolyai University, 400084, Cluj-Napoca, Romania — [4]Faculty of Physics, Babes-Bolyai University, M. Kogălniceanu 1, 400084 Cluj-Napoca, Romania — [5]Institute for Research-Development-Innovation in Applied Natural Sciences, Babes-Bolyai University, Fântânele 30, 400294, Cluj-Napoca, Romania — [6]Department of Applied and Environmental Chemistry, University of Szeged, Rerrich B. sqr. 1, Szeged 6720, Hungary — [7]Faculty of Veterinary Medicine, University of Agricultural Science and Veterinary Medicine, 400372 Cluj-Napoca, Romania — [8]Faculty of Biology and Geology, Babes-Bolyai University, 400015 Cluj-Napoca, Romania — [9]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath Street, 400293 Cluj-Napoca, Romania

In this study, we aimed to enhance the understanding of how chemical bonds form when sodium alginate and gum arabic interact with nanoceria nanoparticles.

CPP 15.18 Mon 19:00 P4

Programming fibril alignment and mechanical response in electron beam-modified collagen type I fibers — •Friedrich Schütte[1,2], Anastassiya Bublikova[1,2], and Stefan G. Mayr[1,2] — [1]Division of Surface Physics, Department of Physics and Earth System Sciences, University of Leipzig, Linnéstr. 5, 04103 Leipzig — [2]Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany

Modifying collagenous systems for tendon and tissue replacements in a controlled manner to produce biomimetic implants has a high potential for future biomedical applications. As a polymeric biomaterial, abundant in human bodies and influencing cellular morphology, collagen type I provides structural integrity and strength to tissues. However, applications are limited because even in crosslinked cases, the biomechanical properties of collagen networks can differ by several orders of magnitude in terms of both elasticity and load capacity. The widely used crosslinker glutaraldehyde has been the subject of controversy due to cytotoxic effects. In contrast, electron-beam-treatment allows reagent free control over a rapid and sterilizing crosslinking method in a non-cytotoxical biomimetic manner, resulting in improved mechanical properties due to high penetration depth and sufficiently high irradiation-induced doses. Subsequently, the modification of collagen type I fibers by energetic electron-beam-treatment during prestrain induced alignment of the inner filaments is shown to achieve and imprint network anisotropies resulting in mechanical properties with Young's moduli bridging orders of magnitude from a kPa range to a MPa range.

CPP 15.19 Mon 19:00 P4

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Jungui Zhou[1], Constantin Harder[1,2], Guangjiu Pan[1], Yusuf Bulut[1,2], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], Sarathlal K. Vayalil[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose has emerged as a promising bio-based template for sensors, smart windows, and bioelectronics. Typically, Surface Enhanced Raman Scattering (SERS), an advantageous analytical technique, allows for the rapid detection and structural analysis of chemical compounds through their spectral patterns in nanotechnology. Crucial for SERS is fabricating the substrates with strong enhancements of the Raman signal over large areas. Herein, we present a straightforward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. GISAXS combined with nano-FTIR spectroscopy was used to confirm a synergistic Raman enhancement mechanism of localized surface plasmon resonance and interface charge transfer. Our approach provides a reference for facile and scalable production of SERS substrates.

CPP 15.20 Mon 19:00 P4

Analysis of folding/unfolding behavior of micro and nano collagen fibers by SFTIRM — •Selcuk Kaan Haciosmanoglu[1], Gihan Kamel[2,3], and Murat Kazanci[1,4] — [1]Nanoscience and Nanoengineering Program, Graduate School, Istanbul Medeniyet University, Istanbul, Turkey — [2]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Biomedical Engineering Department, School of Engineering and Natural Sciences, Istanbul Medeniyet University, Istanbul, Turkey

Collagen nanofibers are essential extracellular matrix (ECM) components widely used in regenerative medicine. While both electrospinning and wet-spinning techniques can produce anisotropic collagen micro- and nanofibers from dissolved collagen solutions, electrospun fibers require crosslinking to maintain water stability for cell culture applications. This study investigates in-situ crosslinking during electrospinning using chemical agents and physical methods. Synchrotron Fourier-Transform Infrared Microspectroscopy (sFTIRM) analysis revealed distinct molecular structural changes in the collagen nanofibers based on processing methods. Protein band positions shifted according to the extraction methods employed. Notably, electrospinning inhibited collagen molecule self-assembly, resulting in lower band positions compared to wet-spun fibers. The choice of crosslinking agent significantly influenced collagen's secondary structure, with genipin-mediated in-situ crosslinking better preserving the native structure of electrospun collagen nanofibers compared to UV crosslinking.

CPP 15.21 Mon 19:00 P4

Enhancing Endothelial Cell Attachment on PNIPAM-Based Microgel Coatings with RGD Ligand Functionalization — •Leonie Beer, Souraj Mandal, and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany

Endothelial cell (EC) attachment is crucial for capillary formation and the success of artificial vascular networks in tissue engineering. Poly(N-isopropylacrylamide) (PNIPAM) microgels offer a promising platform for this application due to their tunable mechanical properties and ability to incorporate bioactive ligands. This study investigates the use of PNIPAM-based microgel coatings functionalized with the integrin-binding peptide sequence arginine-glycine-aspartate (RGD) to enhance EC adhesion. Successful conjugation of RGD peptides was confirmed using infrared spectroscopy and fluorescence microscopy. To evaluate the impact of ligand configuration, we compared three variations of RGD based peptides. The results reveal that increasing the anchor length significantly improves HUVEC recognition of the ligands, resulting in enhanced cell attachment and proliferation. These findings highlight the critical role of ligand design in optimizing biofunctional coatings. This work presents a straightforward chemical strategy for improving endothelial cell adhesion on PNIPAM-based microgel surfaces, paving the way for advanced artificial vascular networks in tissue engineering and regenerative medicine.

CPP 15.22 Mon 19:00 P4

Green plastics: Direct production from grocery wastes and characterization by using S-FTIR — •Onur Aras[1], Gihan Kamel[2,3], and Murat Kazanci[4,5] — [1]Istanbul Medeniyet University, Nanoscience and Nanoengineering Program, Graduate School, 34700 Istanbul, Turkey — [2]SESAME Synchrotron (Synchrotron-light for Experimental Science and Applications in the Middle East), 19252 Allan, Jordan — [3]Department of Physics, Faculty of Science, Helwan University, Cairo, Egypt — [4]Istanbul Medeniyet University, School of Engineering and Natural Sciences, Department of Biomedical Engineering, Istanbul, Turkey — [5]Istanbul Medeniyet University, Science and Advanced Technologies Research

This study investigates the production of cellulosic bioplastics from four green waste sources: hemp, parsley stem, pineapple leaves, and walnut shell, using either trifluoroacetic acid (TFA) or water as solvents. Synchrotron FTIR Microspectroscopy (SR-*FTIR) was employed to analyze structural modifications during biofilm formation and regeneration.Water-based biofilms retained their native cellulose, hemicellulose, and lignin components. In contrast, TFA-dissolved samples exhibited additional spectral bands in the hemicellulose region, attributed to ester bond hydrolysis and subsequent carboxylic acid formation. Principal component analysis revealed distinct groupings based on solvent type and polymer addition.

CPP 15.23 Mon 19:00 P4

How do stiffness patterns, with no topographical or chemical cues, influence cellular and tissue contact guidance? — •Mathis Grelier[1], Carlos Urena Martin[2], Mark Schvartzman[2], and Ana Suncana smith[1,3] — [1]Puls Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Department of Materials Engineering and Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, Israel — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Rudjer Bošković Institut, 10000 Zagreb, Croatia

While current systems cannot disentangle the effects of topography and stiffness

contrasts, our study overcomes this challenge by investigating cell and tissue behavior on substrates with only alternating stiffness stripes. Our experiments and model reveal that wider stripes enhance alignment along stiffer or softer regions due to the higher energy cost of traversing softer substrates. At the cellular level, we employ a stochastic model based on Boltzmann weights applied to possible cell shapes, integrating energy contributions that govern movement across stiffness boundaries. For tissues, we extend this framework using a dissipative particle model to capture collective dynamics and mechanical interactions. To further explore these effects, we applied a Globalized Bounded Nelder-Mead optimization, enabling the efficient recovery of key physical parameters, such as stiffness and contractility, under both untreated and treated conditions.

CPP 15.24 Mon 19:00 P4

Latex film formation investigated by GISAXS and spectral reflectance — •Simon Schraad[1,2], Helder Marques Salvador[4], Nadja Kölpin[1], Nicolae Tomozeiu[4], Peter Müller-Buschbaum[2], and Stephan Volkher Roth[1,3] — [1]Deutsches Elektronen Synchrotron, Notkestraße 85, 22607 Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [4]Canon Production Printing Netherlands B.V., Van der Grintenstraat 10, 5914 HH Venlo, Niederlande

The film formation of latex inks on nanoporous substrates is of high interest for scientific and industrial applications. Inks are multi-component, complex fluids and consist of colloids, pigments and solvents. The film formation is a multistage process. After deposition, solvent begins to evaporate and finally nanoparticles self assembly. To quantitatively analyze latex film formation a combination of in-situ grazing incidence small angle scattering (GISAXS) and light scattering will be employed. Here structural changes during the deformation and coalescence phase of latex colloids will result in changes in the scattering patterns. We present a design of an experimental spray chamber to allow in-situ GISAXS and the spectral reflectance during spray deposition of latex inks to be used at synchrotron facilities.

CPP 15.25 Mon 19:00 P4

Dynamic magnetic response of multicore particles: the role of grain magnetic anisotropy and intergrain interactions — •Ekaterina Novak[1], Elena Pyanzina[1], Andrey Kuznetsov[2], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

This study examines the magnetic properties of multicore magnetic nanoparticles (MMNPs) utilizing Brownian dynamics simulations in conjunction with the Landau-Lifshitz-Gilbert equation. We demonstrate that the magnetic responses of MMNPs, both static and dynamic, are governed by a complex interplay between the cores magnetic anisotropy and the strength of inter-core magnetic interactions. These insights are crucial for refining the design of multicore magnetic particles in various applications, including magnetic hyperthermia, data storage, and targeted drug delivery, where accurate control over magnetic characteristics is vital.

CPP 15.26 Mon 19:00 P4

Kinetics of nanostructure and interface evolution induced by photopolymerization — •Shouzheng Chen[1,2,3], Yufeng Zhai[2], Jungui Zhou[2], Guangjiu Pan[1], Sarathlal Koyiloth Vayalil[2], Rolf A.T.M. van Benthem[4], Johan F.G.A Janssen[5], Mats K. G. Johansson[6], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]FRM II, Lichtenbergstraße 1, 85748 Garching, Germany — [4]Eindhoven University of Technology, Groene Loper 5, 5600, MB, Eindhoven, the Netherlands — [5]Covestro (Netherlands) B.V., Urmonderbaan 22, 6167, RD, Geleen, the Netherlands — [6]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, SE-100 44 Stockholm, Sweden

Photopolymerization offers spatial resolution, low energy consumption, and high curing speeds, making it a widely used technology in additive manufacturing. The kinetics of the physical transformation of the resin from liquid to solid (cross-linked) state induced by photopolymerization and the kinetics of the solid-liquid interface formation of resin multilayer are the key to achieving controllable high-precision manufacturing. By modulating precursor resin components and combining grazing incidence small angle X-ray scattering (GISAXS), the UV-curing induced nanostructure and the buried interface of resin multilayer are probed. We reveal how solvents and additive monomers determine in nanostructure and multilayer interface formation during photopolymerization.

CPP 15.27 Mon 19:00 P4

Effect of grafting density on particle distribution in polymer brush/gold nanoparticle composite materials — •Elias Hallenbach, Hayden Robertson, and Regine von Klitzing — Institute for Condensed Matter Physics, Technical University of Darmstadt, Germany

Metal/polymer nanocomposites are versatile hybrid materials and find use in many fields such as photonics, biomedical engineering and catalysis. A promising realization of this type of hybrid material is the controlled self-assembly of gold nanoparticles (AuNPs) inside a polymer brush, which induces color changes upon exposure to environmental changes enabling sensor applications.

The polymer brushes serve as a matrix for the immobilization of AuNPs. Particle uptake into the brush matrix is affected by parameters such as thickness, particle size and the grafting density. Polymer brushes with varying grafting densities are synthesized by a controlled polymerization (SI-ARGET ATRP) directly from a silicon substrate. The nanocomposite materials are fabricated by dip-coating of polymer brushes into a AuNP dispersion. Characterization of the nanocomposites is performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry (XRR).

Uptake of nanoparticles has proven to be highest at intermediate grafting densities. I will discuss the influence of particle distribution inside the brush on particle uptake, which can be yielded by XRR measurements.

CPP 15.28 Mon 19:00 P4

Multi-material filament fabrication for 3D printing photoelectrocatalytic carbon nitride composites — •Timo Uhlein and Siowwoon Ng — FAU Erlangen-Nürnberg, Erlangen, Germany

Additive manufacturing of electrochemically active 3D structures is of rising interest. In particular, using fused deposition modeling (FDM) based on filament extrusion concept to produce carbon-polymer-based 3D structures offers several advantages, such as accessibility, low-cost and ease of use. Nevertheless, carbon-based filaments are limited with their applications. Therefore, incorporating additional materials to produce a multi-material filament is of interest, to create 3D-printed electrodes with new or targeted functional properties. In this project, we fabricated a multi-material filament consists of carbon nitride, C3N4, and carbon nanotubes, CNTs, for its photocatalytic properties and high conductivity, respectively, and polymer as the backbone of a FDM filament. We examined the performance of the composite C3N4-CNT electrodes for hydrogen evolution and the photocatalytic degradation of a dye. We indicate that further advancements can be achieved by developing multi-material filaments in order to use them for further electrochemical applications.

CPP 15.29 Mon 19:00 P4

Mechanochemical Behavior and Flow Dynamics of Glycerol Aqueous Solutions Confined between Ferrous Surfaces: Atomic-scale Insights from Reactive Molecular Dynamics Simulations — •Vahid Fadaei Naeini[1,2], Andreas Larsson[1], and Roland Larsson[2] — [1]Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden. — [2]Machine Elements, Division of Machine Elements, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden.

This study explores the tribochemical behavior of glycerol and its aqueous solutions confined between ferrous surfaces using reactive non-equilibrium molecular dynamics simulations. Results show that glycerol reduces friction effectively, with viscosity decreasing as water content increases. Pure glycerol achieves lower friction but exhibits significant wall slip and deviations from a linear velocity profile near the surfaces. Glycerol dissociation, influenced by shear stress and pressure, produces water and organic acid by-products, with dissociation rates decreasing at higher water concentrations. Atomic-scale analysis reveals increased surface wear and iron atom dissociation under elevated stresses. These findings highlight the balance between friction reduction, viscosity, and tribochemical reactivity in glycerol-water mixtures, offering insights for sustainable lubricant design under extreme conditions.

CPP 15.30 Mon 19:00 P4

Evaluating the Properties of Nafion PEMFC Membrane via MD Simulations — •Mateja Jovanović[1], Matthias Baldofski[1], Igor Stanković[2], Marcin Rybicki[1], and Miljan Dašić[2] — [1]Freudenberg Technology Innovation SE & Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Understanding the nanoscale interactions within Nafion membranes is crucial for optimizing their performance in Proton Exchange Membrane Fuel Cells (PEMFC). In present a molecular dynamics study of the structural and dynamic properties of Nafion-water systems under varying hydration levels using molecular dynamics simulations. The density of the Nafion-water system is examined to identify deviations from the ideal additivity rule, providing insights into molecular interactions and structural rearrangements. The radial pair distribution function, radius of gyration, pore-water contact surface, and diffusion coefficients for water and hydronium ions are analyzed to reveal the local organization, solvation quality, porosity, and transport properties within the hydrated Nafion membrane. The methodology used to obtain properties of the Nafion-water mixture builds on techniques previously developed for the study of ionic liquids [1].

[1] I. Stanković, M. Dašić, M. Jovanović, A. Martini, Langmuir 2024, 40(17), 9049-9058, doi:10.1021/acs.langmuir.4c00372

CPP 15.31 Mon 19:00 P4

Exploring Polymer Aging: Microscopy and Thermal Analysis — •Judith Bünte, Laila Bondzio, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld

The analysis of polymers and their additives is essential for understanding material performance and longevity, particularly in the context of aging processes. This work emphasizes the synergistic application of advanced microscopy and thermal analysis techniques to investigate polymer composition, structure, and degradation behavior.

Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) were utilized to visualize the microstructural features of polymer matrices, as well as the distribution of particles within the polymer. TEM offered high-resolution imaging to reveal morphological details, while SEM enabled surface characterization. These imaging techniques were further augmented by Differential Scanning Calorimetry to analyze thermal properties.

Polymer aging was studied under controlled conditions to evaluate structural and compositional degradation over time. Changes in microstructure and thermal properties were correlated with aging-related alterations.

The integration of these analytical techniques establishes a robust framework for characterizing polymers and their additives. This approach yields valuable insights into the stabilizing role of additives, such as TiO_2, in protecting polymers against environmental and thermal stressors.

CPP 15.32 Mon 19:00 P4

Atomistic simulations of PEDOT:PSS — •Richard Schömig[1,2], Annalena Riffelt[2], and Alexander Schlaich[1] — [1]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Hamburg — [2]SC SimTech, University of Stuttgart, Stuttgart

PEDOT:PSS is by far the best known conjugated polymer with a broad application in e.g. bioelectronics, energy storing devices or neuromorphic computing due to its electrolyte-dependent swelling behavior and extraordinary conductance in the doped (oxidized) state. However, the insolubility of its films once their dried hinders classic experimental studies, thus making molecular dynamics simulations an indispensable tool to understand its electronic and mechanical behavior on an atomic scale. Here, we employ different established force fields to study the influence of a set of parameters such as different water models, dissociation degrees, partial charges and simulation protocols on the structural changes and polymer physics by water uptake for both the PEDOT and the PSS part. We test the validity of these force fields by benchmarking them against ab-initio MD and experimental results.

CPP 15.33 Mon 19:00 P4

Analysis of the Reciprocity Theorem in the DWBA — •Reinhard Sigel — Independent Scientist, D-88677 Markdorf, Germany

The Distorted Wave Born Approximation (DWBA) is a favored theory among X-ray scientists for the analysis of interface scattering experiments [1,2]. Unfortunately, there is no proper clarification which X-ray specific aspects and approximations enter the DWBA and what is the difference to interface scattering of coherent visible laser light. Based on the differing refractive index approaches for X-rays and for visible light, we identify the spot where an X-ray specific equation enters the derivation [1] of the so-called reciprocity theorem. It involves an intermixing of microscopic and macroscopic Maxwell equations. A much simpler correct derivation valid for both wavelength ranges is discussed.

[1] Daillant, Gibaud, *X-ray and Neutron Reflectivity*, Springer 2009.
[2] Renaud, Lazzari, Leroy, Surf. Sci. Reports 64, 255–380 (2009).

CPP 15.34 Mon 19:00 P4

Dynamic Polarization and Electrostriction of PVDF-Based Copolymer Films as Measured with Double-Modulated Interferometry — Marvin Malchau[1], Philipp Ramming[2], and •Lothar Kador[1] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — [2]University of Bayreuth, Experimental Physics II, 95440 Bayreuth, Germany

Thin films of a ferroelectric copolymer based on polyvinylidene fluoride (PVDF) were exposed to electric ac fields with amplitudes up to 115 MV/m and frequencies between 5 and 100 Hz. The electrical polarization of the material was calculated by integrating the current flow, and the electric-field-induced thickness change (electrostriction) was measured with double-modulated interferometry. Thickness changes up to 60 nm were observed in an 8 μm thick film. The polarization shows a hysteresis loop typical for ferroelectric materials; it is independent of frequency in the investigated frequency range. The electrostriction exhibits a different type of hysteresis with strong frequency dependence. This indicates that the mechanical relaxation of the polymer film is independent of the electric dipole orientation.

CPP 15.35 Mon 19:00 P4

Ternary Organic Solar Cells For Space Applications — •Ivonne A. Zitzmann, Lukas V. Spanier, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

It has been demonstrated that organic solar cells (OSC) are capable of achieving high gravimetric power density, making them suitable for space applications. However, they still exhibit insufficient long-term stability, and there are few studies on their performance under space-like conditions. Here we investigate the ternary OSC system PBDB-T-2F:BTP-eC9:$PC_{71}BM$ by optimizing its efficiency and studying its structure and degradation by optical measurements and grazing incidence wide and small angle X-ray scattering. Space conditions were simulated with AM0 illumination. Further, the OSCs were exposed to temperature cycling to assess their stability in a space environment, subject to rapidly changing temperatures. In addition, data from a suborbital rocket flight was examined for performance and degradation of the solar cells. These results may allow for the furthering of our understanding of photovoltaic power generation in harsh environments.

CPP 15.36 Mon 19:00 P4

Degradation of Printed Organic Solar Cells at High Temperatures — •Christoph G. Lindenmeir[1], Simon A. Wegener[1], Christopher R. Everett[1], Julian E. Heger[1], Sigrid Bernstroff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Elettra, 34149 Basovizza, Trieste, Italy

Organic solar cells (OSCs) have gained significant attention recently due to their non-toxicity, short energy payback times, and fast efficiency improvements. Their high absorbance, potentially flexible design, and easy solution-based manufacturing make them particularly promising. Especially slot-die printing, a fast and low-waste fabrication method, enhances their scalability and potential for various applications, including space use. OSCs are particularly suited for space as their thin, lightweight structure provides a higher power-to-weight ratio than traditionally used solar cells, lowering production and launch costs. However, space conditions like extreme temperatures, high vacuum, and radiation accelerate degradation. This study focuses on the impact of extreme temperature variations on printed OSCs. We optimized their printing process and analyzed their degradation using operando grazing incidence small-angle X-ray scattering (GISAXS), a nondestructive method for studying thin-film morphology. Additionally, we monitored their electrical performance under high vacuum to simulate space conditions.

CPP 15.37 Mon 19:00 P4

Modulate Pre-aggregation to Optimize the Morphology in Organic Solar Cells — •Tim Bohnen, Jinsheng Zhang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Morphology optimization has emerged as a key strategy to effectively improve device performance and stability in organic solar cells. Due to the solution-processing method, the selection of solvents for precursor solutions is crucial, as it directly affects the ultimate the morphology of active layer. Recent research demonstrates that donor and acceptor molecules form aggregates of varying sizes in precursor solutions, subsequently inducing different phase separation and crystallization behavior during drying process. However, the detailed correlation between pre-aggregation behavior and final morphology has yet to be fully elucidated. In this study, the active layer is composed of PBDB-TF-TTz acting as the donor and BTP-4F-24 as the non-fullerene acceptor. Next, we characterize the resulting morphology using atomic force microscopy (AFM) and grazing incidence small- and wide-angle X-ray scattering (GIWAXS and GISAXS).

CPP 15.38 Mon 19:00 P4

Investigation of quenching in exciplex OLEDs under variation of the giant surface potential — •Clarisse Henriques, Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Institut für Physik, University of Augsburg, Augsburg, Germany

An exciplex is a short-lived excited charge transfer state formed between donor and acceptor molecules of different species, in which under radiative decay a photon is emitted. They can either function as efficient host for emitters or directly as emitter because of their apparent thermally activated delayed fluorescence characteristics. Especially the electron accepting materials tend to show a macroscopic film polarization, which is also referred to as giant surface potential (GSP). The presence of GSP in an organic light emitting diode (OLED) promotes charge injection in the electron transport layer (ETL), but causes the accumulation of holes, which can result in exciton quenching. Consequently, studying the impact on the device is of crucial importance. The main interest lies now on the tunability of this parameter by using the material as a co-host or directly as emitter. We investigate OLEDs with different film thickness of the ETL and emission layer. Additionally, devices of donor and acceptor with different mixing ratios were prepared. The major focus is now on studying these systems by current density-voltage-luminance, photoluminescence (PL) and electroluminescence spectra, impedance spectroscopy and their PL quenching under different bias voltages. Such studies are fundamental to understand the impact of SOP in OLEDs for further improvement.

CPP 15.39 Mon 19:00 P4

Tracking degradation of non-fullerene organic solar cells under dynamic environmental conditions — •Lixing Li, Lukas Spanier, Zhaonan Jin, Linus Huber, Guangjiu Pan, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The power conversion efficiency (PCE) of non-fullerene organic solar cells (OSCs) has already approached 20%, but stability and environmental degradation issues have always been one of the biggest challenges limiting their application. Considerable research has been conducted to understand the degradation mechanisms in OSCs, especially under extreme environmental conditions like high and low temperatures. While these studies offer valuable insights, they do not fully represent the dynamic conditions that most organic solar cells face in real-world environments. In practical scenarios, environmental factors such as temperature, humidity, and light fluctuate over time rather than remaining constant. Therefore, it is crucial to investigate how OSCs degrade not only under steady stress but also when exposed to varying environmental conditions. This study explores the degradation of BTP-4F non-fullerene organic solar cells subjected to multiple environmental cycles. Advanced characterization methods, including grazing-incidence X-ray scattering (GIXS) and atomic force microscopy (AFM), are used to monitor both in-situ and ex-situ structural changes in the active layer of OSCs, offering deeper insights into the underlying degradation mechanisms.

CPP 15.40 Mon 19:00 P4

Revealing the Effect of Solvent Vapor Annealing on the Morphology of Non-Fullerene Organic Solar Cells — •Liansong Chu — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Solvent vapor annealing (SVA), as an effective post-treatment technique, has been widely used to optimize the morphology in organic solar cells (OSCs). When exposed to the specific solvent atmosphere, the swelling effect induced by solvent vapor facilitates molecular mobility of both donor and acceptor molecules, leading to modifications in crystallinity and phase separation. Hence, the selection of solvent and annealing duration for SVA is critical for the morphology, which ultimately determines the power conversion efficiency and stability. However, fundamental understanding of solvent selection criteria and the associated kinetic processes during treatment remains unknown. In this work, we systemically investigates the impact of different solvents for SVA on the morphological properties of non-fullerene OSCs (PBDB-TF-TTz as the donor and BTP-4F-24 as the acceptor) using atomic force microscopy (AFM), grazing incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS). Furthermore, we provide real-time insights into the morphological evolution during SVA through in situ UV-Vis absorption spectroscopy and photoluminescence measurements.

CPP 15.41 Mon 19:00 P4

Impact of the electrode area on the local J-V curves of organic photovoltaics — •Paul Schwanitz[1], Fabian Eller[1], Carsten Deibel[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Organic photovoltaics (OPV) are promising candidates for flexible solar cells, which may be more cost efficient to produce than their silicon counterparts. The organic semiconductor materials can be dissolved and printed on large scale, with the attractive advantage that the geometry of the OPV devices can be chosen on demand. The aim here is to analyze the influence of the top and bottom size of the electrodes on the J-V curve measurements. If the active areas are too small, fluctuations in the performance can occur, which are caused by inhomogeneities in the film. As the active area increases, performance is expected to stabilize as it is averaged over a larger area [1]. The different sizes of the anode and cathode also enable in-line measurements during production. The sizes of the electrodes are systematically varied to estimate the influence on the measurements, to interpret the J-V curves correctly and to account for the dark currents.

[1] Herzig, E. M., Gao, F., Bergqvist, J., Loi, M. A., & Meier, S. B. Harmonizing organic photovoltaics research and development among academia and industry. Joule, 8, 2171 (2024). https://doi.org/10.1016/j.joule.2024.07.015

CPP 15.42 Mon 19:00 P4

Thin Films of Substituted Benzo[*b*]fluorenes as Emitting Layers for Blue OLED Devices — •Pascal Schweitzer[1], Christopher M. Leonhardt[2], Cazibe Arslan[1], Hermann A. Wegner[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic light emitting diodes (OLED), despite widespread application in displays, still exhibit major challenges: The search for stable and efficient blue-emitting molecules continues, as these often suffer from degradation. Here we study substituted benzo[*b*]fluorenes (BF) as an alternative for such emitters. Their modular structure allows for tuning opto-electronic properties. Thin films of different BF were prepared by solution-based methods or physical vapor deposition (PVD). Significant blue emission was found by photoluminescence spectroscopy in solid state. Film growth at device interfaces was studied. In-situ Kelvin-probe force microscopy (KPFM) gave insight into electrical contact formation to typical transport materials: Stranski-Krastanov growth was found in PVD onto hole-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), accompanied by the formation of an interface dipole. On the electron-conducting side, a pronounced Volmer-Weber growth of bathocuproine (BCP) on the emissive layer demands a high film thickness for pin-hole-free contacts. Finally, based on these findings, we show a working prototype of a blue OLED based on a substituted BF.

CPP 15.43 Mon 19:00 P4

Excimer as intermediate in singlet fission process for Polydiketopyrrollopyrrole based materials — •Sruthy Asa Rajan, Sergey Bagnich, and Anna Köhler — University of Bayreuth, Bayreuth, Germany

Photovoltaics are essential for renewable energy generation, but the efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which arises from fundamental and practical losses such as thermalisation loss. Singlet fission (SF), a carrier multiplication process, offers a promising pathway to surpass this efficiency limit. However, a key challenge lies in identifying SF molecules with triplet energy levels that align with the silicon band gap, enabling the efficient formation of correlated triplet pairs, 1(TT) and their subsequent separation into individual triplets.

Polydiketopyrrollopyrrole (PDPP) is a molecule with a comparable triplet energy to the silicon bandgap. We investigate the influence of solvent properties on the optical behaviour of N-substituted pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-substituted pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the evolution of different species. We observe excimer emission at intermediate temperature and 1(TT) emission at lower temperature. This observation supports the notion that excimers are involved in the formation of 1(TT).

CPP 15.44 Mon 19:00 P4

Solution processed organic solar cells for agrivoltaic applications — •Sebastian Coen, Yunan Chen, Kerstin Märkle, and Christian Sprau — Karlsruhe Institute of Technology, Light Technology Institute

Organic solar cells (OSCs) offer a wide range of applications due to their light weight, low energy payback time, non-toxicity and mechanical flexibility. This work aims to expand these applications by fabricating semitransparent OSCs for agricultural photovoltaic applications, such as greenhouses and foil tunnels.

To facilitate future industrial production, we explore scalable processes and a fully solution-processed architecture based on non-halogenated solvents. The fabricated solar cells are studied in terms of their electrical and spectral properties and their real space morphology.

CPP 15.45 Mon 19:00 P4

Utilizing Ultrasonic Spray for the Integration of Organic Solar Cells on Cellulose Substrate — •Xinyu Jiang[1], Kang An[2], Qin Wang[2], Nadja Koelpin[1], Arik Willner[1], Ning Li[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [2]Institute of PolymerOptoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology (SCUT), Guangzhou, Guangdong 510641, China — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Cellulose nanofibrils, heralded for their eco-friendly and renewable nature, offer a significant stride toward sustainable energy solutions. Their advantageous attributes such as biocompatibility, flexibility, lightweight nature, transparency, and remarkable mechanical strength render them suitable as a base material for incorporating photovoltaic or electronic devices. We aim to explore the development of functional photovoltaics on transparent cellulose-fabricated curtains, aiming at transforming undesired sunlight into electricity. The inherent flexibility of curtains poses a fabrication challenge for solar cells, adeptly mitigated through ultrasonic spray deposition. This technique manifests as an efficacious means to engender functional layers on a large scale, ensuring a homogeneous surface with minimal roughness. Employing an advanced non-fullerene acceptor system, the resultant organic solar cell curtain showcases the promising performance, delineating a path toward substantial applications in the sustainable energy.

CPP 15.46 Mon 19:00 P4

Multiscale morphological modulation in spray-coated organic solar cells — •Shuxian Xiong[1,2], Benedikt Sochor[1], Constantin Harder[1,2], Sarathlal Koyiloth Vayalil[1], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden

The balance between phase separation and crystallization arising from the aggregations of organic semiconductor molecules defines the film morphology, resulting in multi-length scale phase transitions that enhance device performance. We investigate the morphological evolution driven by molecular self-assembly during the ultrasonic spray-coating of organic functional layers in organic solar cells. An in-depth understanding of phase transition phenomena through an analysis of both temporal (film formation kinetics) and thermal scales (annealing), with the elucidation of the intricate structure-performance nexus linked to morphological evolution and device efficiency, is achieved. We clarify the principles of effective morphological optimization to achieve high-efficiency sprayed organic solar cells, providing valuable guidance for their commercial application.

CPP 15.47 Mon 19:00 P4

Impact of amphiphilic additives on organic solar cells: Enhancing thermal stability for long term performance — •Jose Prince Madalaimuthu[1,2], Tim Matzdorff[1,2], Zhuo Xu[1,2], Md. Moidul Islam[1,2], Yisak Tsegezab Gerase[3], Hassan Ismail[1,2], Rico Meitzner[4], Aman Anand[1,2], Martin Presselt[3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany — [4]Helmholtz-Zentrum Berlin GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The stability of organic solar cells (OSCs) depends not only on the device architecture or effective sealing but also significantly on the morphological stability of the photoactive layer. This stability can be disrupted by alterations in the spatial arrangement of the electron donor and acceptor, which are the fundamental components of OSCs. The extent of phase separation between donor and acceptor regions within the bulk heterojunction (BHJ) plays a pivotal role in determining device performance. Consequently, various strategies have been explored to preserve the distribution of these components. One promising approach is the incorporation of amphiphilic molecules to enhance the stability of the donor-acceptor interface. This method improves thermal resilience, overall OSC performance, and mitigates morphological degradation.

CPP 15.48 Mon 19:00 P4

Interfacial encapsulation of organic solar cells — •Saib Jahan Qazi[1,2], Md Moidul Islam[1,2], Zhou Xu[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany

Organic solar cells are emerging as promising prospects in the field of solar energy technology due to their low-cost, light-weight and simple roll to roll fabrication properties. A record power conversion efficiency above 19% has already been reported. However, long-term stability is still the main obstacle for commercialization of these devices. In this study, we demonstrate solution processed interlayer encapsulation of organic solar cells using polymer-based barriers to prevent interlayer migration of impurities as well as the ingress of oxygen and moisture.

CPP 15.49 Mon 19:00 P4

Modifying spacers for higher efficiency and stability of single-component organic solar cells — •Yakun He[1], Peter Baeuerle[2], Weiwei Li[3], Christoph Brabec[4], and Frederic Laquai[1,5] — [1]King Abdullah University of Science and Technology, Saudi Arabia — [2]University of Ulm, Germany — [3]Beijing University of Chemical Technology, China — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [5]Ludwig-Maximilians-Universität München, Munich, Germany.

Organic solar cells have achieved 20% efficiencies yet still lag regarding stability. Single-component materials incorporating donor and acceptor moieties in a nonconjugated method exhibit intrinsically high stability because of the restriction of morphological evolution. Nevertheless, the efficiency of single-component organic solar cells (SCOSCs) is still low compared to bulk heterojunction structures. We employ a series of dyads with similar structures but modify their spacer type and lengths to investigate the structure-morphology-performance relation. Photophysics has been studied by using steady-state and transient absorption and photoluminescence. Dyad4, with a proper long spacer, has shown the highest efficiency and surprisingly high stability under illumination. Moreover, we investigated the thermal stability of double-cable polymers by tuning the linker length between donor and acceptor moieties. Surprisingly, double-cable polymers do not show a decline of stability with the increase of space linker, and all of them display remarkably excellent stability without degradation after heating for 1000 hours at 90 degree.

CPP 15.50 Mon 19:00 P4

Photoinduced charge transfer and photophysics of functionalized Diethienopyrrole molecules from first principles — •Jannik Theile, Caterina Cocchi, and Michele Guerrini — Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, D-26129 Oldenburg, Germany

Donor-acceptor compounds are key components in organic electronics due to their tunable electronic and optical properties. In this work based on time-dependent density functional theory, we examine diethienopyrrole molecules, which act as electron donors, covalently combined with electron-acceptor units, focusing on their charge transfer dynamics induced by femtosecond laser excitations.

In the current symmetric molecule configuration, we find strong fluctuation patterns of the charge after laser excitation across both intensities and with and without nuclear motion, exceeding the initial changes of charge induced by laser excitation and the charge transfer (CT) remains insufficient and inconsistent throughout time evolution. Further considerations include asymmetric molecule configuration.

CPP 15.51 Mon 19:00 P4

Direct stochastic optical reconstruction microscopy (dSTORM) on cationic copolymer microgels — •Evelyn Gettinger and Thomas Hellweg — Physical & Biophysical Chemistry, University Bielefeld, Bielefeld, Germany

Microgels, three-dimensional polymer networks with colloidal dimensions, are promising candidates for catalysis, sensory and drug delivery applications due to their responsive properties. Cationic copolymer microgels, in particular, are gaining increasing attention in research, as they are suitable for conjugation with biomolecules like peptides, antibodies, and nucleic acids. Poly(NNPAM-co-DAPMA) is one such microgel that exhibits thermoresponsiveness through the monomer N-n-propylacrylamide (NNPAM) and pH responsiveness through the cationic comonomer N-3-(dimethylamino)propylmethacrylamide (DAPMA). This study investigates the network structure of Poly(NNPAM-co-DAPMA) microgels using direct stochastic optical reconstruction microscopy (dSTORM), a high-resolution fluorescence technique. Microgels with varying DAPMA concentrations were synthesized and analyzed for swelling behavior and polydispersity using photon correlation spectroscopy (PCS). Morphological properties were examined with atomic force microscopy (AFM). Post-synthetic fluorescence labeling with the anionic dye DY-654-carboxylic acid revealed a gradient of fluorophore localization from the core to the periphery and concentrated fluorophore domains, indicating a heterogeneous network with random comonomer distribution.

CPP 15.52 Mon 19:00 P4

Volume phase transition of NIPAM based copolymer microgels with non-thermoresponsive comonomers — •Jannis Krüger and Thomas Hellweg — Physical and Biophysical Chemistry, Bielefeld University

We conducted photon correlation spectroscopy (PCS) to obtain swelling curves of *N*-isopropylacrylamide (NIPAM)-based copolymer-microgels with varying content of non-thermoresponsive *N*-tert-butylacrylamide (NtBAM). Increasing NtBAM content reduces the hydrodynamic radius and broadens the volume phase transition (VPT). We analyzed the thermoresponsive contribution to the swelling curves with a cooperative Hill-like model for the Flory-Huggins interaction parameter $\chi_{\mathrm{Hill}}(T)$ [1]. This model effectively describes the microgel swelling at various compositions. The Hill parameter ν estimates the number of water molecules leaving a polymer segment at the phase transition. A linear decrease of ν with BIS content suggests that water stays adsorbed on BIS during the VPT due to the lack of an LCST [2]. We fitted PNIPAM-*co*-NtBAM microgel swelling curves [3] with a hybrid model of χ_{Hill} for NIPAM and the original Flory-Huggins parameter χ_{FH} for NtBAM, revealing an exponential decrease in ν with x_{NtBAM}, indicating that NtBAM inhibits water adsorption of neighboring NIPAM units. Based on these results we propose a steric mechanism, which qualitatively describes the observed inhibition of microgel hydration.

[1] D. C. Leite et al., Langmuir 34 (2018), 10943. [2] S. Friesen et al., Gels 7 (2021), 42. [3] J. Krüger et al., Colloid Polym. Sci. (2024).

CPP 15.53 Mon 19:00 P4

Amphiphilic Monomers Bridge Hydrophobic Polymers and Water — •Guido Kusters[1,2,3], Guogao Zhang[1,4], Zheqi Chen[1,5], and Zhigang Suo[1] — [1]Harvard University — [2]Eindhoven University of Technology — [3]Max Planck Institute for Dynamics and Self-Organization — [4]Xi'an Jiaotong University — [5]Zhejiang University

Water dissolves a hydrophilic polymer but not a hydrophobic polymer. However, many hydrophilic polymer monomers are amphiphilic, with a hydrophobic vinyl group for radical polymerization and a hydrophilic group, and so may form solutions with both water and hydrophobic polymers. Ternary mixtures of amphiphilic monomers, hydrophobic polymers, and water have recently been used as precursors for interpenetrating polymer networks with unusual properties. However, the phase behavior of such ternary mixtures has not been studied. Here we mix the amphiphilic monomer acrylic acid, the hydrophobic polymer

poly(methyl methacrylate) and water. In the mixture, the hydrophobic polymer can form various morphologies, including solution, micelle, gel, and polymer glass. We interpret these findings by proposing that the hydrophobic and hydrophilic groups of the amphiphilic monomer enable it to function as a bridge. That is, the hydrophobic functional group binds to the hydrophobic polymer, and the hydrophilic functional group binds to water. This picture leads to a simple modification to the Flory-Huggins theory, which agrees well with our experimental data. Amphiphilic monomers offer a rich area for the development of materials of self-assembled structures with unusual properties.

CPP 15.54 Mon 19:00 P4

Mechanical Characterization of Epon 862/DETDA Epoxy Networks: Molecular Dynamics Simulations — •Djihed Rezzig[1,3], Wolfgang Verestek[2], Saad Abdeslam[1], Johannes Roth[3], and Siegfried Schmauder[2] — [1]LPMMM, Setif 1 University- Ferhat ABBAS, Algeria — [2]IMWF, Stuttgart University, Germany — [3]FMQ, Stuttgart University, Germany

Epoxy resins are widely used in advanced materials due to their exceptional mechanical properties. Among them, Epon 862/DETDA is a commonly employed thermoset system in aerospace and automotive applications. This study employs molecular dynamics simulations to investigate the mechanical behavior of the Epon 862/DETDA epoxy network. The simulations were conducted using cross-linked molecular models to represent the cured network, incorporating detailed atomic scale interactions. Mechanical behavior was evaluated by simulating stress-strain responses under tensile loading conditions and shear test for the elasticity tensor, revealing the epoxy networks high modulus and strength. Additionally, the study examines the effects of varying cross-link densities and molecular configurations on the materials performance.

CPP 15.55 Mon 19:00 P4

The effect of intracrystalline chain dynamics (ICD) in the stress relaxation of semi-crystalline polymers — •Tonghua Liu, Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Von-Danckelmann-Platz 3, 06120, Halle(Saale)

The intracrystalline chain dynamics (ICD) plays a significant role in semicrystalline polymers (SC), influencing not only the polymer crystallization and morphology but also the stability of crystals and the mechanical properties, such as drawability. Here we investigate how the ICD affects the stress relaxation of SC polymers.

Plane-strain compression test is used to study the relaxation behavior after yielding point. For crystal-fixed polymers like polycaprolactone (PCL), where ICD is absent or significantly hindered, only one relaxation process is observed. In contrast, crystal-mobile polymers like high density polyethylene (HDPE) exhibit two distinct relaxation processes, which can be attributed to the additional mobility within the crystals. The two relaxation processes in HDPE demonstrate markedly distinct time scales. The faster relaxation process is observed to relax faster with increasing temperature, whereas the slower relaxation process remains unaltered within the chosen temperature range.

CPP 15.56 Mon 19:00 P4

The effect of the intracrystalline chain diffusion on the non-linear mechanical behavior of semicrystalline polymers — •Rose Mary Michell, Albrecht Petzold, and Thomas Thurn-Albrecht — Martin Luther University Halle Wittenberg, Institute of Physics, D-06099 Halle, Germany.

This work studies the influence of intracrystalline chain diffusion (ICD) on the mechanical properties of semicrystalline polymers by comparing PEO with fast ICD and PCL with slow ICD. Mechanical tests were performed under plane strain compression at temperatures from -10 to 55 °C and true strain rates from 0.005 to 10 min^{-1}. At large deformations, the PCL always shows a strain hardening effect, while PEO shows softening when the rate decreases, temperature increases, and molecular weight decreases. The data corresponding to the strain hardening part, which describes the network forces, was fitted using the Gaussian model. The stress-strain curve for PCL showed higher stress than the Gaussian chain model predicted. In contrast, PEO had lower stress values; this difference could be attributed to an effect linked to chain mobility. For slow ICD, the crystals act as physical crosslinking points. Otherwise, the chains can be pulled from the crystals and soften the network. In conclusion, we found systematic differences in non-linear mechanical behavior between crystal-fixed and crystal-mobile polymers. This suggests that the competition between ICD and deformation determines the non-linear mechanical behavior at large deformations of semicrystalline polymers.

CPP 15.57 Mon 19:00 P4

Exploring the role of defects in polymer networks through simulations of 4-armed polymers — •Sayam Bandyopadhyay[1,2], Sebastian Seiffert[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Germany — [3]Department of Chemistry, Johannes Gutenberg Universität Mainz, 55128 Mainz, Germany

We simulated polymer networks formed by coarse-grained tetra-PEG (tPEG) macromolecules to investigate the effects of (connectivity) defects on network dynamics. We modeled both homoleptic and heteroleptic systems, where we modeled non-covalent bonds between functionalized end groups using an inverted Gaussian potential to control valency. The network structure was quantified through the fraction of bonded end groups and the radial distribution functions of attractive beads. Polymer mobility was characterized by examining the mean square displacement of individual tPEG molecules after gelation. To explore the impact of defects, we systematically altered the defect density by incorporating tPEG chains with inert end groups in the homoleptic systems and by varying the stoichiometry in the heteroleptic mixtures. Additionally, we examined how the bending stiffness of the polymers influenced network structure and dynamics, finding a marked slowing down with increasing stiffness. These findings provide new insights into the factors governing the role of defects in the structure and dynamics of polymer networks.

CPP 15.58 Mon 19:00 P4

Silicone implementation to car industry — •Yury Ostretsov — Moscow, Russia, Bolshaya Semenovskaya 38

Silicone is a preferred material for manufacturing automotive hoses due to its high heat resistance, resistance to aggressive chemical environments, flexibility, and durability. These properties allow silicone hoses to maintain shape and performance under extreme temperatures and pressure fluctuations, reducing the risk of leaks or failures. Additionally, silicone is lightweight compared to rubber alternatives, contributing to overall vehicle efficiency. Its ability to withstand ozone and UV exposure also enhances longevity, making it a reliable choice for various automotive applications.

CPP 15.59 Mon 19:00 P4

Water flow decrease of track-etched polyethylene terephthalate membranes in filtration applications — •Ana Ambroz[1,2], Zhen Yao[2], Christopher Rojas[3], Polina Angelova[2], Irena Petrinic[1], and Armin Gölzhäuser[2] — [1]Univeristy of Maribor, Maribor, Slovenia — [2]University of Bielefeld, Bielefeld, Germany — [3]CNM Technologies GmbH, Bielefeld, Germany

Track-etched (TE) membranes, with their precise pore size, controlled porosity, and defined pore geometry, are industrially applied as highly sensitive and fast filters for bacteria in the food, cosmetic and pharmaceutical industries, as control barriers in glucose sensors, and as biomolecule selective barrier in implants. Additionally, they are being investigated for their potential in reverse and forward osmosis for water purification and cold concentration. However, their tendency to lose performance over time presents a significant challenge, particularly in high-throughput and durable applications. In this work, we evaluate the performance of track-etched polyethylene terephthalate (TE-PET) membranes as nano- and microfilters in low-pressure reverse osmosis (LPRO) and dead-end filtration systems. Monitoring water flux through the TE-PET membranes at different low pressures (0.02-10 bar) revealed a gradual decrease over time, varying with porosity and pore size. Specifically, membranes with low porosity (<1.5%) and small pore sizes (<1.5 um) exhibited a significant reduction in water flux. The decline is attributed to membrane swelling and the formation of a sol-gel film within the pores, with additional contributing factors discussed.

CPP 15.60 Mon 19:00 P4

Intermolecular bonds - connecting structure and dynamics — •Martin Tress[1], Friedrich Kremer[1], and Jan Philipp Gabriel[2] — [1]Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany — [2]Institute of Materials Physics in Space, German Aerospace Center, Köln, Germany

Descriptions of the glass transition often consider temperature dependent changes in the specific volume to explain the tremendous increase in relaxation time, and empricial data confirm the general role of thermal expansion [Nat Phys 19 (2023) 694]. However, since glassy dynamics happens on molecular scale, macroscopic thermal expansion might be too coarse. Here we use infrared spectroscopy data to extract inter-molecular hydrogen (H)-bond lengths in wide temperature ranges. For water, the H-bond expansion coefficient differs strongly from the macroscopic one, which is easily assigned to considerable structural reorganization in the water network [JCP 160 (2024) 234502]. Their comparison reveals that the most compact molecular arrangement is formed in the range ~316-331 K (i.e. well above the density maximum). This coincides with several pressure-related anomalies which confirms this characteristic point in the supra-molecular arrangement. These results confirm our earlier approach to deduce inter-molecular H-bond lengths in polyalcohols [JCP 154 (2021) 024503] and open a new alley to investigate the role of inter-molecular expansion as a precursor to structural relaxation on a bond-specific level.

CPP 15.61 Mon 19:00 P4

Single-molecule spectroscopy of organic laser gain media — •Janne Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Since the first experiments on pentacene [1], single-molecule spectroscopy has been performed for applications ranging from cell biology and medicine to organic laser media and single-photon emission [2]. To design and use these spe-

cialized molecules, their photophysical properties have to be investigated. Here, we perform single-molecule spectroscopy to study organic laser gain media. To isolate single molecules, we dilute the organic material down to concentrations of the order of nmol/L with ultra-pure solvents and measure characteristic fluorescence lifetimes and spectra.

[1] W. E. Moerner and L. Kador, Physical Review Letters, 62, 2535. (1989)
[2] H. Miller et al, Rep. Prog. Phys. 81 024601 (2018)

CPP 15.62 Mon 19:00 P4

XPS study of redox mechanism in $Na_{2.5-x}Fe_{1.75}(SO_4)_3$ cathode material for high-voltage sodium-ion batteries — •Neama Imam[1], Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], Ehrenfried Zschech[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of $Na_{2.5-x}Fe_{1.75}(SO_4)_3$, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ~3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. $Fe2p_{3/2}$ spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe^{2+} to Fe^{3+} during battery charging while transitioning from its pristine state ($x = 0$) with the presence of only Fe^{2+} at the cathode surface to the highest sodium deintercalation level ($x = 1.61$). This result is consistent with the electrochemical analysis.

CPP 15.63 Mon 19:00 P4

Multiscale dynamics simulations of amorphous polyethylene terephthalate — •Andoni Ugartemendia[1], Alessandro Mossa[2], and Giorgia Brancolini[3] — [1]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [2]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy — [3]Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

In the last decades, multiwall polymers have become widely used in food packaging due to their excellent mechanical and barrier properties. Unfortunately, the recycling of these materials is difficult and costly, leading to environmental problems. An understanding of the polymers properties is crucial towards the development of new recycling technologies. However, their computational modeling poses a great challenge since the dynamics span over several time scales. As a result, a multiscale approach becomes mandatory to gain access to the slower degrees of freedom. In this regard, coarse grained (CG) models have drawn considerable attention recently. CG models neglect the fastest degrees of freedom, flattening the rugged potential and thus, allowing higher time steps. In this work, we adopt a multiscale protocol to characterize several properties of polyethylene terephthalate (PET). First, atomistic molecular dynamics (MD) simulations are performed for amorphous PET systems with varying chain lengths. Then, the atomistic data is employed to derive a CG force field based on the iterative Boltzmann inversion (IBI). Finally, the structural data obtained with atomistic and CG simulaions are compared.

CPP 15.64 Mon 19:00 P4

Fourth-Generation High-Dimensional Neural Network Po- tentials for Molecular Chemistry in Solution — •Djamil Abdelkader Adel Maouene[1,2], Moritz Richard Schäffer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department Physik, Universität Basel, Switzerland

Machine learning has become a powerful tool in chemistry and materials science, as high-dimensional neural network potentials (HDNNPs) provide accurate representations of multidimensional potential energy surfaces for atomistic simulations. In this study, we compare the performance of two types of HDNNPs; 2G-HDNNPs and 4G-HDNNPs, in modeling organic molecules in aqueous solution. While 2G-HDNNPs have proven effective in many systems in capturing local interactions based on atomic environments, they fail in scenarios where long-range charge transfer plays a critical role. These cases are better addressed by 4G-HDNNPs, which take into account atomic charge variations caused by structural or electronic changes even at distant regions in the system. Both methods are demonstrated using a model organic molecule.

CPP 15.65 Mon 19:00 P4

Insights into Machine Learning Interatomic Potentials for simple analytical model systems — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

During the past 10 years Machine Learning interatomic potentials (MLIP) have gained popularity for Molecular Dynamics simulations with quantum chemical accuracy. Although it is a rapidly evolving field, many questions remain open. These include issues of interpretability, modeling different interaction types and how to select training data properly. MLIPs are rarely applied to simple model systems, for which the interactions of particles can be described analytically, to investigate these questions. Instead, MLIPs are mostly applied directly to realistic molecular systems for which the ground truth interactions must be approximated by methods like Density Functional Theory. By training an Atomic Cluster Expansion as a systematic and generally interpretable model for a Lennard-Jones model system, we aim to study how interaction types, system size and temperature affect the learned model in a systematic manner. The obtained interactions can be directly compared to the known true analytical interactions. Moreover, we fit a MLIP for an amorphous silica system to study structure and dynamics in a glass-forming system, where low-energy states are important. The question emerges, how to select the training data best and if such low-energy (low temperature) states must be explicitly included in it or if the MLIP is able to extrapolate from high-energy (high temperature) states to low energy states.

CPP 15.66 Mon 19:00 P4

Efficient Millisecond Timescale Modeling of Hydroxide Ion Dynamics in Aqueous Systems: A Multiscale Simulation Approach — •Jonas Hänseroth[1,2], Daniel Sebastiani[2], and Christian Dressler[1] — [1]Theoretical Solid State Physics, Institute of Physics, Ilmenau Universitiy of Technology, Ilmenau, Germany — [2]Theoretical Chemistry, Institute of Chemistry, Martin-Luther-University of Halle-Wittenberg, Halle (Saale), Germany

An adapted combined Molecular Dynamics/Lattice Monte Carlo (cMD/LMC) approach models hydroxide ion transport across extended systems and millisecond timescales.[1] The method surpasses classical Molecular Dynamics in efficiency while maintaining the accuracy of ab initio Molecular Dynamics, allowing the study of aqueous potassium hydroxide systems over a wide concentration range (3-61 wt.-%). The cMD/LMC algorithm allows simulations involving thousands of atoms at low computational cost, yielding diffusion coefficients consistent with ab initio benchmarks. This framework can provide insights into the dynamics of hydroxide ion in systems such as anion exchange membranes, which are essential for fuel cell technology. [1] J. Chem. Theory Comput. 2014, 10, 10, 4221-4228

CPP 15.67 Mon 19:00 P4

Confinement-induced dynamics in binary liquid mixtures: insights from molecular simulations — •Anam Sara, Pascal Merle, Siegfried Stapf, and Christian Dressler — Technische Universität Ilmenau, Germany

In this work, we investigate the behavior of binary liquid mixtures confined within silica nanopores, examining how confinement impacts the diffusion and relaxation properties of mixtures such as cyclohexane/acetone, cyclohexane/tetrahydrofuran (THF), water/acetone, and water/THF [1]. Experimental NMR measurements revealed deviations in diffusion coefficients and relaxation times of these mixture under confinement [2,3]. To interpret these observations, we perform molecular dynamics (MD) simulations to get atomistic insights into the structure and dynamics of these mixtures within the pores. Our primary objective is to characterize how confinement alters the microphase separation, component density distribution along the pore axis, and preferential interactions with pore walls.

[1] G. Guevara-Carrion, T. Janzen, Y. Muñoz-Muñoz, J.Vrabec, The Journal of Chemical Physics, 144, (2016).
[2] D. Bellaire, H. Kiepfer, K. Münnemann, H. Hasse, J. Chem. Eng.Data, 65, 793-803 (2020).
[3] Stapf, S., Siebert, N., Spalek, T., Hartmann, V., Gizatullin, B., and Mattea, C. (2023).

CPP 15.68 Mon 19:00 P4

Density of states in hard disks: Concentration dependency via SAMC simulation — Timur Shakirov[1,2], Malte Kautzsch[1], and •Viktor Ivanov[1] — [1]Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany — [2]Indivumed GmbH, Hamburg, Germany

We propose a new variant of SAMC sampling for determining the density of states as a function of the concentration of particles. The system is modelled as a set of dimensionless points, i.e., points with zero diameter. The minimal points separation, d_{min}, is chosen as the sampling parameter determining the macrostate. Thus, the density of states and the visiting histogram depend on the minimal distance d_{min} and are accumulated at each step of the algorithm according to the standard SAMC procedure. In a microstate (particular configuration of points' positions) with a given value of the minimal distance between points, d_{min}, one can replace the points with the hard disks of the diameter d_{min} (or less). This creates a system with a specific value of the concentration φ. We apply this algorithm for the two-dimensional system of hard disks to study its phase behaviour at different concentrations and compare the results with KTHNY theory and the previous simulations.

CPP 15.69 Mon 19:00 P4

Multiscale Simulation Framework for Functional Polymer Systems — •Steffen Kampmann[1], Alexander Croy[2], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden — [2]Chair of Theoretical Chemistry, Institute of Physical Chemistry, Friedrich Schiller University Jena — [3]Dresden Center for Computational Materials Science (DCMS)

Functional, mechanically resilient polymer and polymer-based nanocomposite films play an important role for strain gauges or organic light-emitting diode (OLED) displays [1-3]. The modelling and simulation workflow presented here enables the generation of disordered polymer systems and the linking of the mechanical and electronic properties from the atomistic to the microscopic size scale. Here, the focus is on the relationship between deformation and conductivity behavior. To calculate the multi-scale material behavior, we use density functional tight binding (DFTB) calculations, molecular dynamics simulations, and the finite element method. The in-situ processing, evaluation as well as the exchange of the generated data across simulation methods is performed using our Python framework. The multi-scale computational workflow indicated here represents a computationally efficient assessment of the properties of the polymer systems at different scales. [1] K. Grabowski, et al., Computational Materials Science, 135, 169*180, (2017) [2] R. Luo, et al., Progress in Organic Coatings, 162, 106593 (2022) [3] L. Liu, et al., Organic Electronics, 89, 106047 (2021)

CPP 15.70 Mon 19:00 P4

Investigation of electrolyte dynamics with interfaces: Insights from simple MD-models — •Katharina Kintrup[1,2], Youssef Mabrouk[1,2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Deutschland — [2]Helmholtz-Institut Münster, Corrensstraße 48, 48149 Münster, Deutschland

Molecular Dynamics (MD) simulations are a common tool to investigate transport properties of electrolytes. Typically, periodic boundary conditions (pbc) are applied to simulate energetically closed systems, which are contrary to experimental systems with interfaces. Electrophoretic NMR (eNMR) experiments show that the incompressibility is dominating the transport properties of electrolytes, leading to an application of local conservation of volume. [1] Inspired by this, we set up simplified models to simulate binary liquids, imitating ionic liquids (IL), within interfaces, resulting in energetically open systems. After applying external (electric) fields, various properties of the model systems such as average velocities, number densities, volume densities, etc. were evaluated. A transition from local conservation of momentum towards local conservation of volume was observed. The velocities of all systems portrayed oscillations due to sound waves. A general analysis of dynamic processes on different time scales for systems without explicit charges was achieved. A comparison between systems with and without explicit charges was conducted, proving the superiority of the advanced charged model due to higher incompressibility. [1] J. Phys. Chem. Lett, 2022, 13, 8761-8767

CPP 15.71 Mon 19:00 P4

Evidence for unusual solvation shell of aqueous Fe^{3+} at high dilution — •Amrita Goswami, Elvar Örn Jónsson, and Hannes Jónsson — Science Institute and Faculty of Physical Sciences, University of Iceland, VR-III, 107 Reykjavík, Iceland

Solvated Fe^{3+} in water is a particularly important system, relevant, for instance, for the widely studied charge transfer Fe3+/Fe2+. However, the solvation shell of such highly charged cations is still poorly understood, particularly at for concentrations less than 1 M. In this regime of high dilution, experimental data and high-level calculations are sparse. For instance, most density-functional theory calculations are performed at a concentration of 0.8 M or higher, with uniform background charge. Simulations for such dilute solutions can provide insight inaccessible to other techniques. Using extensive molecular dynamics simulations with empirical potentials and DFT geometry optimizations of selected configurations, we study the effect of solution concentration on the solvation structure of aqueous Fe^{3+}. The solvation shell is found to undergo abrupt transitions between two states: an octahedral (OH) state with 6-fold coordination, and a metastable capped trigonal prism (CTP) state with 7-fold coordination. Further, we have developed a QM/MM (quantum-mechanical/molecular mechanical) method to study dilute solutions of aqueous Fe^{3+} with DFT-level accuracy, with a polarizable water model. References: Goswami et al., J. Phys. Chem. Lett., 2024

CPP 15.72 Mon 19:00 P4

Exploring Pathways of Supramolecular Self-Assembly at Liquid-Liquid Interfaces — •Mephin Philip Alamcheril[1], Friederike Schmid[1], and Shikha Dhiman[2] — [1]Institute for Physics, Johannes Gutenberg University Mainz — [2]Department of Chemistry, Johannes Gutenberg University Mainz

A self-assembly process usually occurs through thermodynamic pathways but the co-existence of different intermediates and diverse pathways of self-assembly have been observed. Liquid droplets are one such intermediate in many self-assembly processes, particularly in biological systems, which form through liquid-liquid phase separations (LLPS). Even though LLPS is a very well-known phenomena in polymer chemistry, only little is known about the possible role of LLPS in synthetic small molecule-based self-assembly.

In this project, we aim to study the possible mechanism of self-assembly at the surface of phase separated liquid droplets to explore the structure and dynamics at various stages of self-assembly and provide insights into how it can be controlled and manipulated for various applications. To that end, we develop a simple coarse-grained model for monomers in explicit solvent that self-assemble into fibers. The model is designed to represent BTA-like molecules in water. It is able to capture key characteristics of the experimental system such as the competition of fibril formation and liquid-liquid phase separation. We use it to examine the pathways of fibril formation from phase separated droplets.

CPP 15.73 Mon 19:00 P4

Isoconversional effect in epoxy polymerization process — •Sampanna Pahi[1], Christian Wick[1,2], and Ana Sunčana Smith[1,2,3] — [1]PULS Group, Institute for Theoretical Physics , FAU Erlangen-Nürnberg, Germany — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, Zagreb, Croatia — [3]Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany

Isoconversional methods are essential for understanding the kinetics and predicting thermodynamic data in epoxy polymerization. While these methods have been experimentally validated, their computational modeling remains underexplored. In this study, we use molecular dynamics (MD) simulations and Quantum Mechanics/Molecular Mechanics (QM/MM) transition state (TS) analyses to investigate mechanisms and energetic barriers in epoxy thermoset curing, focusing on isoconversional effects. We generated post-a-priori QMMM reactive sites with hydrogen-bonded systems to examine the influence of hydrogen bonding on the curing process. Initial results without hydrogen bonds showed higher activation energies than experimental values, with some outliers showing lower energies. Adding hydrogen bonds, especially hydroxyl (OH) bonds, reduced activation energies and explained these discrepancies. Radial distribution function (RDF) analyses showed OH bond formation is more likely than amine (NH) bonds, highlighting hydrogen bonding*s critical role in isoconversional effects during epoxy curing.

CPP 15.74 Mon 19:00 P4

A Multiscale MD-QM/MM Approach for Modeling Fracture Behavior in Epoxy Resins — •Barişcan Arican[1], Christian Wick[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen — [2]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute 10000 Zagreb, Croatia

Epoxy resins, with their exceptional mechanical properties, are indispensable in advanced engineering applications. However, understanding their fracture behavior at the molecular level remains a challenge. This study presents a multiscale framework that couples molecular dynamics (MD) simulations with quantum mechanics/molecular mechanics (QM/MM) calculations to analyze bond rupture and crack propagation in epoxy networks. The MD component monitors strain accumulation and identifies critical bond elongation thresholds indicative of imminent fracture. When these thresholds are met, the simulation transitions to QM/MM calculations, where bond breakage is determined dynamically by considering the surrounding chemical environment. This on-the-fly approach enables efficient and accurate modeling of fracture events and their impact on larger-scale material behavior, providing a foundation for future studies of epoxy resin failure mechanisms.

CPP 16: Energy Storage and Batteries I

Time: Tuesday 9:30–11:15 Location: H34

Invited Talk CPP 16.1 Tue 9:30 H34

Multifunctional structural batteries — •Göran Lindbergh — KTH Royal Institute of Technology, Stockholm, Sweden

A multifunctional lightweight material combines several functions in a single material entity able to simultaneously bear mechanical loads by acting as a carbon fibre composite component while providing one or more other functionalities at the same time, e.g. storing energy. In this work, we will show functionalities coming from alkali ion insertion in carbon fibres that goes beyond the battery function, and how these functions can be combined in a single device.

The starting point for these concepts is so called structural batteries, which

are multifunctional composite materials able to carry load while storing electrical energy like lithium-ion batteries. In such a battery, carbon fibres are used as the load carrying material thanks to their excellent strength and stiffness properties, but also as the active negative electrode. They also include a multifunctional matrix system, a structural battery electrolyte (SBE), the material holding the fibres together to make a solid-state load carrying material, but which at the same time is ionically conductive and chemically stable. It includes a multifunctional positive electrode, a composite electrode based on conventional ion inserting materials like lithium iron phosphate (LFP) supported by electrochemically active carbon fibres for load carrying and electrical conduction. This device can then also be used for inherent strain sensing in the material and can also be made to shape-morph with electrical control at low voltages and for harvesting energy by converting mechanical strain to electrical power.

CPP 16.2 Tue 10:00 H34

Structural response of advanced silicon-containing graphite anodes in commercial Li-ion batteries — •Tobias Hölderle[1,2], Dominik Petz[1,2], Vladislav Kochetov[2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany

This study explores the structural behavior of graphite anodes containing silicon additives in commercial lithium-ion batteries (LIBs) through detailed X-ray and neutron powder diffraction analyses. Silicon is increasingly utilized in advanced LIB anodes due to its potential to significantly increase energy capacity. However, its substantial volume expansion and amorphization during lithiation, complicate direct observation of lithium redistribution within the anode via diffraction techniques. Nonetheless, an indirect structural response linked to the lithiation of silicon was identified, indicated by a delayed lithium intercalation into the graphite structure. Furthermore, aging effects on high-silicon-content anodes were explored, showing the role of silicon in accelerating electrode degradation over time. These findings enhance our understanding of the complex relationship between the silicon content in the anode, structural stability, and lithium transport in advanced LIBs.

CPP 16.3 Tue 10:15 H34

XPS study of redox mechanism in Na2.5-xFe1.75(SO4)3 cathode material for high-voltage sodium-ion batteries — Neama Imam[1], •Karsten Henkel[1], Anna Milewska[2], Janina Molenda[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]AGH University of Krakow, Faculty of Energy and Fuels, Krakow, Poland

A multiplet splitting model based on the original work by Gupta and Sen has been used to track the redox mechanism and electronic structure of Na2.5-xFe1.75(SO4)3, a high-performance cathode material for sodium-ion batteries (SIBs). This high-purity, off-stoichiometric open-channel cathode material with a tailored sodium-ion distribution, synthesized using an optimized solid-state route, demonstrates a high operating voltage of ~3.8 V, surpassing the values reported for other cathode materials in the literature. X-ray photoelectron spectroscopy (XPS) was employed to analyze the evolution of the material's electronic structure at various charging potentials. Fe2p3/2 spectra decomposition using the multiplet splitting model revealed the gradual oxidation of Fe2+ to Fe3+ during sodium de-intercalation while transitioning from its pristine state with the presence of Fe2+ at the cathode surface only to the fully charged state (Na0.89Fe1.75(SO4)3 at 4.5 V). This result is consistent with the electrochemical analysis.

CPP 16.4 Tue 10:30 H34

Multipoint Anionic Bridge: Asymmetric Solvation Structure Improves the Stability of Lithium-Ion Batteries — •Tianle Zheng[1], Ya-jun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, 315201, Zhejiang Province, P. R. China

In this study, a novel concept of multipoint anionic bridge (MAB) is proposed and proved, which utilizes anions with different sites to connect with the asymmetric solvation structure (ASS). Compared to usual solvation structures, this study uses the multifunctional groups of difluoro(oxalate)borate anion, which can connect with Li ions. By tailoring the concentration, the anion serves as a bridge between different solvated structures. In-situ techniques and simulations investigate electrolytes to draw correlations between solvation structures and reaction pathways. The proposed design demonstrates remarkable high-temperature performance on both the anode and cathode sides, enabling stable cycling of lithium cobalt oxide (LCO)||graphite (0.5 Ah, 1.0 C) pouch cell for over 200 cycles at 80 °C, and facilitating Li||MCMB and Li||lithium iron phosphate (LFP) cells to deliver stable performance for 200 cycles at 100 °C. This work paves a way to develop high-performance electrolyte systems by designing and using new multipoint anions to construct ASSs.

CPP 16.5 Tue 10:45 H34

In situ Mechanochemical Synthesis of Organic Anodes in Electrode Processing for Ultra-long Sodium Storage — •Ying Qi, Huaping Zhao, and Yong Lei — TU Ilmenau

Currently, hard carbon is commonly used as an anode material in sodium-ion batteries (SIBs). However, hard carbon anodes face several challenges, including time-consuming and energy-intensive synthesis processes, low-voltage operating platforms, and capacity storage with a steep slope. These issues contribute to severe dendrite growth and reduced full-cell capacity, negatively affecting electrochemical performance. In contrast, organic anodes are becoming a focal point in SIBs research due to their abundant availability, low cost, simple synthesis, and stable potential plateaus. In this study, we directly prepared a series of acid anhydrides including perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA), 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA), and pyromellitic dianhydride (PMDA) into electrodes using a one-step milling process during slurry preparation. The prepared Na4PTC electrodes show low potential plateaus and ultra-stable cycling performance in SIBs. It exhibited exceptional performance, demonstrating ultra-long cycling stability lasting nearly one year. Additionally, the assembled full cell delivered a high energy density of ~200 Wh kg-1.

CPP 16.6 Tue 11:00 H34

Localized highly concentrated electrolytes with perfluorocarbonate diluents enable high-energy-density lithium/sodium metal batteries — •Zhuijun Xu[1], Yinghui Li[2], Yajun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, Zhejiang, 315201, P. R. China

Localized high-concentration electrolytes (LHCEs) have been widely recognized for their critical role in managing the reversible plating/stripping of alkali metals. multi-functional diluents with more stable physical and chemical properties are crucial for enhancing battery performance and safety. In this study, a variety of solvents, including 4-fluoro-1,3-dioxolan-2-one, 4,4-difluoro-1,3-dioxolan-2-one, cis-4,5-difluoro-1,3-dioxolan-2-one, trans-4,5-difluoro-1,3-dioxolan-2-one, 4,4,5-trifluoro-1,3-dioxolan-2-one, and 4,4,5,5-tetrafluoro-1,3-dioxolan-2-one, were analyzed using Density Functional Theory (DFT) calculations. Further, molecular dynamics (MD) simulations were conducted on the aforementioned solvents and their corresponding LHCEs for lithium/sodium metal batteries (LMBs/ SMBs). A comprehensive set of physical and chemical properties was examined, including the density of the solvent molecules, their highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, and their binding energies with lithium or sodium ions, distinct solvation structures within various LHCEs.

CPP 17: Modeling and Simulation of Soft Matter I

Time: Tuesday 9:30–11:15 Location: H38

Invited Talk CPP 17.1 Tue 9:30 H38

Continuum models for water's peculiar behavior on the nanoscale — •Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Water at the nanoscale exhibits unexpected properties relevant to many soft matter applications, ranging from the hydration forces that stabilize biological matter, via interfacial viscous effects that dominate wear behavior, to the unique dielectric behavior. Atomistically, these effects can be linked to the strong hydrogen bonding network and the corresponding water orientation and density at interfaces and in confinement – observables directly accessible from molecular simulations. However, relating these properties to experimental, typically macroscopic or at least averaged quantities is a tedious task. Here I will discuss some of the progress we have made in the last few years in deriving effective descriptions of the microscopic details that can be used to apply continuous descriptions and thereby extract, for example, experimentally accessible hydration pressure, permeance, or capacitance. Our recent work has focused on combining concepts from solid state theory and soft matter physics to accurately treat the electrode/electrolyte interface, and I will present our analysis of the unusually high capacitance of pure water capacitors.

CPP 17.2 Tue 10:00 H38

Coupled self and collective dynamics in highly charged colloidal Yukawa-systems — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate binary mixtures of highly charged colloidal particles employing Brownian dynamics simulations. In mixtures of identically charged, but differently sized particles solely the Stokes-Einstein diffusion coefficients differ, while the interactions are practically size-independent. Due to these identical interactions the static structure of all species are identical and independent on dynamical properties of the particles, as observed in partial static pair correlation functions. A dynamical coupling of both self and collective motion is observed in these systems. The long-time self-diffusion coefficient of a larger species is enhanced by the presence of a smaller, more mobile species and vice versa. Similar coupling effects are as well observed in the initial correlation decay of partial, distinct intermediate scattering functions, quantified by relaxation rates and stretching exponents of stretched exponentials. For all the here mentioned parameters, in the limit of strongly electrostatically coupled colloidal systems in first approximation linear dependencies on the size-ratio and reduced number density are observed. Despite we investigated highly dilute colloidal suspensions, where normally hydrodynamic interactions are neglectable, we found especially in binary mixtures an enhancement of the self and collective diffusion coefficients due to hydrodynamic interactions. Contrary, in one-component systems, hydrodynamic interactions do not have significant influence on time-dependent diffusion coefficients.

CPP 17.3 Tue 10:15 H38

Grand canonical molecular dynamics simulation of surface-initiated polymerization — •Bhuwan Poudel and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

The post-characterization of polymer brushes prepared from surface-initiated polymerization (SIP) is challenging because of their unique morphology and limitations in experimental techniques. However, in simulation counterparts, it is much easier to gain control over SIP processes. In this work, we used grand canonical molecular dynamics simulations to investigate the growth kinetics and characterization of polymer brushes. The SIP was studied by varying the grafting density. At low grafting densities, nearly monodisperse brushes were obtained. The dispersity was found to be increased with increasing grafting density; as a result, brushes with broad molecular weight distribution were obtained. We also showed that parameters such as thickness, molecular weight, and dispersity can be precisely controlled during SIP. The results suggests that the method presented here provides strategies to synthesize polymer brushes and tailor their properties more efficiently.

CPP 17.4 Tue 10:30 H38

IR Spectroscopy and Electric Field Simulations Enabled by the Atomic Polar Tensor Neural Network — •Philipp Schienbein — Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

Vibrational spectroscopy is a vital technique for uncovering microscopic structure and dynamics of condensed phase systems. However, interpreting such spectra at the microscopic level often requires theoretical support. While ab initio molecular dynamics (AIMD) has proven effective for this purpose, its high computational cost – especially when using electronic structure methods beyond GGA DFT – can be prohibitive. We have recently introduced a machine learning molecular dynamics (MLMD) approach for accurately calculating IR spectra using the atomic polar tensor, a size-intensive physical observable that can uniquely be defined for each atom and is thus broadly applicable across diverse systems. Notably, the atomic polar tensor also rigorously enables MLMD simulations under external electric fields. In this work, I benchmark this method against explicit AIMD simulations demonstrating comparable accuracy with significantly reduced computational cost and present applications of the atomic polar tensor neural network. These examples highlight its potential to drive novel physical insights, particularly in scenarios requiring large-scale MD simulations or computationally intensive electronic structure methods.

CPP 17.5 Tue 10:45 H38

Reducing dynamical helical polymers to 1D Ising models: long-range effects from polymer self-avoidance — •Keerti Chauhan[1], Marcus Müller[2], and Kostas Daoulas[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Georg-August-Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Cooperative chiral order in dynamic helical polymers (DHP) is commonly understood by reducing them to 1D Ising chains. Each spin can switch between $\sigma = -1$ and $\sigma = +1$ to represent rapid interconvertion between left-handed (M) and right-handed (P) helical twist. Spins are ferromagnetically coupled to capture the energetic disadvantage of boundaries between P and M domains. Currently, all 1D Ising models of DHP assume nearest-neighbor (NN) spin-spin interactions. We use a minimal model to challenge this assumption and investigate whether polymer self-avoidance, due to excluded volume, leads to effective non-local coupling between spins. Polymers are represented by freely-jointed chains with reversible hinges and helicity is described by a NN 1D Ising Hamiltonian with coupling strength J. Ideal and self-avoiding DHP are generated via a Monte Carlo scheme. First, we verify that in ideal chains the spins reproduce the statistics of a NN 1D Ising model with coupling strength J. Next, we find that chain self-avoidance does create effective long-range interactions between spins, as demonstrated by spin-spin correlation functions and free-energy calculations. These interactions renormalize J and create finite-size effects that are inconsistent with a NN 1D Ising behavior.

CPP 17.6 Tue 11:00 H38

Stabilization of Sodium Dodecyl Sulfate Reverse Micelles in Acid Solutions and Toluene from Molecular Dynamics Simulations — •Qixuan Li — Ruhr University Bochum, Bochum, Germany

The anionic surfactant Sodium dodecyl sulfate (SDS) forms reverse micelles (RMs) in two non-miscible components above the critical micelle concentration. Although the RMs in salt or alkali solution has been investigated in previous studies, less is known on the working mechanism of acids in SDS RMs. Here, we employ all-atom molecular dynamics simulations using Generalized Amber Force Field (GAFF) to investigate the effects of chloroauric acid (HAuCl4), fluoroboric acid (HBF4), phosphoric acid (H3PO4) and perchloric acid (HClO4) solutions on the stability of the RMs through spontaneous self-assembly in toluene. We find that all kinds of acids can stabilize micellar structure, and in particular high concentration of acids can significantly enhance the stability of RMs. In addition, H2PO4- anions tend to accumulate close to the RM surface, because they can form stable hydrogen bonds with the sulfate-based headgroup of SDS molecules or hydrated protons. Our findings can help to rationalize the impact of different acids on the RMs stability and in turn on the metallic nanoparticles synthesis where the RMs are used as nanoreactors.

CPP 18: Biomaterials, Biopolymers and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Tuesday 9:30–11:15 Location: H46

Invited Talk CPP 18.1 Tue 9:30 H46

Hybrid materials from colloidally stable nanocellulose and nanoparticles - scattering techniques are needed for characterization — •Eva Malmström[1], Åsa Jerlhagen[1], Benedikt Sochor[2], Korneliya Gordeyeva[1], and Stephan Roth[1,2] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Cellulose nanofibrils (CNFs) have rendered increasing interest during the last decades as their high stiffness, strength, and aspect ratio are attractive features to further explore on the pathway to a more sustainable society.

Controlled radical polymerization procedures allow for the synthesis of well-defined, nearly monodisperse, block-copolymers. The development of the polymerization-induced phase self-assembled (PISA) technique enables the production of well-defined nanoparticles (nanolatexes), with controlled size (typically with a diameter smaller than 200 nm), charge density, chemical functionality, and glass transition temperature.

The combination of CNFs and well defined nanolatexes allows for the design of novel materials with unique properties. Scattering techniques have proven very useful to characterize the corresponding materials, for instance, a method to assess cross-section orientation.

CPP 18.2 Tue 10:00 H46

In situ GISAXS investigation of different protein-templated titania nanostructures — •Linus Fidelis Huber and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Nanostructured titania thin films have been studied for a large variety of applications. An environmentally benign and scalable synthesis route for this material class could be of interest to many state-of-the-art devices, from solar cells to battery materials. Protein-assisted sol-gel synthesis is a low-temperature, low-cost, and highly scalable technique, that can be used to achieve a nanostructured titania thin film. It has been shown that the bovine whey protein β-Lg forms differently shaped aggregates at different solution pH values. With simple changes to the solution chemistry, different domain sizes, porosities, and morphologies are possible. Therefore, it is a promising candidate to create tunable and mesoporous

titania structures. In this work, we investigate the film formation with in situ small-angle/wide-angle grazing incidence X-ray scattering (GISAXS/GIWAXS) techniques. It is found that films printed at acidic pH form significantly different final bulk morphologies than films printed at neutral pH. The crystallite phase is strongly reduced in average domain size and domain-domain distance. Agglomerate size is increased for the acidic template. The in situ data is complemented by SEM, PL, UV-Vis and static GISAXS/GIWAXS measurements.

CPP 18.3 Tue 10:15 H46

With digital luminescence towards minimalistic, biodegradable information storage — •Sebastian Schellhammer, Heidi Thomas, Tim Achenbach, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Materials showing persistent luminescence, characterized by extended excited state decay times in the millisecond range and beyond, have gained much attention. Recently, we have reported a photonic device architecture based on organic functional materials called programmable luminescent tag (PLT) that is well suited for sensing, labelling, and information exchange applications. Information can be erased and rewritten repeatedly by using the design principle of digital luminescence, i.e. the control of the local oxygen concentration in a polymer:emitter blend and accordingly the emission by room temperature phosphorescence (RTP). We present the design of PLTs made from industrially compostable, ready-to-use materials (bioPLTs). As natural emitters, quinoline alkaloids show sufficient RTP when being embedded in a polymer matrix. Polylactic acid is used as matrix material and flexible substrate. RTP can be controlled adding oxygen blocking layers made from Exceval. Although organic semiconductors provide the potential of biodegradable technologies, prototypes do only rarely exist. With this work, a promising technology for compostable information storage and sensing systems is introduced.

CPP 18.4 Tue 10:30 H46

Enhancing drug release at interfaces with photoresponsive surfactant-polyelectrolyte mixtures — •Ipsita Pani, Michael Hardt, and Björn Braunschweig — Institute of Physical Chemistry, Center for Soft Nanoscience (SoN), University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Using micellar nanocarriers of a photoresponsive arylazopyrazole (AAP) surfactant, we have recently demonstrated the drug release at air-water interface.[1] In this work, we use a biopolymer poly-L-lysine (PLL) to form surfactant-polyelectrolyte mixtures to enhance the drug release of a chemotherapeutic drug doxorubicin. We observe a strong binding between the negatively charged AAP and the positively charged PLL at equimolar ratio. The information from UV-visible spectroscopy, light scattering studies, surface tensiometry and SFG spectroscopy has been utilized to identify the concentration of PLL at which the light-induced drug release is enhanced at the interface. We found that at higher PLL:AAP ratio, the complexes have low net charge and colloidal stability and the release of Dox from the bulk solution to the air-water interface is not observed. However, at lower PLL:AAP ratio, when the system is colloidally stable with a net negative charge, the drug release to the air-water interface is significantly enhanced. Further, the kinetics of drug release to the interface is faster in presence of PLL-AAP mixtures in comparison to pure AAP micelles.

[1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

CPP 18.5 Tue 10:45 H46

Proteins as foam stabilizers: From single foam lamellas to macroscopic foams — •Kevin Gräff, Sebastian Stock, Luca Mirau, Matthias Kühnhammer, Olaf Soltwedel, and Regine von Klitzing — Terchnische Universität Darmstadt, Darmstadt, Germany

Foams consist of foam lamellas, which separate single air bubbles from each other. Investigation of lamellas is crucial to understand foam properties. In order to untangle electrostatic, steric and network stabilization effects, we compare two globular proteins (β-lactoglobulin and Lupine Protein Isolate) and a disordered, flexible protein (whole casein) at different pH values. The Thin Film Pressure Balance (TFPB) device based on image intensity measurements generates spatially resolved disjoining pressure isotherms. We introduce feature tracking for the measurement of interfacial mobility and stiffness of lamellas as a novel method. Around the isoelectric point, Newton Black Films (NBFs) form, which are stable for the globular proteins while they are unstable for the disordered flexible one. This difference in film stability is explained by different characteristics of network structures in the lamellas from the respective protein solutions. Small-Angle Neutron Scattering (SANS) evaluation with a new model for foams proves the presence of NBFs within macroscopic foams. For a complete picture we compare the TFPB findings with X-ray reflectometry as well as with Brewster Angle Microscopy on single interfaces.

[1] Gräff, K. et al, (2022), Untangling effects of proteins as stabilizers for foam films, Front. Soft. Matter 2:1035377.

CPP 18.6 Tue 11:00 H46

What makes a polysaccharide biomaterial a good candidate for tissue engineering applications? — •Emma Bobu Cimpoi[1], Codrut Costinas[1], Emilia Licarete[2], Tamás Gyulavári[3], Klara Magyari[4], and Monica Baia[4,5] — [1]Doctoral School of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Centre for Systems Biology, Biodiversity and Bioresources "3B", Cluj-Napoca, Romania — [3]Department of Applied and Environmental Chemistry, University of Szeged, Hungary — [4]INSPIRE Research Platform, Babes Bolyai University, Cluj-Napoca, Romania — [5]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Biomaterials are inovative systems used to solve medical issues. Daily, injuries produce major bleeding that affects people and, without proper care, leads to other health problems. Traditional care methods are limited and outdated, so the focus is on natural materials with hemostatic properties, that are biocompatible and non-toxic. The aim of this work was to develop biomaterials based on pullulan, alginate and gelatin in various combinations, which could stop the bleeding and regenerate the wound. The developed sponge-like materials were characterized by FT-IR spectroscopy and X-ray diffraction. Then they were evaluated in vitro in terms of porosity, toxicity, swelling and charge on the surface, using SEM, cell viability assays, water up-take and mechanical tests. The investigations revealed good results as the synthesis was succesfull, the samples swell a lot, have good shape memory properties, are porous and non-toxic. These indicate their potential to stop bleeding, and therefore further in vivo tests will be carried out.

CPP 19: Active Matter III (joint session DY/BP/CPP)

Time: Tuesday 9:30–13:00 Location: H47

CPP 19.1 Tue 9:30 H47

From micro to macro: systematic coarse-graining of active particle models and implications on phase separation — •Sumeja Burekovic[1], Filippo De Luca[2], Cesare Nardini[1,3], Ananyo Maitra[4,5], and Michael E. Cates[2] — [1]CEA, Paris-Saclay, France — [2]DAMTP, University of Cambridge, UK — [3]LPTMC, Sorbonne Université, France — [4]LPTM, CY Cergy Paris Université, France — [5]LJP, Sorbonne Université, France

Significant insights into collective phenomena of active systems, such as phase separation, have been obtained through minimal field theories developed in a top-down manner. In contrast, the bottom-up approach seeks to link these continuum models to the microscopic dynamics of active particles, often formulated as Langevin equations for their position and orientation. This connection is typically achieved via explicit coarse-graining and allows active field theories to be expressed in terms of physically meaningful parameters. A major challenge in coarse-graining is the consistent elimination of irrelevant fast degrees of freedom to derive closed equations for the hydrodynamic variables or order parameters, such as the density field. We propose a systematic extension of standard homogenization/projection-operator techniques. As we show in minimal examples with few degrees of freedoms, our technique allows to go beyond the state of the art of homogenization in the mathematical literature. We then discuss the predictions of our coarse-graining methods for the large-scale phenomenology of non-aligning active particles, including cases in which microphase separation - rather than full phase separation - emerges due to activity.

CPP 19.2 Tue 9:45 H47

Active Quadrupolar Dumbbells — •Margaret Rosenberg[1], Marco Musacchio[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf — [2]Università di Roma Sapienza, P.le Aldo Moro 2, 00185 Rome, Italy

The field of Active Matter has thrived in recent years, driven both by the insight that it underlies fundamental processes in nature, and by its vast potential for applications. Although the self-propulsion mechanisms of Active Matter allow us to consider and control a wide range of motions, there is - by default - no obvious control over the orientation and rotation of the particles. One approach to resolve this is the use of anisotropic particles and interactions. This contribution presents a computational study of a novel system composed of active, quadrupolar dumbbells, the phase behavior of which is determined by the competition between active motion and the orthogonal alignment favored by quadrupolar attraction. We explore the novel phase behavior unlocked by these anisotropic interactions, and discuss options for experimental realizations and applications.

CPP 19.3 Tue 10:00 H47

Order by disorder in a swarm with obstacles — Pradeep Kumar[1], Sanjay Puri[1], and •Martin Weigel[2] — [1]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Simple models of swarming and active matter such as the Vicsek model [1] have been studied in detail, and the phase diagram as a function of noise strength and particle density is by now well understood. Real active systems are usually affected by impurities and random disorder, however. The presence of a quenched distribution of disc-like obstacles in the domain of the Vicsek model is observed to have a dramatic effect on the ordering behavior [2]: in contrast to the model without obstacles, where the strongest alignment is observed for the lowest noise, as soon as obstacles are added only the presence of a certain amount of noise leads to a global alignment of particles. This order by disorder phenomenon for active systems is traced back to the interplay of multiple length scales in the system: the typical inter-obstacle distance, the typical cluster size, and the resulting mean-free-paths of cluster-obstacle and cluster-cluster collisions. We present scaling arguments explaining these connections and provide an outlook towards similar phenomena in related systems.

[1] T. Vicsek, Phys. Rev. Lett. 75, 1226 (1995).
[2] O. Chepizhko, E. G. Altmann, and F. Peruani, Phys. Rev. Lett. 110, 238101 (2013).

CPP 19.4 Tue 10:15 H47

Autonomous navigation in synthetic microswimmers: solving mazes with chemical echolocation — •Aritra K. Mukhopadhyay[1], Linhui Fu[2], Kai Feng[2], Ran Niu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems.

We propose and experimentally demonstrate a mechanism enabling synthetic microswimmers, such as autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, creating echoes that carry structural information about the environment. Remarkably, these echoes invoke automatic responses, such as synthetic chemotaxis, enabling the swimmers to avoid dead ends and autonomously find paths through complex mazes.

Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities, which could be useful for developing self-navigating micromachines with potential applications in targeted drug delivery and environmental sensing.

CPP 19.5 Tue 10:30 H47

Active Particles in Tunable Colloidal Environments — •Abhimanyu Nowbagh[1], Venkata M.S.G. Tanuku[2], Thomas Palberg[2], and Ivo Buttinoni[1] — [1]Institute of Experimental Colloidal Physics, Heinrich-Heine University, 40225 Düsseldorf — [2]Institute of Physics, Johannes-Gutenberg University, 55128 Mainz

Active colloids are microscopic particles which propel through aqueous media by converting the externally available energy into directed motion. Using non equilibrium thermodynamics to understand biological systems: interactions of active colloids with crowded systems, and emergent phenomena of ensembles of active particles, remain an important and open question.

In this work, we investigate the dynamics of active particles in crowded environments subjected to alternating-current (AC) electric fields. The AC electric field is used to control: i) the velocity of active particles and ii) the inter-particle interaction between passive colloids. As we increase electric field strength, the velocity of active particles increases and the inter-particle interaction between passive colloids becomes stronger. We study the behaviour of active particles as a function of: i) the frequency of the applied AC electric field, ii) the area fraction of the passive crowd, iii) the active to passive particle number ratio, and iv) the velocity of the active particles.

Our experimental findings show that the active particles reorient faster with an increasing electric field strength. With an increase in the active to passive particle ratio, we show that cluster formation is non-monotonically sensitive to the passive crowd density.

Invited Talk CPP 19.6 Tue 10:45 H47

Beyond spheres - active matter in new shapes — •Juliane Simmchen — University of Strathclyde, Cathedral street 295, Glasgow UK

Surface minimisation for a given volume is energetically favourable on the small scale - this is why most colloidal particles are spherical. In active matter they have the added advantage of facilitating comparison between experiment and theory, one of the reasons why spherical Janus particles dominate the field.

However, broadening the range of materials has led to interesting discoveries - behaviour that would not have been observable in the spherical regime. This talk will give an overview of the intriguing behaviour of non-spherical active materials at the microscale - from plates to truncated bipyramids and rods.

15 min. break

CPP 19.7 Tue 11:30 H47

Modeling Filamentous Cyanobacteria — •Elias Fischer and Holger Stark — Institute Of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet, both in the present and the past. They triggered the great oxygenation event about 2.5 billion years ago, generating the atmospheric oxygen of our planet while contributing large parts of our fossil fuel record.

Filamentous cyanobacteria exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood. Furthermore, the gliding of cyanobacteria is strongly affected by external cues, most importantly light. They aggregate in regions with the highest light intensity, which means best environmental conditions for photosynthesis.

Following recent advances in understanding the self-organization of cyanobacteria, we present a novel approach for modeling the mechanical and behavioral aspects of individual cyanobacteria filaments, including force synchronization and response to light. Each filament is modeled as a bead-spring chain in 3D with bending and torsional elasticity, as well as a hard-core repulsion between the filaments. Notably, the propulsion forces that drive the individual parts of the filament forward are only considered locally where the filament comes into contact with another surface. First results on the 3D bending and twisting motion of a filament and its reaction to light are presented.

CPP 19.8 Tue 11:45 H47

Self-assembly and control of active and passive triblock Janus colloids — •Juri Franz Schubert, Salman Fariz Navas, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Triblock Janus colloids belong to the family of patchy particles, interacting with hydrophobic attraction at opposite poles and electrostatic repulsion in the equatorial region. They are known to self-assemble into a colloidal kagome crystal from experiments [1] and theory [2,3,4]. However, investigating the self-assembly of such systems via Brownian Dynamics can result in timescales inaccessible to brute force simulations, often requiring complex sampling techniques [3]. Recently, it has been shown that introducing self-propulsion can significantly accelerate self-assembly and enhance the Kagome yield [4]. Here, we study the model introduced in [4] and further investigate the self-assembled structures in active and passive systems. Using simple time-dependent activity protocols, we are able to sample a temperature-density state diagram of the passive system. Our results closely match with earlier studies [2,3], where different triblock models and sampling techniques were used.

[1] Q. Chen, S. C. Bae, S. Granick, Nature 469, 7330 (2011).
[2] F. Romano, F. Sciortino, Soft Matter 7, 12 (2011).
[3] K. Bahri, H. Eslami, and F. Müller-Plathe, JCTC 18, 1870 (2022).
[4] S. A. Mallory, A. Cacciuto, JACS 141, 6 (2019).

CPP 19.9 Tue 12:00 H47

Enhanced Diffusion and Universal Rouse-like Scaling of an Active Polymer in Poor Solvent — Suman Majumder[1], Subhajit Paul[2], and •Wolfhard Janke[3] — [1]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India — [2]Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India — [3]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

By means of Brownian dynamics simulations we study the steady-state dynamic properties of a flexible active polymer in a poor solvent condition. Our results show that the effective diffusion constant of the polymer D_{eff} gets significantly enhanced as activity increases, much like in active particles. The simulation data are in agreement with a theoretically constructed Rouse model of active polymer, demonstrating that irrespective of the strength of activity, the long-time dynamics of the polymer chain is characterized by a universal Rouse-like scaling $D_{\text{eff}} \sim N^{-1}$, where N is the chain length. We argue that the presence of hydrodynamic interactions will only have an insignificant effect on the observed scaling behavior.

CPP 19.10 Tue 12:15 H47

A Pulsating Active Solid — •Umang A Dattani[1], Francesco Serafin[1], Jonas Ranft[2], and Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institut de Biologie de l ENS, Ecole Normale Superieure, CNRS

Active matter has garnered significant attention in recent decades due to its numerous parallels with biological systems. Inspired by recent studies of biological tissues, such as cardiac cells, where constituent cell sizes periodically vary, a new form of activity termed "pulsating active matter" has been introduced recently. We propose a model of a pulsating active solid, consisting of size-changing particles linked by a triangular spring network. Despite the fixed connectivity, our model exhibits a variety of patterns and topological phase defects, akin to previous studies. Additionally, we explore the elastic continuum limit, which successfully predicts several essential features of the microscopic model. We conclude by highlighting intriguing properties of this system and its different potential parallels.

Invited Talk CPP 19.11 Tue 12:30 H47

Emergent correlations and boundary fluctuations in epithelial cell sheets — •Silke Henkes — Lorentz Institute, Leiden University, Leiden, The Netherlands

In soft active materials, the driving motion of individual constituents competes with their mechanical interactions, giving rise to active liquids, solids or glasses. An especially important example of this are epithelial cell sheets, which form a barrier function in the body and where the active crawling motion of cells over the substrate acts against cell-cell adhesion and repulsion.

I will show that a minimal model of cell sheets with uncorrelated activity, based on active Brownian dynamics and a vertex model, is a good quantitative match to data from two experiments on corneal and MDCK cell sheets. Its core feature is an emergent correlation length, arising from the diffusive spread of active forces through an elastic solid. This is a very general result that emerges in many active solids.

The boundary of such cell sheets exhibits a 'fingering instability' where the initially straight boundary develops large, spatiotemporally correlated fluctuations. Despite previous interpretations within many frameworks as an instability, I will show that it can be fully explained as arising from the active correlations of the cell sheets driving the boundary.

CPP 20: Interfaces and Thin Films I

Time: Tuesday 11:30–13:00 Location: H38

Invited Talk CPP 20.1 Tue 11:30 H38

Tailored polymer thin films enabled by initiated chemical vapor deposition (iCVD): From fundamentals to functional applications — •Stefan Schröder — Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Functional polymer thin films are of great interest in vast application fields ranging from electronic devices to biomedical interfaces. Device miniaturization and the consequent need for new polymer films on the nanoscale demand precise thickness control and defect free films. Solvent-free initiated chemical vapor deposition (iCVD) meets these demands, because it circumvents de-wetting and surface tension effects encountered in conventional solution-based polymer thin film fabrication. The process provides conformal polymer coatings on the nanoscale on large-area substrates as well as complex geometries. In addition, it enables deposition on delicate substrates like flexible organic substrates, copy paper and biomedical patches at room temperature. This talk demonstrates the versatility of the iCVD process and highlights recent results from fundamental studies based on density functional theory (DFT) on the underlying reaction processes up to the application of iCVD films in sensors, biomedicine and electronic devices.

CPP 20.2 Tue 12:00 H38

Highly Electrically Conductive PEDOT:PSS films via Layer-by-Layer Electrostatic Self-Assembly — •Muhammad Khurram, Sven Neuber, Annekatrin Sill, and Christiane A. Helm — muhammad.khurram@uni-greifswald.de

Electrically conductive films of Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonic acid) (PEDOT:PSS) are usually formed by spin coating of aqueous dispersions with PEDOT:PSS nanoparticles. The adsorption conditions are investigated using dip coating and a flow cell with different flow rates. Multilayer films are formed by sequential adsorption of oppositely charged macromolecules. PEDOT:PSS serves as polyanion, and PDADMA is the polycation. In dip coating, the first layer consists of approximately 70 nm thick monolayer of PEDOT:PSS nanoparticles. Subsequent PDADMA/PEDOT:PSS bilayers have a low, constant thickness (9.5 nm). Using the flow cell (0.2 mL/min) for film preparation also resulted in a constant PDADMA/PEDOT:PSS bilayer thickness (7.5 nm). PEDOT:PSS nanoparticle monolayers could also be observed with the flow cell, but only if the washing step after PEDOT:PSS adsorption was omitted. The films prepared by flow cell showed the highest conductivity (230 kS/m) and the lowest roughness (2 - 4 nm). We propose that the adsorption in a flow cell leads to a nearly flat orientation of the PEDOT molecules, increasing charge carriers' mobility. We also find that the relative humidity strongly influences the volume density and mobility of the charge carriers

CPP 20.3 Tue 12:15 H38

DFT Study of Catalyst-Ionomer Interactions in Hydrogen Fuel Cells — •Johanna Weidelt[1], Fabian Tipp[1], Tobias Binninger[1], and Michael Eikerling[1,2] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Proton exchange membrane fuel cells (PEMFCs) are promising devices for electricity generation from hydrogen. High efficiencies at low temperatures are achieved with platinum (Pt) as catalyst and Nafion as ionomer material. Because of the environmental persistence of the perfluorinated Nafion chains, fluorine-free ionomer materials are searched that maintain PEMFC performance and durability. To this end, the influence of the ionomer on the catalysis of the oxygen reduction reaction (ORR) in the cathode catalyst layer must be considered. Previous studies suggested that interactions between ionomer and Pt surface can compete with the adsorption of oxygenated ORR intermediates and negatively affect the catalytic activity. In this talk, we present a computational study investigating the competitive adsorption of ionomer species and reaction intermediates at a Pt(111) surface using grand-canonical density functional theory simulations. The Pt-adsorbate interaction strength was evaluated and surface phase diagrams were derived from adsorption energies calculated in implicit water environment under constant electrode potential.

CPP 20.4 Tue 12:30 H38

Dynamical and morphological changes of polyethylenimine thin films in relation to its CO2 absorption performance — •Maximilian Brückner[1], Martin Tress[1], Soma Ahmadi[2], and Shiwang Cheng[2] — [1]Peter Debye Institute for Soft Matter Research, Physics Department, Leipzig University, Germany — [2]Department of Chemical Engineering and Materials Science, Michigan State University, United States

Chemical reactions between carbon dioxide (CO2) and amine have been extensively characterized, however, their influence on the dynamics of polyamines remains largely unexplored. In this work, we compare the dynamics of polyethylenimine (PEI) before and after CO2 absorption through broadband dielectric spectroscopy (BDS). The molecular processes of bulk PEI are very different from those of thin film PEI, highlighting an interesting interface and nanoconfinement effect. Detailed analyses show CO2 absorption slows down the PEI dynamics, which is consistent with an elevated glass transition temperature of PEI upon CO2 absorption. Further aspects of thin-film-preparation, namely the impact of molecular weight, film thickness, used solvent and plasma treatment of the substrate on surface roughness were investigated by atomic force microscopy and reveal pronounced de-wetting which did not occur in high-molecular-weight PEI on plasma-treated surfaces. The observed changes in dynamics and morphology are likely to reduce the performance of large-scale CO2 capture devices based on low-molecular weight PEI in porous silica, thus suggesting modifications of this approach.

CPP 20.5 Tue 12:45 H38

Thermo-Responsive Surface Structure and Wetting of Polymer Brushes with Octadecyl Side Chains — •Billura Shakhayeva[1], Franziska Neuhaus[1], Luciana Buonaiuto[2], Sander Reuvekamp[2], Sissi de Beer[2], Frieder Mugele[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Münster (Germany) — [2]University of Twente, Physics of Complex Fluids, Enschede (The Netherlands)

Polymers are extensively studied as coatings due to their ability to respond to environmental changes, such as temperature or humidity variations, which greatly influence their wettability. This study investigates the effect of temperature on the molecular structure of poly-octadecylmethylacrylate (P18MA) brushes and their wetting behavior with hexadecane. Vibrational sum-frequency generation (SFG) spectroscopy was used to examine the molecular structure at the brush surface, both in air and in contact with hexadecane, by recording in situ SFG spectra near the three-phase contact line. The SFG spectra showed strong CH stretching bands of the octadecyl side chains at the air interface, indicating partial chain ordering that varies with temperature. For brushes in air, a phase transition at 311 K was identified as the surface melting temperature, 3 K higher than the bulk melting point. In the presence of hexadecane, surface melting occurred at 309 K, likely due to liquid penetration. Optical microscopy also revealed halo formation around the drop, suggesting local brush swelling. Below the surface melting point, the contact angle gradually decreased, while crossing the melting point enhanced hexadecane spreading.

CPP 21: Modeling and Simulation of Soft Matter II

Time: Tuesday 14:00–15:30 Location: H34

CPP 21.1 Tue 14:00 H34

Hard anisotropic particles: Excluded volume and second virial coefficients in arbitrary dimensions of space — •Markus Kulossa and Joachim Wagner — University of Rostock, Rostock, Germany

Precondition for investigations of phase behavior and equation-of-state data of many-particle systems are closed expressions for their free energy. The virial series gives access to the compressibility factor and therewith to the excess free energy of real supercritical fluids formed by hard, anisometric particles. Using Parson's approach, in many cases expressions solely based on the second virial coefficient accounting for the initial departure from ideal-gas behavior are used. In this contribution, we provide analytical expressions for the excluded volume of hard convex particles in arbitrary-dimensional Euclidean spaces. In addition to the detailed influence of the geometry and aspect ratio, we investigate the influence of singularities in the surface curvature. Analytical expressions for the excluded volume and second virial coefficients are of crucial importance for numerical calculation of higher-order virial coefficients. We provide so far unknown expressions for geometrical measures of uniaxial solids of revolution such as hyperellipsoids, hyperspherocylinders, hypercylinders, and hyperdoublecones in higher-dimensional Euclidean spaces.

CPP 21.2 Tue 14:15 H34

Navigating Chemical Space: An Active Learning Strategy Using Multi-Level Coarse-Graining — •Luis Walter and Tristan Bereau — ITP, Heidelberg University

Exploring the vast chemical compound space remains a significant challenge due to the immense number of possible molecules and limited scalability of conventional screening methods. To approach chemical space exploration more effectively, we have developed an active learning-based method that uses transferable coarse-grained models to compress chemical space into varying levels of resolution. By using multiple representations of chemical space with different coarse-graining resolutions, we balance combinatorial complexity and chemical detail. To identify target compounds, we first use an autoencoder to transform the discrete molecular spaces into continuous latent spaces. We then perform Bayesian optimization within these latent spaces, using molecular dynamics simulations to calculate target free energies of the coarse-grained compounds. This multi-level approach allows for an effective balance between exploration at lower and exploitation at higher resolutions. We demonstrate the effectiveness of our method by optimizing molecules to enhance phase separation in phospholipid bilayers. Our funnel-like strategy not only suggests optimal compounds, but also provides insight into relevant neighborhoods in chemical space. We show how this neighborhood information from lower resolutions can be used to guide the optimization at higher resolutions, thereby providing an efficient way to navigate large chemical spaces for free energy-based molecular optimization.

CPP 21.3 Tue 14:30 H34

Tuning Pore Size in Integral-Asymmetric, Isoporous Membranes via Bidisperse Diblock Copolymers — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Integral-asymmetric isoporous membranes, widely used in water filtration, are fabricated using a combination of evaporation-induced self-assembly (EISA) and nonsolvent-induced phase separation (NIPS). Membranes must have pores of an optimal size; small enough to block target substances but not so small as to cause excessive water resistance. While pore size can technically be adjusted by varying the copolymer's degree of polymerization, this approach requires synthesizing new copolymers for each desired pore size. A more economical alternative is blending polymers, where tuning the blending ratio of different components offers a feasible way to control pore size. However, mixing different copolymers could lead to macrophase separation. In this study, we focus on bidisperse diblock copolymers, and employ self-consistent field theory and particle-based simulations to explore the range of pore sizes over which this blending strategy is effective in fabricating membranes. Specifically, we aim to (1) establish correlations between system parameters and pore size and (2) elucidate the effects of these parameters on the dynamic behavior during SNIPS and the resulting membrane morphologies. Our findings provide valuable insights for the cost-effective fabrication of filtration membranes with tailored pore sizes.

CPP 21.4 Tue 14:45 H34

Machine-Learning potentials to understand pairing and stacking at the origin of life — •Laurie Stevens[1], Riccardo Martina[2], Alberta Ferrarini[2], and Marialore Sulpizi[1] — [1]Faculty of Physics and Astronomy, Ruhr-Universität Bochum, Germany — [2]Chemical Science Department, Università degli Studi di Padova, Italy

When exploring the origin of life, one main question remains open: how did we get from single nucleotides to long RNA and DNA chains which then led to more complex biological structures, following the RNA world hypothesis. More specifically, we are interested in how the nucleotides interactions are able to promote the synthesis of long polynucleotides. Experimental studies suggest that free nucleotides in water spontaneously organize into small molecular columnar phases, promoting the ligation of nucleic acid chains. To uncover the mechanisms behind this self-assembly, we use Molecular Dynamics simulations combined with Machine-Learning approaches.

Ab initio methods are too computationally expensive for the timescale of interest and for the complexity of the investigated systems. To overcome this limitation, we use Neural Network Potentials (NNPs) trained with DeepMD-kit and reinforced by metadynamics. After mastering the static and dynamical properties of a single Adenosine Monophosphate (AMP) in water, we are now investigating the stacking and pairing interactions between several AMPs by predicting the free energy landscape of this system as a function of the relevant degrees of freedom.

CPP 21.5 Tue 15:00 H34

Influence of hydroxyl groups on the dielectric constant of polyethylene — •Roshal Perepadan Shaju[1], Guido Roma[1], and Xavier Colin[2] — [1]Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif sur Yvette, 91191, France — [2]PIMM, Arts et Métiers Institute of Technology, CNRS, CNAM, HESAM University, 151 Boulevard de L'Hôpital, 75013 Paris, France

Polyethylene (PE) is widely used as an insulation for electric cables in various environments, including nuclear power plants. PE is susceptible to chemical modifications when exposed to ionizing radiation and oxidative environments. Introducing polar functional groups to this semi-crystalline PE, such as carbonyls and hydroxyl (OH) groups, has been observed to modify its dielectric response. However, the precise influence of hydroxylation on the dielectric properties of semi-crystalline PE is still inadequately understood. In this paper, we employ DFT and Density Functional Perturbation Theory (DFPT) to systematically investigate the effect of OH groups on the dielectric properties of semi-crystalline PE. By modeling PE with distinct surface, amorphous, and crystalline regions, the complexity of its semi-crystalline nature is explored. The static and high-frequency dielectric constants of polyethylene systems with different concentrations of OH groups were determined. The orientation of the OH defect relative to various crystallographic axes is thoroughly examined in order to determine how the alignment of the defects in the crystal lattice may affect the dielectric tensor.

CPP 21.6 Tue 15:15 H34

Load-induced shear band formation in microscale epoxy materials — •Julian Konrad, Janina Mittelhaus, Bodo Fiedler, and Robert Meissner — Hamburg University of Technology

Thin epoxy films ($\approx 30\ \mu$m) exhibit unexpected ductile behavior under mechanical load, challenging the conventional view of thermoset materials as inherently brittle. This behavior is characterized by the formation of shear bands, as revealed by mechanical testing and infrared spectroscopy. Analysis of vibrational spectra shows redshifts in *para*-phenylene stretching vibrations due to bond elongation, and blueshifts in out-of-plane hydrogen vibrations, resulting from polarization effects in the aromatic backbone. Molecular dynamics simulations support these findings, revealing a cascade of molecular realignments driven by deformation. Notably, these structural changes are reversible upon heating, suggesting a form of frozen entropy elasticity rather than plasticity. To further investigate, we employed a novel method using the MACE neural network potential to compute vibrational spectra with *ab initio* accuracy. This approach captures strain-dependent spectral shifts, accounts for interface and size effects, and highlights key implications for the design of composite materials.

CPP 22: Organic Electronics and Photovoltaics II

Time: Tuesday 14:00–15:15 Location: H38

CPP 22.1 Tue 14:00 H38

Spontaneous orientation polarization in mixed films of organic semiconductors — •Albin Cakaj, Alexander Hofmann, and Wolfgang Brütting — Experimental Physics IV, Institute of Physics; University of Augsburg, 86135 Augsburg, Germany

Small organic molecules processed by physical vapor deposition (PVD) can exhibit a preferential alignment, despite their tendency to form glassy amorphous films. This alignment can additionally lead to a macroscopic polarization of the film, if the molecules have a permanent dipole moment (PDM). The additional field, also referred to as giant surface potential (GSP), can impact the properties of organic light emitting diodes (OLEDs) significantly. Therefore, understanding the formation and control of this effect is of crucial importance.

We investigated different GSP forming polar molecules mixed with non-polar organic compounds. We found combinations with enhanced PDM alignment, where the impact of suppressed dipole-dipole interactions by dilution is far more significant than the effect on the film-formation process by a change in the effective glass temperature of the blend. Additionally, our data hint to the conclusion that molecules with an already high degree of PDM alignment keep their magnitude of alignment in mixed films without significant enhancement. Therefore, we can conclude that mixing of polar molecules with a non-polar compound can enhance the degree of PDM alignment significantly, if the polar molecules exhibit only a small degree of PDM alignment in the first place.

CPP 22.2 Tue 14:15 H38

Ultrafast Response in Unbalanced Mobility Organic Photodetectors — •Felix Hergenhan, Tianyi Zhang, Karl Leo, and Johannes Benduhn — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, TU Dresden, Dresden, 01187 Germany

Organic photodetectors (OPDs) have attracted growing interest due to their potential in various optoelectronic applications. However, the slower response speed of OPDs compared to their inorganic counterparts, primarily influenced by low charge carrier mobilities, has hindered their application in high-speed technologies. In this presentation, we will discuss the dynamic behavior of OPDs, focusing on how ultrafast response times can still be achieved despite significant mobility imbalance and overall low mobility. Importantly, the role of RC (resistance-capacitance) limitations is emphasized, as they significantly impact the achievable response speed of the devices. We systematically investigated the effects of device design, device dimensions, light intensity, and applied bias on OPD performance and its dynamic behavior. Notably, special features could be identified in their dynamic response that led to improved rise and fall times of only a few nanoseconds and a cutoff frequency beyond 10 MHz. We propose a model explaining the origin of these features and demonstrate how to utilize them to achieve faster response times. By exploring the entire picture of device design, material choice, and operational conditions, we provide an outlook on the future development of ultrafast OPDs.

CPP 22.3 Tue 14:30 H38

Systematic variation of acceptor and donor moieties in donor-accerptor-donor small molecules for efficient room-temperature phosphorescence — •Uliana Tsiko, Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) from purely organic materials promises unique application in diverse fields including molecular sensing, bioimaging, information storage, and anti-counterfeiting. With the design of programmable luminescent tags (PLTs), we recently reported a novel photonic device architecture that is well suited for various labelling and information exchange applications and even allows a biodegradable design. However, improved RTP emitters are required to fully exploit this technology.

In our contribution, we systematically analyze the impact of the acceptor and donor moieties on the photophysical properties of newly synthesized RTP emitters to gain an understanding of structure-property relationships. While the electron-accepting character does not significantly affect the emission properties, the electron-donating ability of the donor unit can strongly improve RTP emission, leading to pronounced sky-blue phosphorescence in purely organic materials, which has been rarely observed before. These emitters are further characterized in PLTs as a prototypical excitonic application scenario.

CPP 22.4 Tue 14:45 H38

Efficient room-temperature phosphorescence in small-molecule hosts for applications in information storage — •Yana Bui Thi, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) from organic materials promises unique applications in molecular sensing, bioimaging, and information storage. Typically, RTP is achieved by embedding emitter molecules in a rigid matrix to suppress non-radiative decay. The integration of such emitters into polymer hosts has enabled advancements in photonic technologies, such as programmable luminescent tags. However, a comprehensive understanding of host-guest interactions, particularly with small-molecule hosts suitable for vacuum processing, is widely missing. This work investigates the photophysical properties of RTP emitters embedded in wide bandgap small molecules, typically used in OLEDs. Thin films are fabricated either by spin coating or thermal evaporation, the latter offering superior film quality and compatibility with patterning techniques. RTP can be promoted or impaired depending on the choice of the host material, partially even allowing for RTP in the presence of oxygen. A significant enhancement of photoluminescence can be obtained due to favorable energy transfer from host to emitter. These results highlight the importance of the host selection in optimizing emitter performance and present valuable insights for polymer-free RTP-based photonic devices.

CPP 22.5 Tue 15:00 H38

Regulated Growth of Benzoperylene-TCNQ Charge-Transfer Complex Crystalline Networks — •Kirill Gubanov, Yana Reva, Stevie Furxhiu, Fabian Streller, Yifan Bo, Phillip Greissel, Dirk M. Guldi, and Rainer H. Fink — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Highly ordered luminescent organic micro- and nano-crystals of charge-transfer complexes (CTC) are generating a considerable interest due to their prospective applications in miniaturized and multifunctional optoelectronics. We propose a strategy of controlled crystallization growth of Benzoperylene (BP)-TCNQ-CTC nanorods network. As a result of the distinct polarity-based solubility of BP and TCNQ, 2D microsheets of BP of tunable sizes can be used as templates for the CTC nanorod meshes growth in solution. The optical and electronic properties of the respective CTC were additionally investigated. Emission spectroscopy revealed a significant quenching of the BP strong fluorescence upon CTC formation: electron excitation in BP leads to a charge transfer to a non-emissive TCNQ and to non-radiative relaxation. Using NEXAFS micro-spectroscopy, we examined the electronic structure and a temperature-dependent band gap modification. Thus, collective insights into the BP-TCNQ CTC properties provide valuable information for material optimization for future applications in optoelectronic devices. The research is funded by the BMBF (contract 05K19WE2) and SolTech initiative.

CPP 23: Polymer and Molecular Dynamics, Friction and Rheology

Time: Wednesday 9:30–11:15 Location: H34

Invited Talk CPP 23.1 Wed 9:30 H34

Advanced combined rheometer setups to in-situ correlate molecular dynamics and molecular structure formation with mechanical properties — •Manfred Wilhelm — Karlsruhe Institut für Technologie, Karlsruhe, Germany

Molecular understanding of mechanical properties over a broad length and time scale is crucial to develop advanced materials. Our research aims to design and built unique combined rheometer setups that can monitor in-situ molecular observables, such as molecular dynamics or chemical functional groups that are directly correlated to the macroscopic mechanical responses. These combined experimental setups overcome the experimental challenges associated with offline measurements and facilitate the understanding of structure-property relationships.

CPP 23.2 Wed 10:00 H34

Nonequilibrium Dynamics of the Helix-Coil Transition in Polyalanine — •Maximilian Conradi[1], Henrik Christiansen[1,2], Suman Majumder[3], Fabio Müller[1], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]NEC Laboratories Europe GmbH, Kurfürsten-Anlage 36, 69115 Heidelberg, Germany — [3]Amity

Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

In this work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. At the start of the transition short 310-helices form, leading to the molecule becoming more rod-like midway through the collapse. Afterwards, α-helix formation becomes the prevalent ordering mechanism leading to multi-leg hairpin structures, representative for the equilibrium behavior of longer chains. The dynamics of this transition is explored in terms of the power-law scaling of various associated relaxation times as a function of the chain length.

CPP 23.3 Wed 10:15 H34

Porous Particles Formation in the Drying of Polymer Solution Droplets — •Mengmeng Wu, Hsiao-Ping Hsu, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, Germany

Due to the unique properties such as large specific surface area, high permeability and low density, porous polymer nano- or micro-spheres are promising for various applications including biomedical, pharmaceutical, tissue engineering and degradable electronic applications. We develop a coarse-grained polymer solution droplet model to study the particle structure formation of drying polymer solution droplets. By maintaining below the glass transition temperature, highly porous particles are generated followed by a fast evaporation and cavitation of solvents. For a drying droplet in an environment with low thermal conductivity, the temperature experiences a decrease owing to solvent vaporization. Such temperature reduction results in a decrease in evaporation rate during evaporation, consequently impacting the drying dynamics of polymer droplets. Our investigation explores how the cooling of droplets during solvent evaporation influences the final morphology of polymer particles.

CPP 23.4 Wed 10:30 H34

Polymer chains under oscillatory force in solvents of variable quality — •Bogumiła Szostak[1,2], Ron Dockhorn[2], Jens-Uwe Sommer[2], and Jarosław Paturej[1,2] — [1]University of Silesia in Katowice, Bankowa 12, 40-007 Katowice, Poland — [2]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6 D-01069 Dresden, Germany

Polymers are key materials in soft condensed matter with diverse applications. Recently, significant attention has been given to understanding the micromechanical behavior of single macromolecules under applied forces. Using molecular dynamics, we examined how constant and periodic forces affect polymer chain conformations in dilute solutions, modeled for good and poor solvents. We systematically calculated the projection of the end-to-end vector in the force direction as a function of the applied force. This analysis led to the construction of force-extension diagrams, which revealed conformational transitions of polymers from a globular state to an extended chain. Analysis of hysteresis loops for periodic forces showed that longer force periods allowed more time for the system to respond, resulting conformational reorganization. These results were compared with analytical solutions of the Rouse model under periodic perturbation and scaling laws, providing a valuable benchmark and deeper insight into the observed dynamics. We also characterized the relationship between dissipated energy and the frequency of the applied sinusoidal stretching force. These findings provide new insights into the mechanical behavior of polymer chains under oscillatory forces, enhancing our understanding of their dynamic properties and potential applications.

CPP 23.5 Wed 10:45 H34

Role of Trapped Water Molecules at Sliding Contacts in Lattice-Resolved Friction Investigated with Molecular Dynamics — •Miljan Dašić and Igor Stanković — Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Understanding nanoscale friction within an environment which contains water, is crucial for engineering friction-based mechanisms and characterizing surfaces. From the point of view of Friction Force Microscopy (FFM) experiments, it has been understood that the lattice resolution in water environments originates from a dry contact state, in case of which all water molecules get expelled from the gap between the microscope's tip and the studied substrate.

We have developed an All-Atom Molecular Dynamics simulation setup, for revisiting this understanding by performing a detailed analysis of the impact of water molecules present in the system on the dynamic behavior of the nanotribological contact between an amorphous SiO2 probe and a monolayer MoS2 substrate.

Our analysis of stick-slip patterns shows the entrapment of water molecules at the contact interface. These trapped water molecules act as an integral part of the probe and participate in its interaction with the substrate, hence affecting the probe's dynamics and preventing long slips. Surrounding water molecules from the capillary or layer of water exhibit a replenishing effect, acting as a water reservoir during the sliding process. Such a phenomenon enables the preservation of lattice-scale resolution across a range of normal loads.

CPP 23.6 Wed 11:00 H34

The analytical investigation of star polymers in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Maciej Dudek[3] — [1]Cracow University of Technology — [2]Institute of Nuclear Physics — [3]Academy WSB

The analysis of the influence of star polymer topology on the depletion interaction potentials, the depletion forces and Pincus force was carried out analytically. The method of calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star polymers with f=3, 4, 5 legs in a Θ - solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other inert surface was proposed. Besides, we performed the investigation of the elastic properties of star polymers with different number of legs in a semi-infinite space confined by single wall with different boundary conditions and calculated Pincus force in the above mentioned cases. Calculations were carried out for star polymers with f=3,4,5 legs attached to the substrate by one or two arms. The acquired results showed that the Pincus force is affected by the number of arms attached to the surface. The obtained results are interesting from scientific and industrial point of view, because of their potential use in the production of paints, varnishes and new functional materials. Star polymers, due to their topology and shape can find practical application in nano - technology, as well as in biotechnology and medicine for drug and gene transmission.

CPP 24: Hybrid and Perovskite Photovoltaics III

Time: Wednesday 9:30–11:15 Location: H38

CPP 24.1 Wed 9:30 H38

Tailored perovskite crystallization by passivation molecule engineering for efficient light-emitting diodes — •Jungui Zhou[1,2], Min Zhu[1], Yufeng Zhai[2], Shouzheng Chen[2,4,5], Benedikt Sochor[2], Sarathlal Koyiloth Vayalil[2], Lei Cai[3], Man-Keung Fung[1,6], Peter Müller-Buschbaum[5], and Stephan V. Roth[2,7] — [1]Soochow University, Suzhou, China — [2]DESY, Hamburg, Germany — [3]Shandong normal university, Shandong, China — [4]FRM II, Garching, Germany — [5]TUM School of Natural Sciences, Garching, Germany — [6]MUST, Macau, China — [7]KTH Royal Institute of Technology, Stockholm, Sweden

Metal halide perovskite light-emitting diodes (PeLEDs) are regarded as alternative candidates for next-generation display technologies.Various additives have been widely used in perovskite precursor solutions, aiming to improve the as-obtained perovskite film quality through passivating defects and controlling the crystallinity. Although the defect passivation of additives has been intensively investigated, a deep understanding of how additives influence the crystallization process of perovskites during the spin-coating and annealing processes is still lacking. Here, by combining In-situ photoluminescence (PL) and grazing-incidence wide/small-angle X-ray scattering (GIWAXS/GISAXS) techniques, a systematic study of the perovskite film-formation process, perovskite structure, and inner morphology of CsPbBr3 perovskite films modified by various additives is conducted, revealing the influence of additives on the formation of high-quality perovskite films and efficient PeLEDs.

CPP 24.2 Wed 9:45 H38

Optical In-Situ Methods as Process Optimization Toolbox — •Lennart Reb — Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109, Berlin

In the field of perovskite photovoltaics, precursor optimization is often guided by the visual inspection of film quality by experienced researchers. However, combined optical in-situ techniques can help shift toward rational, evidence-based process design. In-situ characterization methods are frequently used for studying the reaction kinetics during processing: Optical techniques to monitor solvent evaporation, such as spectral absorption, reveal changes in halido-plumbate spectral signatures that correlate with the increasing density of polynuclear plumbate species. Photoluminescence (PL) measurements further elucidate early perovskite nucleation during quenching processes and crystal growth. Structural insights from grazing-incidence X-ray scattering (GIWAXS) track intermediate phases, the formation of perovskite structures, and the evolution of secondary phases. This work briefly reviews the state-of-the-art multimodal in-situ characterization techniques and introduces the multimodal μ slot-die coater, a small-scale platform integrating UV-vis, PL, imaging, and GIWAXS capabilities. Initial results of combined measurements demonstrate its power for studying perovskite film formation during scalable processing, offering insights into reaction kinetics and showcasing the capabilities of in-situ imaging techniques in scalable perovskite deposition. For example, in-situ PL measurements show the changes of PL signal over time upon the inclusion of chloride-based additives.

CPP 24.3 Wed 10:00 H38

Metal halide perovskite solar cells under space like temperature conditions — •Simon Alexander Wegener[1], Altantulga Buyan-Arivjikh[1], Kun Sun[1], Zerui Li[1], Xiongzhuo Jiang[1], Matthias Schwarzkopf[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany

Perovskite solar cells hold great promise for space applications due to their exceptional properties, including high power-to-weight ratios and efficiencies comparable to silicon cells. Their solution processability lowers both manufacturing and launch costs, presenting a cost-effective alternative to gallium arsenide cells. However, their viability in space is challenged by harsh conditions such as high vacuum, extreme temperatures, and radiation. This study investigates the impact of extreme temperature fluctuations in low Earth orbit, ranging from -100*C to +100*C, on perovskite solar cell performance. Operando GIWAXS measurements enable real-time analysis of the crystal structure under simultaneous illumination and thermal cycling. Measurements of I-V curves and optical absorption spectra further assess electrical and optical properties. Results reveal temperature-dependent efficiency variations and degradation influenced more by device layers and interfaces than the active layer itself. Understanding the mechanical, optical, and electrical behavior of the entire cell assembly under such conditions is key to optimizing durability and performance.

CPP 24.4 Wed 10:15 H38

Simulation of the impact of processing conditions for solution-processed thick perovskite layers — •Martin Majewski[1], Shudi Qiu[2], Larry Lüer[2], Vincent M. Le Corre[2], Tian Du[2], Olivier J.J. Ronsin[1], Christoph J. Brabec[2], Hans-Joachim Egelhaaf[2], and Jens Hartin[1] — [1]Helmholtz Institue Erlange-Nuernberg, Cauerstraße 1, 91058 Erlangen, Germany — [2]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander Universitaet Erlangen Nuernberg

Fabricating thick (1000 nm) solution-processed perovskite layers is expected to increase the efficiency of carbon-contact-based solar cells compared to thinner (500 nm) films. However, increasing only the deposited layer thickness often results in buried voids inside the dry film. Recently, we have developed a theoretical framework based on Phase Field simulations. With the help of the simulations, it is possible to explain why voids form in the film. The crystals nucleate at random spots inside the liquid film. The movement of the condensed-vapor interface, due to evaporation, leads to an agglomeration of the crystals at the film surface. The crystals block further evaporation and the remaining solvent is the origin of the buried voids inside the dry film. We explain how adding seeds on the substrate before coating the thick film can prevent this. In this case, processing conditions have to be modified compared to standard operating procedures for thin films. The theoretical expectations can be verified experimentally, leading to a performance improvement of the devices.

CPP 24.5 Wed 10:30 H38

First-principles modelling of hybrid perovskites — •Udo Schwingenschlögl and Aleksandra Oranskaia — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The photoconversion efficiency record of silicon-perovskite solar cells exceeds 30% owing to hybrid perovskites with organic cations that stabilize the perovskite by non-covalent bonding. To address the electronic properties and stability issue from the perspectives of the bulk crystal phases, point defects, and surfaces and interfaces (requiring large simulation cells) the computational methods must be chosen carefully: (1) For the structural relaxation an exchange-correlation functional is required that adequately describes materials rich in NH$\cdots$I bonding (between organic cations and I) and I$\cdots$I bonding (between PbI_6 octahedra or between PbI_6 octahedra and I-related defects). (2) For the electronic structure calculation an exchange-correlation functional is required that adequately describes the spin-orbit coupling of the Pb and I electrons. Comparing the PBE, PBE-TS, PBE-D3, PBEsol, vdW-DF2, and rVV10 functionals for relaxing FAI, $C_4N_2H_{12}(I_3)_2$, $C_6H_7NI(I_3)$, I_2, In, $Cs(I_3)$, $Cs_2(I_3)_2(I_2)$, and PbI_2 crystals, we show that the rVV10 functional provides the most balanced prediction for the types of non-covalent bonding relevant for hybrid perovskites. We also discuss problems related to the HSE06 functional and show that the PBE functional with a Hubbard correction for the Pb 6p and I 5p orbitals (together with fully relativistic pseudopotentials) provides promising results.

CPP 24.6 Wed 10:45 H38

An effective Population balance model for evaporation-driven precursor-mediated crystallization — •Kai Segadlo, Olivier Ronsin, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IET-2), Erlangen, Germany

Although tremendous progress has been made in recent years in Experimental and Material Design for solution-processed photoactive Perovskite thin films, this progress has not likewise been followed by a corresponding improvement in the theoretical understanding of these systems. In particular, the high computational demands arising from the plethora of potentially relevant thermodynamic processes, such as evaporation, crystallization, chemical reactions, demixing, and advection, as well as the high costs of in situ multichannel screening experiments, lead to uncertainties about the underlying physical mechanisms, which in practice often facilitate the use of narrow empirical models. As a first step towards theoretical coherence, we combine empirical mass transport models into a single population balance model accounting for evaporation, crystallization, and chemical reactions. We validate the drying subpart against drying curves, and the crystallization subpart against crystallinity curves from Ultraviolet Imaging Spectroscopy, and Phase field simulations, respectively. The model allows us to gauge the relevances of the processes during precursor-mediated methylammonium lead iodide crystallization measured with in situ Grazing Incidence Wide Angle X-ray scattering and to shed light on the experimentally highly relevant but hard-to-access coupling between evaporation and crystallization.

CPP 24.7 Wed 11:00 H38

Modeling and Analysis of Spectral and Thermal Effects in 2-Terminal Perovskite-CIGSe Tandem Solar Cell Configurations — •Yokozuna Schirmer[1], Nicolas Otto[1], Guillermo Farias Basulto[2], Rutger Schlatmann[1,2], Bert Stegemann[1], and Christof Schultz[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, D-12459 Berlin, Germany — [2]PVcomB / Helmholtz-Zentrum Berlin für Materialien und Energie, Schwarzschildstr.3, D-12489 Berlin, Germany

Tandem solar cells are being developed to exceed the efficiency limits of single-junction cells. Typically, they are designed in a 2-terminal (2T) current-matched configuration, which can result in a reduced energy yield due to current mismatch caused by spectral variations throughout the day. To overcome this limitation, tandem solar cells can be configured in a 2T voltage-matched setup, which could mitigate the impact of spectral sensitivity on performance. The aim of this work is the development of a computational model to analyse the energy yield of each configuration. This model combines temperature-dependent electrical cell parameters with spectrally resolved real-world outdoor data to simulate the operational behaviour and to evaluate the advantages of each interconnection approach. The model is validated by measured I-V cell data from single- and multi-junction cells. Moreover, a comprehensive analysis of the calculated results provides valuable insights into the performance trade-offs under real-world conditions, enabling the identification of the optimum design for specific applications.

CPP 25: Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)

Time: Wednesday 10:00–12:00 Location: P3

CPP 25.1 Wed 10:00 P3

Enhanced stability and chaotic condensates in multi-species non-reciprocal mixtures — •Laya Parkavousi[1], Navdeep Rana[1], Ramin Golestanian[1,2], and Suropriya Saha[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), D-37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Random non-reciprocal interactions between a large number of conserved densities are shown to enhance the stability of the system towards pattern formation. The enhanced stability is an exact result when the number of species approaches infinity and is confirmed numerically by simulations of the multi-species non-reciprocal Cahn-Hilliard model. Furthermore, the diversity in dynamical patterns increases with increasing number of components and novel steady states such as pulsating or spatiotemporally chaotic condensates are observed. Our results may help to unravel the mechanisms by which living systems self-organise via metabolism.

CPP 25.2 Wed 10:00 P3

Non-reciprocal Model B and the role of mobilities and non-reciprocal interfacial forces — •Bibhut Sahoo[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Mathematics, King's College London, London

Recently the effects of non-reciprocal interactions have been widely studied in the Cahn-Hilliard model for phase separation, which is based on a magnetic analogy. Here we explore the corresponding nonreciprocal model B, as the continuum theory for non-reciprocal particle mixture. We focus on the effect of mobility matrix on topology of the phase diagram and find that changing mobility can change stability of a homogeneous state, which for reciprocal interactions

would be impossible. We study spinodal dynamics in regions of instability, where static or travelling spinodal patterns can occur. This aspect is as in non-reciprocal Cahn-Hilliard but, the transitions between these instabilities are novel: they occur not via exceptional points, but via first order transitions in the length scale of the dominant unstable modes. At transition, a static and a travelling spinodal pattern with two different scales coexist. We show that more complicated transitions involving coexistence of three length scales can also occur. We finally argue, based on a nonreciprocal version of Dean's equation, that coarse graining into a model B description should lead to non-reciprocal interface terms, rather than only in the bulk as assumed in theories to date. We show that such interfacial terms can significantly enlarge the travelling spinodal regions in the phase diagram.

CPP 25.3 Wed 10:00 P3

Mixed active fluids of two kinds — •Astik Haldar — Universität des Saarlandes, Saarbrücken 66123, Germany

We explore here the polar active fluids of two types, characterizing by their different aligning and propulsion strengths. We example here the fluids as the collections of moving living creatures, which could fuel itself through chemical reactions in their body . We called this system as active system, and consider their brilliant interactions. We here try to model those through considering some parameters and physically observable quantities. We find the parameters region where they have their oriented flocking as parallel or antiparallel, ordered rotating phase coherently meaning chiral phase. Our study finds the transition between the phases as saddle node as well as pitchfork bifurcation in mean field theory scheme. We find different kind of pattern formed states appear through the analytical as well as numerical study.

CPP 25.4 Wed 10:00 P3

Verification, efficiency analysis and extension of the kinetic Event-Chain Algorithm — •Nico Schaffrath, Tobias Kampmann, and Jan Kierfeld — TU Dortmund, Dortmund, Germany

The novel cluster kinetic Monte-Carlo algorithm, which is based on the event-chain Monte-Carlo method, is specifically designed to simulate systems of two-dimensional self-propelled hard particles. We verify this algorithm from scratch by analysing various single-, two- and many-body systems, as well as some algorithm-specific quantities. To gain insight about the applicability of the algorithm, we compare its performance to that of an Event-Driven Brownian-Dynamics simulation. Finally, we investigate the possibility to simulate particles with soft interaction energies as well as an extension to three-dimensional systems. Regarding the latter, the phase diagram of self-propelled hard spheres is calculated.

CPP 25.5 Wed 10:00 P3

AMEP: Analyzing Active Matter Simulations in Python — Kay-Robert Dormann[1], Lukas Hecht[1], Kai Luca Spanheimer[2], Aritra K. Mukhopadhyay[1], Mahdieh Ebrahimi[1], Suvendu Mandal[1], and •Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany

The **A**ctive **M**atter **E**valuation **P**ackage (AMEP)[1] is an easy-to-use Python library for analysing simulation data of particle-based and continuum simulations. It provides a powerful interface for handling complex analysis of large data sets from different simulation software such as LAMMPS, HOOMD-blue, GROMACS and others. A plethora of methods to calculate observables and visualise results make AMEP suitable to calculate complex observables not only for beginners but also for advanced studies of active and soft matter. AMEP is written in pure Python and leverages powerful and well-known libraries such as NumPy, SciPy and Matplotlib. Computationally expensive methods are parallelized to run on laptops and workstations as well as high-performance computing clusters.

The methods range from order parameters, cluster methods, spatial and time correlation functions to thermodynamic properties and coarse-graining methods. More information and examples are available at https://amepproject.de. AMEP can be installed via conda and pip.

[1] L. Hecht et al., arXiv:2404.16533 [cond-mat.soft]

CPP 25.6 Wed 10:00 P3

Fluctuation induced network patterns in spatially correlated noise — •Sebastian Fehlinger[1], Kai Cui[2], Arooj Sajjad[1], Heinz Koeppl[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Institut für Physik Kondensierter Materie, Hochschulstraße 8, 64289 Darmstadt — [2]Technische Universität Darmstadt, Selbstorganisierende Systeme, Merkstraße 25, 64283 Darmstadt

Fluctuations play an important role in many fields of physics, from quantum electrodynamics to statistical mechanics. In active matter physics, so far, most works have focused on active particles that are subject to thermal fluctuations caused by the surrounding solvent. Here, we explore the collective behaviour of active particles under the influence of spatially correlated noise, that can arise, e.g., from fluctuating external fields. Therefore, we introduce a minimal model which describes the dynamics of (chiral) active particles with alignment interactions in a time-dependent Gaussian random field, that features a characteristic spatial correlation length, but no temporal correlations. Using Brownian dynamics simulations, we find, that the active particles aggregate to system spanning, percolated networks. These structures are (i) fluctuation-induced, (ii) feature local alignment of the contained particles, but no global alignment, and (iii) hardly show any coarsening. We systematically characterize the emerging patterns with tools from topological data analysis (persistence diagrams, Vietoris-Rips complexes and Betty numbers).

CPP 25.7 Wed 10:00 P3

Reconfiguring hydrodynamic flow fields of active particles by light — Lisa Rohde, Tom-Hannes Hemann, Gordei Anchutkin, and •Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Microscopic active particles propel themselves via localized energy conversion, generating hydrodynamic flow fields that govern their boundary interactions and collective behaviour. The long-range behaviour of the flow patterns classifies them as either pushers, which expel fluid along their swimming axis, or pullers, which draw fluid inward. In nature, some microorganisms can adaptively switch between pusher and puller modes in response to their environment. However, synthetic active particles are currently limited to a fixed pusher or puller configuration during fabrication, constraining our ability to study their dynamic responses to environmental cues. Here, we present a self-thermophoretic active particle that can reconfigure its flow field on demand during the experiment. This is achieved by illuminating the particle with an inhomogeneous light field shaped by a spatial light modulator. The illumination patterns create surface temperature fields inducing thermo-osmotic flow fields that propel the particle and shape the hydrodynamic interactions. By using gold nanoparticles, we trace and characterize the hydrodynamic flow field of the active particle. The ability to dynamically alter the propulsion characteristics will enable us to investigate and control their interactions and collective dynamics.

CPP 25.8 Wed 10:00 P3

Brainbots as smart autonomous active particles with programmable motion — •Isa Mammadli[1], Martial Noirhomme[2], Nathan Vanesse[2], Jayant Pande[3], Ana-Sunčana Smith[1], and Nicolas Vandewalle[2] — [1]PULS, Institute for Theoretical Physics, FAU Erlangen-Nürnberg, 91058, Erlangen, Germany — [2]GRASP, Institute of Physics B5a, University of Liege, B4000 Liege, Belgium — [3]Department of Physical and Natural Sciences, FLAME University, Pune, India

We introduce an innovative robotic device designed to enable controlled motion for the study of active matter. Motion is driven by an internal vibrator, powered by a compact rechargeable battery. The system integrates acoustic and magnetic sensors alongside a programmable microcontroller. Unlike conventional vibrobots, this device employs a motor that generates horizontal vibrations, producing cycloidal trajectories that have been thoroughly characterized and optimized. Specific segments of these trajectories can be harnessed to create tailored motion patterns. As a proof of concept, we demonstrate how this versatile system can be used to develop active particles exhibiting diverse dynamics, ranging from ballistic motion to run-and-tumble diffusive behavior. Based on experimental data, we provide a simulation routine capable of replicating these trajectories, enabling the generation of extended datasets and the exploration of various input velocity configurations. This approach facilitates the determination and prescription of optimized input parameters for applications such as enhanced search strategies and precise path following.

CPP 25.9 Wed 10:00 P3

Fundamental Measure Theory for active hard discs — •Jonas Buba and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The behavior of active soft particles has been studied extensively and provides a good model for many active matter systems [1]. However, some systems might be described more accurately by considering hard particles instead. While active soft particles have been described with a Phase Field Crystal approach (e.g., in [2]), a similar description of active hard particles is still lacking. In our approach we use Fundamental Measure Theory [3] to model hard discs and add activity. We expect to gain further insight into the role that the particle type can play in dynamical pattern formation.

[1] Marchetti M C, Joanny J F, Ramaswamy S, Liverpool T B, Prost J, Rao M and Simha R A. Hydrodynamics of soft active matter. Rev. Mod. Phys. 85 1143, 2013. [2] Arold D and Schmiedeberg M. Mean field approach of dynamical pattern formation in underdamped active matter with short-ranged alignment and distant anti-alignment interactions. J. Phys.: Condens. Matter 32 315403, 2020. [3] Roth R, Mecke K, and Oettel M. Communication: Fundamental measure theory for hard disks: Fluid and solid. The Journal of Chemical Physics, 136(8):081101, 2012.

CPP 25.10 Wed 10:00 P3

Many-Body Dynamics of actively rolling fibers — •Alex Arnhold[1], Falko Ziebert[1,2], and Igor M Kulic[3,4] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany — [3]Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg, France — [4]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany

Fiberboids are active filaments, capable of self-propulsion, whose dynamics were recently described in [A. Bazir, A. Baumann, F. Ziebert, I. M. Kulić, Soft Matter 2020]. So far, only single and simple 2-body dynamics of fiberboids were described.

In this work we will take a first look at the many-body dynamics. Specifically, we analyze a system of multiple nylon-rods, which when heated from below display self-propelled rolling motion. Confining the rods to roll on a single axis only, implements a simple realization of an 1D active gas. We analyze the experiments concerning clustering and nonequilibrium fluctuations and rationalize the system by simple lattice models.

CPP 25.11 Wed 10:00 P3

Pumping currents and formation of flocks in 1D Ising model — •Adrian Morais Cabral and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Non equilibrium systems create phenomena that are not observed in equilibrium counterparts, such as long range order in two or less dimensions and breaking of detailed balance.

We use an effective description of coupled Langevin equations to study a 1D system where an Ising order parameter is coupled to a charge density. Our assumption is that the charge current has a contribution proportional to the order parameter for the driven system. The formation of domain walls leads to a source of dynamical frustration for the charge. Driving disallows the formation of domain walls and creates flocking blob like states in addition to constant ordered and disordered states and a non moving spike phase. These solutions are studied numerically in 1D for $T \geq 0$.

At $T = 0$, we characterize existing flocking solutions and compare analytical predictions to numerical simulations which agree well with only one fitting parameter.

At finite temperatures we find new dynamics for the flocking state such as reversals similar to the active Ising model and (quasi) crossings. However, we have not yet been able to answer whether the existing ordered phase is stable in 1D.

CPP 25.12 Wed 10:00 P3

Statistical Field Theory for Vicsek-type models — •Carsten Littek, Falko Ziebert, and Matthias Bartelmann — Institut für Theoretische Physik, Universität Heidelberg, Germany

Dry, aligning, dilute active matter systems display a wide range of emergent phenomena such as collective, orientationally ordered motion and phase separation. The self-propelled particles in such systems undergo noisy aligning interactions with their neighbours, but they do not exchange momentum with their surrounding. While microscopic and hydrodynamic descriptions, whose connection involves approximations, exist, their predicted behaviour - such as scaling exponents - do not match.

Here we present a microscopic statistical field theory for active Brownian particles inspired by Mazenko (2010). In our formulation we interpret the particles' two-dimensional positions and their direction of motion as Martin-Siggia-Rose (MSR) fields to obtain a path integral representation of the N-particle partition function. The MSR action is augmented by a two-particle interaction that aligns particle directions either ferromagnetically as in the Vicsek model or nematically. Similar to quantum many-body theory the benefit of our field theoretic formulation of Vicsek-type models is that it allows for developing a self-consistent perturbation theory and using renormalization techniques. Our aim is the calculation of density and velocity correlation functions in the homogeneous ordered phase and the transition into the ordered phase.

CPP 25.13 Wed 10:00 P3

Coupling reaction-diffusion and locomotion in vegetative cells — •Blaž Ivšić[1], Piotr Nowakowski[2], Igor Weber[2], and Ana Sunčana Smith[3,2] — [1]Institut za fiziku, Zagreb, Croatia — [2]Institut Ruđer Bošković, Zagreb, Croatia — [3]Friedrich-Alexander- Universität, Erlangen, Germany

Cellular locomotion involves the dynamic interplay between signaling molecules, cytoskeletal activity, and membrane deformation. We present a computational model coupling protein Rac1 reactiondiffusion dynamics to cell locomotion to study vegetative state of amoeba Dictyostelium discoideum. Rac1 regulates actin polymerization via effectors like WASP and Arp2/3, while GAP modulates its activity. The model captures Rac1 dynamics on a deforming membrane, reproducing experimentally observed spatiotemporal patterns.

Cell shape is modeled using a Level-set method to track membrane dynamics, driven by forces linked to Rac1 concentration. Specifically, surface tension and normal forces (due to interaction of the cell with the substrate) proportional to Rac1 concentration influence membrane movement. The dynamics are conveyed through a fluid velocity field obtained by solving a time-dependent Stokes equation.

Our model replicates Rac1 activity patterns seen in live-cell imaging and links these patterns to cell motility. By bridging Rac1 reactiondiffusion dynamics with membrane mechanics, the model provides insights into the mechanisms of actin-driven locomotion in vegetative cells.

CPP 25.14 Wed 10:00 P3

Numerical Simulation of Microplastic Permeation in Soil: from Solutes to Particles — •Hao Liu[1], Yifan Lu[2], Christina Bogner[2], Martin Lörder[1], and Stephan Gekle[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]University of Cologne, Cologne, Germany

Microplastics have become significant environmental pollutants, raising concerns about their accumulation and distribution across ecosystems. Although terrestrial environments, particularly soils, often exhibit high levels of microplastic contamination, they remain relatively understudied. Microplastic transport in soil involves complex interactions among particle properties, soil structure, and fluid dynamics. Understanding mechanisms such as permeation, aggregation, and degradation is essential for effective environmental risk assessments and strategies to control microplastic pollution.

This study aims to simulate and predict soil hydraulic conductivity in microplastic-laden flows. Challenges include modeling behaviors of microplastic particles as they transport in soil with complex porous structures. High-resolution μCT scans of soil samples will provide the necessary porous media data, and simulations will be conducted using FluidX3D software. The research progresses in two phases: first, disregarding particle size and shape to analyze solute transport mechanisms; second, incorporating detailed particle properties to study transport and accumulation in pores. The goal is to model microplastic dynamics for accurate predictions of microplastic distribution in soil systems.

CPP 25.15 Wed 10:00 P3

Thermo-Osmotic Flows via Anti-Stokes Cooling — •akshay kallikkunnath[1], kamil bruchal[2], pawel karpinski[2], and frank cichos[1] — [1]Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Germany — [2]Faculty of Chemistry, Institute of Advanced Materials, Wroclaw University of Science and Technology, Poland

Fluidic manipulation has gained huge interest over time especially with the studies on metal nanoparticles as optically controlled heat sources generating temperature gradients. With recent developments in the synthesis of lanthanide doped crystals which can be cooled by anti- stokes cooling, we try to bring laser cooling of microcrystals to the field of fluidics. In this work, we optically trap and cool ytterbium doped NaYF4 crystals by means of anti-stokes cooling. Temperature measurements for such microscale cooled crystals are done using a technique which utilizes the phase transition of liquid crystals. With such a thermal gradient created using cold sinks in liquid, we study and provide for the first time experimental and numerical results for flows generated at solid-liquid boundary, i.e., thermo-osmotic flows. The results will provide further scope for studying dipolar thermo-osmotic and corresponding thermo-electric fields in an electrolyte solution generated by arranging optically heated and cooled particles together. Our findings can have direct implications on the study of temperature-dependent biochemical processes which inhibit with lower temperature or on response of a biological specimen to low temperature stress or may even find application in local cryotherapy.

CPP 25.16 Wed 10:00 P3

Thermodynamically consistent coarsening model of crossover placement in meiosis — •Marcel Ernst[1,2] and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universität Göttingen, Germany

Crossovers play an important role in meiosis, ensuring correct segregation of homologous chromosomes and increasing genetic variability. A recently proposed model suggests that crossover placement is determined by biomolecular condensates that coarsen by exchange and diffusion of a protein along chromosomes, consistent with experiments. We here present an extended model including exchange with the nucleoplasm based on thermodynamic principles. We study theoretically and numerically the initial protein loading onto the chromosome, the droplet growth regime, the coarsening regime, and the final equilibrium. We derive scaling laws for the number of crossovers analogous to Lifshitz-Slyozov-Wagner theory in different limits. Finally, we investigate the effect of protein exchange with the nucleoplasm on crossover placement and compare the results with empirical data from several species. In conclusion, our model allows us to explain key features of meiotic crossover placement in wild type and several mutants.

CPP 25.17 Wed 10:00 P3

A lattice Boltzmann approach to electrolytic multiphase flows — •Alexander Reinauer and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

Simulating electrolytic multiphase flow presents significant challenges, often requiring either the detailed modeling of large numbers of particles or solving complex, nonlinear partial differential equations, such as the Navier-Stokes and Nernst-Planck equations. While particle-based simulations provide molecular details, continuum-scale approaches, including the Navier-Stokes and Nernst-Planck equations, enable the study of larger systems relevant to applications in oil recovery, biological processes, and waste treatment.

In this work, we extend the Lattice Boltzmann Method using a Color-Gradient approach to simulate immiscible two-phase flow, coupled with a custom Nernst-Planck solver for the transport of dissolved charged species. This coupling allows to incorporate the preferential solubilities of chemical species.

Our implementation, based on the pystencils/lbmpy framework, generates highly optimized code for both CPU and GPU architectures. To validate the model, we performed simulations of freely suspended liquid droplets subjected to an external electric field. Additionally, we explored contact angle models and initiated studies on applying the approach to porous media under varying conditions.

CPP 25.18 Wed 10:00 P3

Coarsening of chemically active droplets — •Stefan Köstler[1,2], Yicheng Qiang[1], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Droplets formed by phase separation play an important role in cellular organization and are widely used in the design of synthetic cells and lab-on-chip devices. Droplet emulsions typically coarsen due to surface tension and hydrodynamic effects, which generally prevents precise control over droplet sizes. While coarsening can be suppressed by active chemical reactions, it is unclear how these reactions affect the coarsening dynamics and control droplet sizes. To elucidate this, we numerically simulate a binary mixture that phase separates and undergoes reactions. We find three different dynamical regimes: Small droplets are dominated by coalescence due to hydrodynamic advection, then transition to an Ostwald ripening regime dominated by diffusion, and finally exhibit size control by active chemical reactions. We predict the transition from ripening to size control analytically, and we validate our analytical estimate of the final size using a numerical minimization of a surrogate equilibrium free energy. Our theory provides an improved understanding of coarsening mechanisms, allowing to achieve greater control of emulsions.

CPP 25.19 Wed 10:00 P3

Zetapotential of Gold Surfaces in a Flow Cell — •Mattis Rasenat, Peter Vogel, Marcus Witt, and Thomas Palberg — Johannes Gutenberg Universität Mainz

We present a case study on the zeta-potential of gold surfaces in a continuous flow cell. The charge of dielectric surfaces is of high interest for technological applications. Therefore, we measure the zeta potential of polymer particles in a custom-made electrokinetic flowthrough cell with exchangeable sidewall. The zeta potential is measured with a super-heterodyne light scattering setup.

CPP 25.20 Wed 10:00 P3

Use of molecular CO_2 for surface charge regulation — Peter Vogel[1], Markus U. Witt[1], David Beyer[2], Christian Holm[2], Muhammad Navaz Qaisrani[3], Marialore Sulpizi[4], and •Thomas Palberg[1] — [1]Inst. of Physics, JGU, Mainz, Germany — [2]Inst. of Computational Physics (ICP), U Stuttgart, Stuttgart, Germany — [3]MPI for Polymer Research, Mainz, Germany — [4]Dept. of Physics, RU Bochum, Bochum, Germany

In deionized water CO_2 forms carbonic acid which partially dissociates. Such 'realistic' salt free systems contain a significant background electrolyte concentration and a pH of 5.5. Both lowers the effective charge of dielectric surfaces. Surprisingly, the remaining molecular CO_2 causes an additional drastic decharging effect, even to complete decharging in water equilibrated against pure CO_2. Molecular CO_2 acts directly on the degree of dissociation and thus lowers the bare charge, while effective charges merely follow suit. MD simulations show the formation of a diffusely adsorbed monolayer of CO_2, which locally lowers the dielectric constant. Based on this we suggested dielectric charge regulation as novel decharging mechanism. If then salts are added to the carbonized surfaces, one finds recharging by co-ion adsorption. This process is favoured by hydrophobicity, by co-ion size and, most important, also by the amount of adsorbed CO_2. Given the ubiquity of dielectric surfaces in contact with aqueous electrolytes, this very general charge regulation processes appear to be of great fundamental and practical importance.

CPP 26: Nanostructures, Nanostructuring and Nanosized Soft Matter I

Time: Wednesday 11:30–13:00 Location: H34

Invited Talk CPP 26.1 Wed 11:30 H34

Polyelectrolytes in the confined space of mesopores for transport regulation — •Annette Andrieu-Brunsen — Technische Universität Darmstadt, Macromolecular Chemistry - Smart Membranes, Germany

Nanopores are a key component in various technologies from oil production, separation and sensing, to drug delivery or catalysis and energy conversion. In contrast to technological pores, biological pores and channels demonstrate highly precise transport being directed, highly selective, and gated. A key factor to this performance is their nanoscale structure, and their local control on charge regulation and polarity in confined space. Inspired by this performance and precision we are interested in understanding the relation between the design of polymers in nanoscale space and its resulting properties to for example understand and advance transport performance of technological pores.

This talk will give insights into the interplay of polymer functionalization of mesoporous layers and resulting ionic mesopore accessibility. Among others, the effect of increasing polyelectrolyte amount and thus increasing charge density as well as the influence of polymer chain composition and the observation of confinement-induced pKa shifts will be discussed. Furthermore, ionic transport regulation by gradually adjusting the wettability of mesopores will be demonstrated including the influence of nanoscale wettability step-gradients in mesoporous silica layers. To indicate next steps our activities towards increasing precision in polymer functionalization of mesoporous silica materials will be outlined.

CPP 26.2 Wed 12:00 H34

Infrared Scanning Near-Field Spectroscopic Insights into Self-Assembled Block Copolymer Nanostructures — •Nadine von Coelln[1], Britta Weidinger[2], Christian Huck[1], Irene Wacker[3], Ronald Curticean[3], Rasmus R. Schröder[3], Eva Blasco[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]IMSEAM — [3]BioQuant, Heidelberg University, Germany

Block copolymers (BCPs) are known for their ability to self-assemble into a variety of morphologies on the nanometer scale. While the self-assembly of 2D thin films has been extensively investigated, less attention has been paid to 3D bulk morphologies. In this work, the internal nanostructure of long-range ordered 3D bulk morphologies of a well-defined diblock copolymer consisting of polystyrene and a methacrylate-based copolymer is studied by means of infrared scanning near-field optical microscopy (IR-SNOM). We demonstrate that by irradiation at an absorption band specific to one polymer block, it is possible to chemically image the blocks nano-ordered spatial arrangement [1]. Representative images were successfully correlated with scanning electron microscopy (SEM) data. By altering the molar fraction of polymer blocks, a variety of nanostructures was imaged. For some polymer compositions, the nanostructure formed was observed to change upon post-functionalization. Additionally, nanotomography of the bulk material is approached by imaging and volume reconstruction of serial sections.

[1] B. Weidinger, N. von Coelln et al., Polym. Chem., **15** (2024) 4093-4100.

CPP 26.3 Wed 12:15 H34

Star-like molecular brushes with poly(2-oxazoline)-based amphiphilic diblock copolymer side arms — •Wenqi Xu[1], Laura Fietzke[2], Rustam A. Gumerov[3], Feifei Zheng[1], Peiran Zhang[1], Cy M. Jeffries[4], Dmytro Soloviov[4], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Faculty of Chemistry and Food Chemistry, Technical University of Dresden, Dresden, Germany — [3]DWI Leibniz Institute for Interactive Materials, RWTH Aachen University, Aachen, Germany — [4]EMBL at DESY, Hamburg, Germany

Poly(2-oxazoline)s (POx) are synthetic, non-toxic, and biocompatible polymers developed to replace the increasingly immunogenic poly(ethylene glycol) in biomedicine. Among many architectural variants of POx, studies on POx-based star brushes are still scarce. In the present work, we investigate molecular brushes, in which diblock copolymers from hydrophilic poly(2-methyl-2-oxazoline) and hydrophobic poly(2-*n*-butyl-2-oxazoline) are grafted onto star-shaped poly(methyl methacrylate) backbones with the stars having functionalities ranging from 2 to 5. The size and shape of the star brushes were investigated in dilute aqueous solutions using computer simulation, dynamic light scattering, and synchrotron small-angle X-ray scattering. Our results show that these star brushes form ellipsoids with different degrees of elongation. Moreover, a size growth is found for the star brushes at high temperatures, which is attributed to the aggregation of the amphiphilic side arms.

CPP 26.4 Wed 12:30 H34

STED-inspired optical lithography beyond acrylates — Sourav Islam, Georgii Gvindzhiliia, and •Thomas A. Klar — Institut für Angewandte Physik, Johannes Kepler Universität Linz, Austria

STED-inspired[1], and hence sub-diffractional, nanolithography was so far restricted to free radical polymerizations, predominantly of (meth)acrylates.[2] We now expand the STED-inspired toolkit to cationic[3, 4] and oxidative polymerizations,[5] comprising the technologically important classes of epoxides and pi-conjugated polymers. In both cases, we achieved structure sizes below 100 nm using transient-state absorption depletion (TAD) in systems comprising depletable photosensitizers, optionally combined with onium salts. The pi-conjugated nanostructures are particularly intriguing, because they potentially will allow for sub-diffractional organic electronic devices.

[1] Klar, Hell, Opt. Lett. 24, 954 (1999). [2] Fischer, Wegener, Las. Phot. Rev. 7, 22 (2013). [3] Islam, et al., J. Phys. Chem. C 127, 1873 (2023). [4] Islam, Klar, ACS Omega 9, 19203 (2024). [5] Islam, et al., Proc. SPIE 1299503(2024).

CPP 26.5 Wed 12:45 H34

In-situ investigation of the lateral and vertical structure of PNIPAM-microgels at the air-liquid and solid-liquid interfaces — Olaf Soltwedel, Joanne Zimmer, •Hayden Robertson, and Regine von Klitzing — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

The novel surface characterisation approaches presented here highlight, for the first time, the use of both specular and off-specular X-ray reflectivity (XRR) to probe the vertical and lateral structure of adsorbed polymer microgels particles at various interfaces, offering *in situ*, non-invasive insights without the need for doping or transfer-induced artefacts. In particular, we demonstrate the complementarity of two readily accessible laboratory techniques on characterising the structure of adsorbed microgels: atomic force microscopy (AFM) and XRR. Initial *ex situ* AFM scans of Langmuir-Blodgett deposited microgels at the solid interface revealed strong lateral 2D hexagonal ordering across a broad range of surface pressures. However, for the first time, these results are confirmed by off-specular XRR, demonstrating the existence of the hexagonal long-range ordering at low and intermediate surface pressures for *in situ* conditions at the air-water interface. Upon uniaxial compression of the interface, the microgel lattice constants decrease monotonically, indicating tighter packing. At these higher surface pressures, both AFM and off-specular XRR also reveal the formation of microgel domains; hexagonal short-range ordering is maintained whereas long-range ordering is diminished.

CPP 27: Molecular Electronics and Excited State Properties II

Time: Wednesday 11:30–13:00 Location: H38

CPP 27.1 Wed 11:30 H38

Break-junctions beyond single-molecule conductance — •Joseph Hamill — Department of Chemistry and Nanoscience Center, University of Copenhagen, Denmark

The challenge in nanosciences is to reliably manipulate and probe objects on the atomic and molecular scale. Single-molecule break junctions cleverly integrate a single molecule into an electric circuit, enabling measurement of its thermal, electrochemical, and electrical properties. These studies explore candidates for waste heat capture, quantum information technologies, sensors, nanomedicine, and other novel materials applications. Over the past 20 years, single-molecule break junction methods have advanced to measure current, resistance, rectification, and thermopower. Despite this progress, they are not yet a staple in every chemist's toolbox like NMR spectroscopy. Recent studies using these junctions to monitor and induce chemical reactions may change this. I will present two recent studies demonstrating their sensitivity to changes in bonding chemistry and the tautomer state of single molecules in the junction. This sensitivity is unlocked through frequency domain spectroscopy using flicker noise analysis[1] and improved machine learning approaches, such as principal component analysis and k-means clustering.[2]

[1] U. Rashid, W. Bro-Jørgensen, K. Harilal, P. Sreelakshmi, R. R. Mondal, V. Chittari Pisharam, K. N. Parida, K. Geetharani, J. M. Hamill, and V. Kaliginedi. JACS, 146, 9063-9073. [2] P. Sreelakshmi, R. Mahashaya, S. Leitherer, U. Rashid, J. M. Hamill, M. Nair, P. Rajamalli, and V. Kaliginedi. JACS, 10.1021/jacs.4c12423.

CPP 27.2 Wed 11:45 H38

Charge transport in organic semiconductors with a mapping approach to surface hopping — •Johan Runeson[1], Thomas Drayton[2], and David Manolopoulos[2] — [1]Institute of Physics, University of Freiburg, Germany — [2]Physical and Theoretical Chemistry Laboratory, University of Oxford, UK

Coupled charge-phonon systems are challenging to simulate in the intermediate regime between traditional delocalized band theory and localized polaron theory. In particular, it remains unclear which methods are suitable to describe organic semiconductors. Conventional trajectory-based methods, such as Ehrenfest dynamics and surface hopping, do not capture the correct equilibrium of mixed quantum-classical systems. In this talk, I will present a simple solution to this problem. Based on a recently developed "mapping approach to surface hopping" [1,2], we propagate trajectories on the adiabatic state with the highest population, which in contrast to previous methods is consistent with the correct quantum-classical equilibrium. We applied this methodology to charge diffusion in crystalline rubrene [3] and obtained a well-defined diffusion constant, without having to introduce the phenomenological relaxation time approximation (RTA). Our results give 30-60 % higher charge mobilities than conventional RTA calculations and shed light on experiments of the optical conductivity.

[1] J. R. Mannouch and J. O. Richardson, J. Chem. Phys. 158, 104111 (2023). [2] J. E. Runeson and D. E. Manolopoulos, J. Chem. Phys. 159, 094115 (2023). [3] J. E. Runeson, T. J. G. Drayton, and D. E. Manolopoulos, J. Chem. Phys. 161, 144102 (2024).

CPP 27.3 Wed 12:00 H38

Influence of Classical Molecular Motion on Energy Transport in Molecular Aggregates — •Ritesh Pant[1], Sebastian Wüster[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Indian Institute of Science Education and Research, Bhopal, India

Molecular aggregates can transport electronic excitation energy over large distances due to dipole-dipole interactions [1]. We explore the impact of classical thermal motion of entire monomers on this transport, considering a chain of molecules [2]. Such motion induces changes in the aggregate's geometry, thereby altering the exciton states and enabling, in certain regimes, the adiabatic transport of excitation energy. We find that, in the absence of intramolecular vibrations, the interplay between molecular motion and exciton dynamics induces oscillatory behavior in site populations, which are coupled to the motion. These oscillations occur specifically when the molecular motion is slow enough to be considered adiabatic with respect to the exciton dynamics, and their characteristics depend on the chain length, with shorter chains exhibiting more pronounced effects. We also explore the effect of intramolecular vibrations on this oscillatory behavior and investigate the conditions under which the oscillations persist or are suppressed.

[1] T. Brixner et. al., Adv. Energy Mater. 7, 1700236 (2017).
[2] R. Pant et. al., Phys. Chem. Chem. Phys. 22, 21169 (2020).

CPP 27.4 Wed 12:15 H38

Enhancing excitonic properties in organic semiconductors by aqueous ions — •Filip Podjaski — Department of Chemistry and Centre for Processable Electronics, Imperial College London, UK

While organics semiconductors (OSC) promise tailorable structure-function relationships for enhanced solar energy conversion abilities, advancement is often hindered by limiting knowledge of interwoven photo-physical processes and properties that lead to recombination losses on ultrafast time scales.[1] Herein, I discuss possibilities to measure and modify functionalized OSC' exciton behaviour, to address their recombination. For photocatalysis, interactions with aqueous ions, which are also relevant for enabling sea water use, are typically disregarded. Our time-resolved optical spectroscopy study on suspended polymer nanoparticles in presence of different salts shows how they can improve stabilization of excitons. We further introduce Terahertz permittivity measurements as convenient tool to probe the complex permittivity / dielectric properties of OSCs on ps-time scales. The permittivity defines exciton binding energy and is hence relevant for charge carrier photogeneration and transport. But its highly frequency dependent values are commonly extracted orders magnitude off the ps-regime. Our study focussing on carbon nitrides now reveals dielectric screening and transport properties at the early time scales of solar energy conversion process chains, and illustrates environmental enhancements enabled by ions.[2]

References: [1] Nat. Rev. Mater. 6, 168-190 (2021). [2] R. Jahangir, F. Podjaski et al., submitted, arxiv.org/abs/2411.06226

CPP 27.5 Wed 12:30 H38

Computational insights into open-shell molecules for applications in molecular electronics — •Susanne Leitherer[1] and Gemma C. Solomon[1,2] — [1]Department of Chemistry and Center of Nanoscience, University of Copenhagen, Denmark — [2]Niels Bohr Institute, University of Copenhagen, Denmark

Recent studies have explored a range of molecules with unpaired electrons, represented by their spin. These investigations focused on the charge transport characteristics of the molecules when interfaced with electrodes, as well as their structural rearrangements in electric fields and interactions with surfaces. The theoretical analysis of these systems frequently employs spin-polarized or symmetry-broken unrestricted density functional theory (DFT). This method has proven effective in modeling oxidized molecules exhibiting highly conductive low-energy states, characterized as 1D topological insulators[1]. However, it is well known that DFT can pose challenges for open-shell structures due to their multiconfigurational nature. We demonstrate how for a selection of polycyclic aromatic hydrocarbons - previously investigated in recent scanning probe experiments[2] - the ground state can be accurately determined using a multiconfigurational short-range DFT approach[3]. [1] High Molecular Conductance and Inverted Conductance Decay over 3nm in Aminium-Terminated Carbon-Bridged Oligophenylene-Vinylenes, Krieger et al, JACS (2024); [2] Atomically resolved single-molecule triplet quenching, Peng et al., Science 373 (2021); [3] Multiconfigurational sr-DFT for open-shell systems, Hedegard et al, J. Chem. Phys. 148, 214103 (2018)

CPP 27.6 Wed 12:45 H38

Exceptionally High Two-Photon Absorption Cross Sections in Quinoidal Diazaacene-Bithiophene Derivatives — •Gabriel Sauter[1], Antonia Papapostolou[2], Audrey Pollien[1], Kathleen Fuchs[3], Kerstin Brödner[3], Jan Freudenberg[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Universität Heidelberg

In nonlinear optics, materials with high two-photon absorption (2PA) cross sections are crucial for bioimaging, photodynamic therapy, and 3D nanoprinting [1]. Our study highlights quinoidal diazaacene-bithiophene derivatives with exceptional 2PA cross sections, reaching 53,600 GM (850-950 nm) and 4,100 GM (1400-1600 nm), unmatched by organic chromophores of this size [3].

Using experimental z-scan techniques and TDDFT calculations, we attribute these properties to the chromophores acceptor-π-donor-π-acceptor structure, which ensures high oscillator strength and strong state coupling. These features optimize transition dipole moment alignment, maximizing 2PA efficiency.

These findings advance the development of efficient NIR-2PA materials for photonic and biomedical applications.

References:
1. F. Kröger et al., *RSC Appl. Polym.* **2024**, 2, 847.
2. K. Fuchs et al., *Angew. Chem. Int. Ed.* **2024**.

CPP 28: Modeling and Simulation of Soft Matter III

Time: Wednesday 15:00–16:00 Location: H34

CPP 28.1 Wed 15:00 H34

Many-body potentials and optimized mapping schemes for systematic coarse-graining of small conjugated molecules — •Sayan Dutta[1,2,3], Muhammad Nawaz Qaisrani[4], Denis Andrienko[4], and Arash Nikoubashman[1,2,3] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Leibniz-Institut für Polymerforschung, Dresden, Germany — [3]Technische Universität Dresden, Dresden, Germany — [4]Max-Planck Institut für Polymerforschung, Mainz, Germany

Bottom-up coarse-graining approaches frequently focus on reproducing structural order parameters, ensuring consistency with structural properties from the underlying atomistic model. However, these methods often struggle to predict thermodynamic quantities accurately, leading to challenges in transferability. Furthermore, the coarse-grained (CG) potential is typically highly sensitive to the mapping scheme, introducing representability issues. Recent CG models increasingly enhance traditional pair potentials by incorporating a potential that depends on the local density around each CG particle, which effectively includes many-body interactions in a mean-field approximation. We introduce local density dependent potentials based framework in the CG force-field for small conjugated molecules, which are widely used in the field of organic photovoltaic materials. Our framework captures the local density around each mapped CG site to ensure structural and thermodynamic accuracy, while enhancing computational efficiency compared to its atomistic counterparts.

CPP 28.2 Wed 15:15 H34

Simulation of the fabrication of integral asymmetric polymer membranes using continuum modeling — •Gregor Häfner and Marcus Müller — University of Göttingen, Germany

Integral asymmetric polymer membranes represent a promising class of functional macromolecular systems with a wide range of potential applications, including water purification and protein separation. Their synthesis is achieved through a two-step procedure: (i) the controlled self-assembly of diblock copolymers upon solvent evaporation, to form a cylindrical morphology that is oriented perpendicular to the solution-gas interface. (ii) a solvent-non-solvent exchange, raising the polymer concentration above its glass transition, thereby freezing the matrix phase while allowing the entry of the non-solvent through the cylindrical minority domains. Below, the non-solvent macrophase separates from the polymer to form a porous sub-structure.

In order to gain insight into the physical processes, we perform computer simulations. A continuum model is employed which treats the local concentrations as order parameters and minimizes a free-energy functional. In the limit of high viscosity, the dynamics are purely diffusive, enabling comparison with a particle-based model. We use the continuum model to optimize the final membrane morphology and identifying optimal parameter regions and dependencies. Additionally, this model enables the treatment of finite viscosities. We demonstrate that in the presence of a bariocentric flow, the frozen top layer can be transported downwards to prevent the formation of macro voids beneath the isoporous top layer.

CPP 28.3 Wed 15:30 H34

Highways in pore networks — •Werner Napetschnig[1], Ekaterina Baikova[1,2], Maximilian Fuchs[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper

When simulating Stokes flow of gases through porous media, the volume flow is often explained by microstructural properties. However, most of these properties do not adequately account for the arrangement of pathways, which is strongly material dependent. Here, we highlight the importance of considering these pathways and explore different techniques to identify flow paths. A pore network model based on micro-computed tomography scans of paper samples serves as the basis for air flow simulation. Two methods are evaluated to identify transport pathways and locate the most critical flow regions. In the first method, the maximum flow rate between individual pores determines the paths. It is shown that the highest flow rate travels between fiber network layers and clusters at a few exit pores. The second method identifies paths iteratively through a stochastic approach where the flow rate is the weighting factor. We identified the most frequently used highway regions. In addition, we studied the orientation and geometric properties of these highways. Our results show that only a few segments within the highways significantly influence the overall flow. Therefore, these highways need to be numerically represented when defining the explanatory microstructure properties.

CPP 28.4 Wed 15:45 H34

A lattice Boltzmann study of bijels as a novel type of catalyst support structure — •Johannes Martinus Peter Beunen and Jens Harting — Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Cauerstraße 1, 91058 Erlangen, Germany

Due to their high surface area to volume ratio porous media are very suitable as catalyst support materials. However, the stochastic morphology of commercially available supports generally results in poor reaction product transport and inefficient use of the therein-contained catalyst material. These issues can be alleviated by making use of catalyst supports acquired from spinodally derived architectures due to their beneficial percolation properties. In particular, architectures obtained from bicontinuous interfacially jammed emulsion gels (bijels) seem to provide a viable route to manufacture stable catalyst supports that resolve the aforementioned issues. In this work, this type of porous support is further investigated by means of the three-dimensional lattice Boltzmann method. First, we simulate the formation of bijels by an extension of the lattice Boltzmann method, to allow for multi-component fluids and particles with non-neutral wetting properties. We report on the improved properties of the resulting porous structures compared to stochastic equivalents for usage in chemical reactors. Hereafter, the lattice Boltzmann method is employed again to further validate the enhanced performance of bijel-derived geometries by means of reactive flow simulations. Our findings suggest that bijel-derived catalyst support structures allow for an almost threefold increase in reactor effectiveness.

CPP 29: Organic Electronics and Photovoltaics III

Time: Wednesday 15:00–16:00 Location: H38

CPP 29.1 Wed 15:00 H38

Energy band structure of image potential states of organic semiconductor on graphite studied by angle-resolved low-energy inverse photoelectron spectroscopy — •Tomoko Onishi[1] and Hiroyuki Yoshida[1,2] — [1]Chiba university, Chiba, Japan. — [2]Chiba university MCRC, Chiba, Japan.

The image potential state of the organic semiconductor molecule on the conductive surface is of particular interest because the image potential states can be sensitive probes of interfacial electronic states. Their energy band structure (the energy-momentum relation) provides detailed information about the electron behavior. Recently, we have developed the angle-resolved low-energy inverse photoelectron spectroscopy (AR-LEIPS) [1,2]. This technique allows direct observation of the unoccupied states without sample damage and with the resolution better than 0.3 eV. In this study, we applied AR-LEIPS to a monolayer of copper phthalocyanine (CuPc) on highly oriented pyrolytic graphite (HOPG). The observed band structure of the image potential state was parabolic, indicating that its nature is free-electron-like along the surface plane. By fitting the band structure to a quadratic function, we obtained the effective masses of the image potential states on HOPG and CuPc/HOPG to be (1.14 * 0.02) m0 and (1.33 * 0.08) m0, respectively, where m_0 is the electron mass. The effective mass becomes heavier due to the periodic potential induced by the CuPc molecule.[1] H. Sato, H. Ishii, H. Yoshida, et al., Nature Mat. 21, 916 (2022) [2] Y. Kashimoto, H. Yoshida et al, Rev. Sci. Instrum., 94, 063903 (2023).

CPP 29.2 Wed 15:15 H38

Fluorination of Thieno-quinoxalines enables tunable excitonic and electronic bandgaps — •Md Moidul Islam[1,2], Arthur Markus Anton[3], Shahidul Alam[4], Patrick Irmisch[3], Alexander J. Much[7], Ulrich S. Schubert[1,2], Christos Chochos[5,6], and Harald Hoppe[1,2] — [1]IOMC, FSU Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]CEEC Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig — [4]KAUST Solar Center, PSE, MSE, Thuwal 23955-6900, Kingdom of Saudi Arabia — [5]Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece — [6]Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece — [7]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Thieno-quinoxaline conjugated polymers are an interesting class of organic semiconductors. While it is known that fluorination causes shifts in the molecular energy levels to deeper binding energies, the mechanisms behind are, so far, not well characterized. In this study, six thieno-quinoxaline polymers with a systematically increased number of fluorinated sites were investigated in solutions and films. Our results indicate a strong correlation between the extend of fluorination, the molecular planarity, and its ability to form aggregates. We also demonstrate, in unprecedented detail, how these structural properties influence various behaviors related to optical and electronic properties.

CPP 29.3 Wed 15:30 H38

Extending the design space of carbazole-based TADF emitters: From photophysical insights to OLED performance — •Karolis Leitonas[1], Łukasz Łapok[2], Sebastian Schellhammer[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden — [2]Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Kraków, Poland

Although organic light-emitting diodes (OLEDs) dominate the market for mobile displays, e.g., in smartphones, designing efficient and long-lasting blue pixels remains challenging. Enhancing OLED efficiency requires effective singlet and triplet exciton harvesting - a key mechanism to minimize energy losses via non-radiative decay. Emitter materials exhibiting thermally activated delayed fluorescence (TADF) can achieve up to 100 % internal quantum efficiency (IQE) providing a promising approach for the design of efficient OLEDs. Still, their potential is not yet fully exploited due to incomplete insights into the underlying structure-property relationships and chemical design challenges. We discuss the photophysical properties of new emitters extending the class of carbazole-based TADF emitters introduced by Adachi et al. [1] and analyze their application in OLEDs.

[1] Uoyama et al. Nature 2012

CPP 29.4 Wed 15:45 H38

Predicting the molecular arrangement of organic optoelectronic materials — •Alexey Gudovannyy[1], Julia M. Schäfer[2], Olga Gerdes[2], Dirk Hildebrandt[2], Gunter Mattersteig[2], Martin Pfeiffer[2], and Frank Ortmann[1] — [1]Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Heliatek GmbH, 01139 Dresden, Germany

The morphology of the most promising molecular semiconductor materials remains highly challenging to predict from scratch. If possible, it would still require a lot of computational time and sometimes experimental data. The main obstacle here is the exponential growth with the number of molecular degrees of freedom for bulky side groups, which forces one to search on extremely complex energy surfaces. However, organic semiconductors mostly exhibit a limited set of structural motifs, primarily herringbone and two-dimensional brickwork patterns. Constraining the search to such dimensionally reduced packing possibilities simplifies the process while preserving 3D structural features. Here, we present a cost-efficient workflow for predicting thermodynamically stable 2D arrangements of molecular periodic associates, where only the molecular structural formula is required. We theoretically and experimentally investigated a set of known and newly crystallized compounds of evaporable flexible molecules with interesting optoelectronic properties, predicted their packing in two-dimensional layers, and compared them with experimentally resolved crystal structures, obtaining a very good agreement in the packing.

CPP 30: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Wednesday 16:15–18:30 Location: H34

Invited Talk CPP 30.1 Wed 16:15 H34

Challenges and Opportunities in Bringing Machine Learning to a Synchrotron — •Alexander Hexemer[1], Tanny Chavez[1], Wiebke Köpp[1], Dylan McReynolds[1], Stephan Roth[2], Tim Snow[3], and Sharif Ahmed[3] — [1]Lawrence Berkeley National Lab, Berkeley, CA 94720 — [2]DESY, Hamburg, Germany — [3]Diamond Light Source, Didcot, UK

Artificial intelligence (AI) and machine learning (ML) are transforming scientific research, offering innovative solutions to longstanding data collection, analysis, and interpretation challenges. Synchrotron facilities, which generate vast amounts of complex, high-dimensional data, present unique opportunities to leverage ML to advance materials science. Building on this potential, significant progress is being made at the Advanced Light Source (ALS) to integrate ML tools into various synchrotron applications, including tomography segmentation, autonomous scattering analysis, and multimodal data fusion. Efforts are focused on implementing ML as a service, simplifying adoption by providing web-based solutions designed for seamless use across facilities. These tools aim to enable reliable and scalable ML applications for tasks such as the segmentation of complex 3D tomography datasets and automated experimental feedback in scattering experiments. This talk will explore the evolving role of ML at synchrotrons while addressing key challenges.

CPP 30.2 Wed 16:45 H34

Deep Learning-Driven GISAXS Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Shachar Dan[1], Julian Heger[2], Peter Müller-Buschbaum[2], and Stephan Roth[1,3] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Notkestr. 85, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, Garching 5, Germany — [3]Royal Institute of Technology (KTH), Stockholm, Sweden

Nanostructured materials, are at the forefront of advanced applications in various fields, owing to their unique physical and chemical properties. Grazing incidence small-angle X-ray scattering (GISAXS) has emerged as a powerful technique for probing the morphology of these nanostructures, offering valuable insights into electron density distributions both at the surface and within thin films. In our approach, we first simulate GISAXS pattern using the Distorted Wave Born Approximation (DWBA) model to generate high-quality training datasets. We then apply deep learning techniques, specifically convolutional neural networks (CNNs), to predict size distributions from GISAXS data. Our results demonstrate that CNNs are highly robust under varying noise conditions and present a promising, time-efficient approach for overcoming the challenges of conventional scattering analysis. This study highlights the potential of integrating advanced computational methods and new analytical tools to enhance the characterization of nanostructures.

CPP 30.3 Wed 17:00 H34

Towards Closing the Autonomous Loop at Multiple Facilities: Developing Web-based User Interfaces and Data Infrastructure for Autonomous Experiments and Automated Data Reduction Workflows — •Benedikt Sochor[1,2], Wiebke Koepp[2], Tanny Chavez[2], Runbo Jiang[2], Dylan McReynolds[2], Marcus Noack[3], Raja Vyshnavi Sriramoju[2], Aidan Coffey[2], Ronald Pandolfi[3], Eric Schaible[2], Chenhui Zhu[2], Frank Schlünzen[1], Stephan V. Roth[1,4], Alexander Hexemer[2], and Sarathlal Koyiloth Vayalil[1,5] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, 94720, CA, USA — [3]Applied Mathematics and Computational Research Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, 94720, CA, USA — [4]KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [5]UPES, Applied Science Cluster, 248007 Dehradun, India

This project focuses on establishing a robust infrastructure for autonomous scattering experiments at two different synchrotrons: X-ray scattering beamlines at PETRA III (DESY, Hamburg) and at the Advanced Light Source (ALS, Berkeley), initially beamline P03, the micro- and nano-focus small- and wide-angle X-ray scattering beamline (MiNaXS) at DESY, and the SAXS/WAXS/GISAXS/GIWAXS beamline 7.3.3 at the ALS. For selected science cases, the infrastructure's capabilities to handle large datasets during time-resolved and scanning X-ray scattering experiments will be highlighted.

CPP 30.4 Wed 17:15 H34

Imaging techniques for characterization of organic photonic devices utilizing digital luminescence — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

The generally spin-forbidden T_1-S_0 transition of organic molecules gives access to pronounced long-lived room temperature phosphorescence in surprisingly many molecules, but is easily quenched by environmental oxygen. Controlling and utilizing these competing processes has led to the development of digital luminescence as a photonic design principle and its usage in programmable luminescent tags (PLTs) for application in sensing and information storage. To study and utilize this persistent luminescence, a spatially and temporal resolved imaging technique allows us to extend the characterization of these phenomena beyond spectroscopic measurements. By analyzing high-resolution images, differences in intensity and activation time within a single PLT can be detected, allowing conclusions as to structural irregularities. Evaluating each pixel individually also provides great insight into the statistical distribution of these values without the extensive need for samples and measurements. Thus, imaging techniques offer an excellent extension to the characterization of material systems for digital luminescence and by that allowing us to understand and optimize structure-property relationships. This represents an important step towards the use of PLTs for information storage and exchange.

CPP 30.5 Wed 17:30 H34

3D Nanoprinted Polarization Optics Directly on Optical Fibers — •Tim Stechel — Leibniz Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena, Germany

Polarization is a fundamental property of electromagnetic radiation, influencing numerous areas of physical sciences and optical technologies. Developing functional interfaces that seamlessly integrate polarization control with fiber optics opens new opportunities for advancing these technologies. Using two-photon polymerization, we fabricate 3D structures on the sub-micron scale, directly on optical fibers. This high-resolution additive manufacturing technique enables the creation of tailored microstructures that can precisely control the polarization state of light as it enters and exits fibers. These custom interfaces are highly adaptable to different fiber types and optical configurations, allowing for enhanced polarization shaping and analysis. In this talk, we present the design process, fabrication process and characterization of the fabricated structures. Our approach combines the versatility of 3D printing with the precision required for nanoscale optical engineering, providing a robust platform for research into light-matter interactions and advancing fiber-based photonic technologies. Potential applications span diverse fields, from telecommunications to advanced optical metrology, demonstrating the broad impact of integrating 3D-printed microstructures with fiber optics.

CPP 30.6 Wed 17:45 H34

Phase-cycling and double-quantum two-dimensional electronic spectroscopy using a common-path birefringent interferometer — Daniel Timmer[1], •Daniel C. Lünemann[1], Moritz Gittinger[1], Antonietta De Sio[1], Cristian Manzoni[2], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany — [2]Politecnico di Milano, Italy

Ultrafast coherent spectroscopy techniques provide unique insights into the coherent dynamics of atomic, molecular and solid state quantum systems. For this, an experimentally challenging but all the more powerful technique is two-dimensional electronic spectroscopy (2DES), which allows to selectively probe coherent and incoherent couplings and to isolate individual excitation pathways by controlling the absolute phases of the ultrashort optical pulses that interact with the system (phase-cycling, PC). Its experimental implementation can be greatly simplified by employing birefringent in-line interferometers (TWINS) which are inherently phase stable. However, TWINS is so far considered to be incapable of this phase control. Here, we demonstrate PC capabilities for 2DES using an adapted TWINS interferometer by recording rephasing, non-rephasing, zero-quantum and double-quantum 2DES on a molecular J-aggregate. This extension is easy to implement and enables new experimental capabilities for TWINS-based 2DES in multidimensional all-optical and photoemission spectroscopy and microscopy.

[1]: D Timmer, DC Lünemann, et al., Optica (accepted, DOI: 10.1364/OPTICA.543007)

CPP 30.7 Wed 18:00 H34

Real-time structure-transport investigation under mechanical strain in flexible carbon-based conductive polymer nanocomposites — •Sarathlal Koyiloth Vayalil[1,2], Vaishnav B[2], Benedikt Sochor[1], Stephan V. Roth[1,3], Ajay Gupta[2], Tobias Kraus[4,5], and Debmalya Roy[6] — [1]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [2]Department of Physics, Applied Science cluster, UPES, Dehradun 248007, India — [3]Division of Coating Technology, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — [4]INM Leibniz-Institute for New Materials, 66123 Saarbruecken, Germany — [5]Colloid and Interface Chemistry, Saarland University, 66123 Saarbruecken, Germany — [6]DMSRDE, Kanpur 208013, India

In this work, an in situ ultra-small angle X-ray scattering combined with electrical transport measurements under mechanical strain has been carried out in flexible, conductive carbon polymer nanocomposite to observe the real-time structural variations in nanofiller morphologies and distribution. For this purpose, the non-polar and polar elastomers viz. polydimethylsiloxane and polyurethane respectively, loaded with 0D Carbon black, 1D Carbon nanotubes, and 2D Graphene has been employed. The study has elucidated that, it is the filler′s fractal dimension that varies rather than aggregate distribution upon stress that decides PNC′s electrical conduction. Further, a novel relationship has been established between fractal dimension and composite′s conductivity, which invincibly guides in designing wearable and flexible conductors.

CPP 30.8 Wed 18:15 H34

In Situ Synchrotron X-Ray Computed Tomography Studies of Specialty Optical Fibers — •Ali Karatutlu[1], Zehra Gizem Mutlay[1], Andriy Budnyk[1], Gianluca Iori[2], Philipp Iori[3], and Bülend Ortaç[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Paul Scherrer Institute PSI Forschungsstrasse 111 5232 Villigen PSI Switzerland — [3]SESAME - Synchrotron-light for Experimental Science and Applications in the Middle East, Allan, 19252, Jordan

Specialty fibers have complex structures due to their geometry, including glass core and cladding, multilayered polymer coatings, and the variations of their elemental compositions. Such complex structures of the specialty and microstructured fibers with air holes and the deformation due to manufacturing fiber lasers during fiber splicing can be investigated by X-ray computed tomography (XCT). The fiber fabrication process includes deposition and post-processes with a subsequent fiber drawing. Here, we present the first official results performed at the station BEATS, SESAME, for the synchrotron XCT imaging of specialty optical fibers all in one, such as polarization-maintaining, active, and photonic crystal fibers. In addition, temperature-dependent XCT measurements provided information on how inner structures, such as polymer coatings, could evolve for PM fibers. The conditions of the XCT measurements and the inner structure of the same type of fibers were found to be crucial and act as the guidelines that will be presented for the structures with sizes close to the voxel size.

CPP 31: Responsive and Adaptive Polymers

Time: Wednesday 16:15–18:00 Location: H38

Invited Talk CPP 31.1 Wed 16:15 H38

Moving with minimum effort – Optimal work protocols for systems with memory — •Sarah Loos[1], Samuel Monter[2], Felix Ginot[2], and Clemens Bechinger[2] — [1]DAMTP, University of Cambridge, UK — [2]University of Konstanz

Energy optimization is crucial in engineering and may also govern nonequilibrium processes in chemical and biological systems. Finding optimal solutions for microscale processes–dominated by thermal or nonthermal fluctuations and often displaying memory effects arising from internal degrees of freedom or coupling to viscoelastic environments–posses additional challenges, necessitating general guiding principles. We demonstrate such a general principle for the fundamental problem of dragging a harmonic trap containing a single particle over a finite distance within a given time while minimizing work input. We show that the optimal dragging protocol and the corresponding mean particle trajectory both exhibit time-reversal symmetry, which is a universal and exclusive feature of the optimal solutions. The symmetry principle holds across all media described by a linear generalized Langevin equation, irrespective of the memory kernel or noise properties, including glassy, granular, and active media. For intrinsically driven systems, such as active particles, we show that the optimal protocols remain identical to those for passive systems, but work fluctuations are always increased [2]. [1] S.A.M. Loos, S. Monter, F. Ginot, and C. Bechinger, Phys. Rev. X 14, 021032 (2024). [2] R. Garcia-Millan, J. Schüttler, M.E. Cates, and S.A.M. Loos, ArXiv:2407.18542 (2024).

CPP 31.2 Wed 16:45 H38

Influence of Azobenzene Moieties on the Swelling Behavior of Poly(Dimethylacrylamide) Films in Water Vapor under UV-Irradiation — •David P. Kosbahn[1], Julija Reitenbach[1], Morgan P. Le Dû[1], Lukas V. Spanier[1], René Steinbrecher[2,3], André Laschewsky[2,3], Robert Cubitt[4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm, Germany — [3]Fraunhofer Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — [4]Institut Laue-Langevin, 38000 Grenoble, France

This study investigates the swelling behavior of p(AzAm-co-DMAm) films in both isomeric states of the photoswitchable molecule azobenzene (Az). The impact of UV irradiation on swelling in water vapor is examined, with the aim of controlling water uptake, expansion, and nanoscale morphology. This material shows potential for applications in light sensors, photo-actuators, and drug delivery systems. We employ time-resolved FTIR spectroscopy to monitor group vibrations during swelling and irradiation, gaining insights into molecular interactions throughout the isomerization process. Additionally, in situ time-of-flight neutron reflectometry on a thin film provides time- and depth-resolved data on the water distribution along the surface normal. The results shed light on the influence of azobenzene moieties on the polymer's microscopic properties.

CPP 31.3 Wed 17:00 H38

Critical analysis of adhesion work measurements from AFM-based techniques for soft contact — Dmitrii Sychev[1,2], Simon Schubotz[1,2], Quinn A. Besford[1], Andreas Fery[1,3], and •Günter K. Auernhammer[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]TU Dresden, Germany — [3]Chair of Physical Chemistry of Polymeric Materials,TU Dresden, Germany

The work of adhesion is a thermodynamic quantity that is frequently measured by atomic force microscopy (AFM). Its determination requires quasi-equilibrium measurements. Here, we address the question of to what extent atomic force microscopy qualifies for quasi-equilibrium measurements. To measure the work of adhesion, we combined soft colloidal probe AFM (SCP AFM) with reflection interference contrast microscopy (RICM). We extract the work of adhesion either from the pull-off force or from the contact radius to measure the adhesion behavior of poly(N-isopropylacrylamide) (PNIPAM) polymer brushes in the swollen and solvent-induced collapsed state. In the swollen state, the adhesion to the PNIPAM brush was fivefold larger and exhibited significant time dependencies when measured with SCP AFM. A strong rate dependence of the pull-off force method was indicative of a non-equilibrium process. In order to reliably determine the equilibrium work of adhesion, the contact radius method was found to be the better because it is not rate dependent. In summary, using optical measurements to determine the contact radius is beneficial when deriving the works of adhesion between colloidal probes and polymer brush surfaces.

CPP 31.4 Wed 17:15 H38

Chain conformation of thermo- and photo-responsive polymers — •Peiran Zhang[1], René Steinbrecher[2], Cy M. Jeffries[3], André Laschewsky[2], Peter Müller-Buschbaum[1], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Institute of Chemistry, University of Potsdam, Potsdam-Golm, Germany — [3]European Molecular Biology Laboratory, DESY, Hamburg, Germany

Endowing thermoresponsive polymers with additional photoresponsivity is of interest for applications such as drug delivery and soft robotics, owing to the non-invasive nature of these stimuli and the high temporal and local resolution of the photostimulus. The lower critical solution temperature (LCST) behavior in aqueous solution, characterized by a coil-to-globule transition at the cloud point (CP), can be finely tuned by incorporating photoswitches. Among these, azobenzene (AB) is the most widely used due to its pronounced trans-cis isomerization without side reactions. However, due to the weak change of dipole moment, its influence on the CP is only small. To enhance this photo effect, we used various amino acids as flexible linkers between the thermoresponsive backbone and the AB moiety. Dynamic light scattering reveals that a higher AB content leads to a larger shift of the CP, while small-angle X-ray scattering indicates that the amino acid linker reduces the influence of the inherent rigidity of the AB side groups, making the entire polymer chain more flexible. This approach allows adjusting the CP in wide ranges of temperature, thereby enhancing the range of applications.

CPP 31.5 Wed 17:30 H38

Acoustic levitation for dynamic studies of poly(N-isopropylacrylamide) microgels at the air-water interface — •Atieh Razavi[1], Regine von Klitzing[1], Romain Bordes[2], and Amin Rahimzadeh[1] — [1]Soft Matter at Interfaces, Institute for condensed Matter Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany — [2]Applied Surface Chemistry, Chalmers University of Technology, Gothenburg, Sweden

Acoustic levitation provides a unique platform for studying the surface dynamics of an air-water interface covered with poly(N-isopropylacrylamide) (PNIPAM) microgels. By utilizing standing acoustic waves, droplets are trapped at nodal positions, creating a contact-free environment to examine the effects of microgel stiffness, droplet evaporation, and amplitude modulation on droplet deformation. The research focuses on quantifying the aspect ratio (AR) of levitated droplets as a function of frequency of amplitude modulation, microgel concentration, and cross-linker content over time. In addition, we modulate the amplitude of the acoustic pressure at different frequencies (0.005 Hz0 to 05 Hz) to get insight into the interfacial rheology. With this new method, we can qualitatively characterize the interfacial behavior of microgels at the air-water interface such as the elastic modulus of the interface and adsorption kinetics[1].

CPP 31.6 Wed 17:45 H38

Structure and dynamics in injectable hydrogels from thermoresponsive triblock terpolymers — •Feifei Zheng[1], Pablo A. Álvarez Herrera[1], Wenqi Xu[1], Joachim Kohlbrecher[2], Sohila Abdelhafiz[3], Anna P. Constantinou[4], Theoni Georgiou[4], Aristide Dogariu[3], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]CREOL, University of Central Florida, Orlando, USA — [4]Imperial College London, Department of Materials, London, UK

Block copolymers with blocks featuring lower critical solution temperature behaviour have attracted great interest for 3D bioprinting because they form a runny solution at room temperature, but a hydrogel at body temperature. The structure of the solution and the hydrogel as well as dynamic information and their changes upon gelation are essential for understanding. Here we address an ABC triblock terpolymer consisting of a hydrophilic A block, a hydrophobic B, and a thermoresponsive C block. The results from small-angle neutron scattering on 15 wt% polymer solutions indicate that ABC form spherical core-shell micelles, that transform into cylinders in the gel state and form a more compact structure upon heating. By the combination of dynamic light scattering (DLS) and spatiotemporal coherence-gated DLS measurements, the dynamic information of gelation process was retrieved, which reveals the thermoresponsive C block contracts and the micelles aggregate to from the gel upon heating.

CPP 32: Poster Session II

Time: Thursday 9:30–12:00 Location: P3

CPP 32.1 Thu 9:30 P3

Influence of Salt Addition on the Ionic Conductivity, Hydration Behavior, and Structure of Poly(sulfobetaine) Hydrogels for Electrolyte Applications — •Friederike Ganster[1], Marcell Wolf[2], Gilles Wittmann[2], Peter Müller-Buschbaum[1], and Lucas P. Kreuzer[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany

Polyzwitterionic hydrogels are promising candidates for electrolytes in aqueous solid-state batteries, such as zinc-ion batteries (ZIBs), due to their ability to retain water molecules that facilitate ionic transport. The retained water acts as a lubricant, coordinating with the charged groups of the polyzwitterion and reducing interactions with mobile Zn^{2+} ions, thereby promoting the dissociation of ions and improving ion mobility. We systematically investigate how the addition of cosmotropic $ZnSO_4$ or rather chaotropic Zn(acetate) affects the ionic conductivity of poly(sulfobetaine)-based hydrogels. Our findings reveal that while ionic conductivity is generally increased, the extent and nature of this enhancement strongly depend on the specific salt type. We attribute this to unique and salt-type sensitive structural and hydration changes. X-ray scattering techniques resolve the electrolyte structure, and FTIR and Raman spectroscopy provide insights into the altered hydration behavior. Electrochemical impedance spectroscopy correlates these structural and hydration changes with variations in ionic conductivity and ion transport efficiency.

CPP 32.2 Thu 9:30 P3

Exploring pressure effects on the coil-globule transition of a pH sensitive polymer — •Ved Mahajan, Varun Mandalaparthy, and Nico F. A. van der Vegt — Technical University, Darmstadt

Macromolecules like polymers and proteins are essential to everyday life, with their structure and function influenced by environmental changes. The coil-globule transition is ubiquitous and is influenced by factors like hydrophobic interactions. External conditions, such as pressure, impact this transition differently in proteins and thermoresponsive polymers like PNiPAM[1].

This study investigates the effect of pressure on the coil-globule transition of a pH-sensitive hydrophobic polymer using constant-pH molecular dynamics. Our Results show that both pH and pressure significantly influence the transition. While pressure and charge both cause chain swelling, charge counteracts pressure-induced chain extension at high pressure. We observe distinct water structuring around positively and negatively charged sites with consequence to the polymer's pressure response. Additionally, we explore zwitterionic polymers under pressure, providing insights into biologically relevant secondary structures.

[1] Papadakis, C. M.; Niebuur, B.-J.; Schulte, A. Thermoresponsive Polymers under Pressure with a Focus on Poly(N-isopropylacrylamide) (PNIPAM). Langmuir 2024, 40 (1), 1* 20, DOI: 10.1021/acs.langmuir.3c02398

CPP 32.3 Thu 9:30 P3

Microscopic Insights into NaTFSI Based Thermoelectric Polymer Electrolyte by Raman Spectroscopy — •Julian-Steven Schilling[1] and Jens Pflaum[1,2] — [1]University of Wuerzburg, 97074 Würzburg — [2]Center for Applied Energy Research (CAE Bayern e.V.), 97074 Würzburg

The variety of chemical components, solution-based processability, and intrinsically low thermal conductivity have positioned polymers as leading materials in the field of organic thermoelectrics. Since materials facilitating ionic transport provide significantly higher thermoelectric voltages compared to electronic ones, we have analyzed the thermoelectric transport properties of a methacrylate-based solid polymer electrolyte. This study pursued our previous work [1] on this solution processed electrolyte by revealing new insights into the interaction of the conducting NaTFSI salt and the polymer backbone on microscopic length scales. By means of Raman spectroscopy, we use e.g. the S-C stretching modes and their salt concentration dependency to identify free TSFI Ions inside the polymer matrix which are responsible for the thermoelectric properties. In addition, we highlight the concentration dependent characteristics of the liquid versus solid electrolyte phase as well as the impact of the photoinitiator used for UV-curing on the electrolyte behaviour. [1] arxiv:2403.09340

CPP 32.4 Thu 9:30 P3

Ion Transport in Block Copolymer Electrolytes: Insights from Atomistic MD Simulations — •Jignesh Dhumal[1], Diddo Diddens[2], and Andreas Heuer[3] — [1]IGS BACCARA, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH — [3]Institut für physikalische Chemie, Universität Münster

Electrolytes are essential in batteries to facilitate ion transport between electrodes. Block copolymer electrolytes, have emerged as a promising class due to their high ionic conductivity and enhanced mechanical strength. However, despite several experimental and computational studies demonstrating their significance, an atomistic-level understanding of ion transport in Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI)-doped polystyrene-block-poly(ethylene oxide) (PS-b-PEO) block copolymers remain limited. In this study, we employ atomistic molecular dynamics simulations over extended timescales up to a microsecond examining the structural stability of the polymeric system and determine ion co-ordination within. We also quantify ion dynamics and transport properties in the PEO bulk region and the behavior at the PS/PEO interface, providing new insights into the mechanisms governing ion transport in this material.

CPP 32.5 Thu 9:30 P3

Advanced Synchrotron Characterization of NDI based acceptor thin films — •Subhalakshmi Suresh Kumar[1,2], Eva M. Herzig[1], and Christopher R. McNeill[2] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]McNeill Research Group, Department of Materials Science and Engineering, Monash University, Wellington Road, Clayton, Victoria, 3800 Australia

The transition to renewable energy has brought polymer solar cells (PSCs) to the forefront due to their lightweight, flexible, and environmentally friendly properties. The alignment of conjugated polymers within PSCs is critical for improving charge transport and overall device performance. This study aims to enhance the alignment of NDI-based acceptor thin films by employing fabrication methods such as blade coating and post-treatment annealing. Thin films were methodically prepared by varying coating speeds, substrate temperatures, and annealing conditions, followed by characterization using UV-Vis spectroscopy, Near-Edge X-ray Absorption Fine Structure (NEXAFS), and Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS). The analyses demonstrated a significant enhancement in molecular alignment after annealing, particularly in PNDITBT films, which showed pronounced backbone alignment. These findings highlight the potential of synchrotron-based techniques in optimizing thin-film microstructures, paving the way for the production of highly efficient laminated organic solar cells with bilayer heterojunctions.

CPP 32.6 Thu 9:30 P3

Morphologies in Thin Films of Charged Pentablock Terpolymers During Solvent Vapor Annealing — •Yujia Gu[1], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TU Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films from block copolymers containing charged blocks offer enhanced possibilities for precise structural modulation. In our previous work on thin films from a symmetric ABCBA pentablock terpolymer with cationic B and C midblocks and hydrophobic end blocks A, the pH-dependent degree of ionization of the charged midblocks was found to significantly influence the thin-film morphology [1]. In this study, we explore the possibilities to tune the thin film structures during solvent vapour annealing (SVA) using the same ABCBA pentablock terpolymer. Spin-coated films are prepared at various pH values and are subjected to SVA using selective solvents. Depending on the solvent selectivity, SVA may alter the film structure, e.g. by promoting reorganization toward equilibrium morphologies. We utilize in-situ atomic force microscopy (AFM) and spectral reflectometry (SR) to monitor structural transitions during SVA. By systematically examining the effects of pH and solvent selectivity, this study aims to provide insights into controlling nanostructure morphology in charged pentablock copolymers, with implications for advanced thin-film design.

CPP 32.7 Thu 9:30 P3

Adaptive Air-Water Interfaces with Spiropyrans and Arylazopyrazoles — •Michael Hardt[1], Javier Carrascosa-Tejedor[2], Philipp Gutfreund[2], Richard A. Campbell[3], and Björn Braunschweig[1] — [1]University of Münster (Germany) — [2]Institut Laue-Langevin (France) — [3]University of Manchester (UK)

Interfaces that can be tuned in their properties by external stimuli such as light or temperature are of great interest to drive macroscopic properties of interface-controlled soft matter materials. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned, and a low level of adaptivity can be integrated, extending the possibilities of soft matter interfaces beyond responsive functions. We explore the adaptive behaviour of air-water interfaces decorated by spiropyran (SP) and arylazopyrazole (AAP) photo-responsive surfactants. When exposed to UV light, the SP surfactants become more surface active, while the AAP surfactants undergo E/Z photoisomerization, significantly reducing their surface activity. By adjusting the intensity and duration of the UV exposure, the interfacial properties can be shifted from a simple responsive state (upon weak UV irradiation) to a more complex conditioned response (upon intense UV irradiation), accompanied by a dramatic

alteration in interfacial chemistry. Vibrational sum-frequency generation (SFG) and neutron reflectometry suggest that prolonged UV exposure induces SP and AAP surfactant aggregation at the air-water interface, driving the conditioned response where thick SP layers up to 5 nm form in the presence of Z-AAP.

CPP 32.8 Thu 9:30 P3

Is Anomalous Underscreening Detectable via AFM? — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Since colloidal dispersions have a significant importance in our daily life, it is of special interest to gain a deeper understanding of which interfacial forces govern their stability and how this stability can be tailored.

For aqueous electrolyte solutions, the DLVO theory is a powerful and well-established framework to describe these interactions at low and intermediate ionic strengths. In contrast, the situation at high ionic strength is less understood and the main methods for direct force measurements give inconsistent results. While the surface force apparatus (SFA) provides clear evidence for a reentrant behavior of the double layer repulsion in the highly concentrated regime - termed anomalous underscreening - for a wide range of different electrolytes, similar observations weren't possible with the atomic force microscope (AFM) to date. The reason for this fundamental difference is still unclear.

To elucidate the underlying mechanism, we performed colloidal probe AFM (CP-AFM) measurements in aqueous salt solutions. We systematically varied the type of salt, the surface chemistry of the confining surfaces (silica vs mica) as well as their curvature to bridge the gap between CP-AFM and SFA.

CPP 32.9 Thu 9:30 P3

Dynamic Wetting of Adaptive Polyelectrolyte Substrates: A multiscale approach — •Mona Meltschoch, Tünde Benedek, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Wetting phenomena are of great importance across various scientific disciplines and the wettability dynamics of adaptive substrates, such as polyelectrolyte (PE) multilayers (PEM), have gained significant attention. An interesting property of PE substrates is their propensity to swell in a liquid environment. However, complexities like the disparity between time and length scales make experimental investigations quite challenging. We prepared PE substrates by the layer-by-layer method, with a focus on their wettability at the nanoscale. We used atomic force microscopy (AFM) as the main characterisation technique. An optical contact angle (CA) tensiometry method is used for macroscopic measurements, layer thickness is determined by ellipsometry and X-ray reflectometry (XRR). Previous results show a decrease in water CA on silicon wafers coated with polystyrene sulfonate (PSS) as outermost layer in water-saturated atmosphere. To investigate the dependence on thickness, chain length and charge of the outer layer, different PEMs were fabricated and characterised. Here, the substrates were investigated with an AFM and showed to exhibit smooth surfaces while linearly increasing in thickness. The decrease in water CA is more pronounced with an increasing thickness and differs if PSS or PAH are outermost layer.

CPP 32.10 Thu 9:30 P3

Molecular Imprinting of PEDOT in Polyelectrolyte Multilayers — •Martin Hunger, Muhammad Khurram, Sven Neuber, and Christiane A. Helm — martin.hunger@uni-greifswald.de

Electrically conductive films of Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonic acid) (PEDOT:PSS) are formed by sequential adsorption of oppositely charged macromolecules. PEDOT:PSS serves as polyanion, and PDADMA is the polycation. When the top layer is PEDOT:PSS, the electrical conductivity is large (8 kS/m), when the top layer is PDADMA, the electrical conductivity is three orders of magnitude lower. In addition, vis-IR absorption spectroscopy shows that the PEDOT density in PEDOT:PSS-terminated films is high, while it is low in PDADMA-terminated films. When a PDADMA layer is adsorbed, turbidity measurements of the adsorption solution show that PEDOT diffuses out of the film. This can be explained entropically: a few PDADMA molecules with many positive charges replace many small molecules with few positive charges. Furthermore, exposure to solutions with divalent or trivalent cations reduce the conductivity of PEDOT-PSS-terminated films. We discuss whether PSS returns to previous binding sites upon adsorption of PEDOT:PSS, a behaviour that is typical for molecular imprinting.

CPP 32.11 Thu 9:30 P3

Extension of initiated chemical vapor deposition to new polymers via silylation — •Lynn Schwäke[1], Artjom Businski[2], Thomas Strunskus[1], Franz Faupel[1], Rainer Herges[2], and Stefan Schröder[1] — [1]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, 24143 Kiel, Germany — [2]Otto Diels Institute of Organic Chemistry, Kiel University, 24143 Kiel, Germany

Initiated Chemical Vapor Deposition (iCVD) is a powerful technique for the solvent-free and conformal deposition of polymer thin films on sensitive substrates and complex geometries. The utilisation of a variety of monomers enables the fabrication of films with specifically tailored properties and functionalities. However, the evaporation of monomers is a prerequisite for iCVD processes. Consequently, this limits its applicability, for example, in the synthesis of hydrogels. The hydrophilic nature of potential monomers and the presence of other strong intermolecular interactions result in low vapor pressures, which in turn hinders their use in iCVD. A well-known strategy, e.g. in the context of drug detection by gas chromatography-mass spectrometry (GC-MS), is silylation, which is used to weaken inter-molecular forces. Here silylation was employed to enhance the vapor pressure of hydrophilic 2-hydroxyethyl methacrylate (HEMA), an important monomer in the synthesis of hydrogels. Consequently, silylation is proposed as a general route for the introduction of low vapor pressure monomers into iCVD systems, which would lead to a significant expansion of the available monomer toolbox.

CPP 32.12 Thu 9:30 P3

In-Situ Neutron and Raman spectroscopy on polymer thin films at varying humidity — •Marcell Wolf[1], Lucas Kreuzer[1], Friederike Ganster[2], Christopher Garvey[1], and Peter Müller-Buschbaum[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Straße 1, 85748 Garching, Germany

Here we present a new sample environment for in-situ neutron and Raman spectroscopy on polymer thin films at varying humidities and temperatures. The combination of in-situ Raman and neutron spectroscopy shows the advantage that no difference within the sample composition, temperatures and humidity variations at the sample can be neglected, compared to separated single measurements. The structural changes can be directly related to the dynamic changes while varying the environment. We plan to describe our setup and present the first results of this new sample environment measured at the neutron time-of-flight spectrometer FOCUS at the PSI, Switzerland. For our knowledge this is the first time, that both spectroscopy techniques in comibination with varying humidity are applied at in-situ measurements. The new sample environment will be available to all users at time-of-flight spectrometer TOFTOF at the MLZ, as soon as the reactor restarts. Different variations of the sample cell, especially designed for different neutron experiments are available at other neutron instruments at the MLZ.

CPP 32.13 Thu 9:30 P3

Second order nonlinear optical properties of hexagonal boron nitride nanosheets h-BNNs — •Dina Atwa Khalil and G. Omar — Laser Institute for Research and Applications, Beni-Suef University, Egypt

The superior optical characteristics of hexagonal boron nitride nanosheets (h-BNNs) have been drawing more attention in the past few years. However, scientists have not yet thoroughly studied the nonlinear optical (NLO) properties of such innovative material. Here, NLO characteristics of h-BNNs are investigated for the first time utilizing the Z-scan approach that had been irradiated with 100 fs laser pulses using different excitation wavelengths that started from 740 to 820 nm at a constant incident power of 1 W. The studied 2D nanomaterial was prepared by a straightforward and effective technique for producing (h-BNNs), which is mechanical exfoliation. Their morphology and crystal structure have been investigated using different techniques, including UV-vis spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Raman spectroscopy. The measurements of nonlinearity show that by increasing the excitation wavelength, the nonlinear absorption coefficient decreases in a linear trend. The as prepared h-BNNs performed fascinating optical limiting with excellent two-photon absorption. This innovative optical nanomaterial makes them promise for sensitive optical components and laser protection applications.

CPP 32.14 Thu 9:30 P3

Highly oxidized Graphene Oxide as a Drug Delivery platform: Functional Group Interactions and Controlled Release Mechanisms — •Codrut Costinas[1], Liviu Cosmin Cotet[2], Monica Baia[1], Klara Magyari[3], and Lucian Baia[1] — [1]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania — [2]Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Cluj-Napoca, Romania — [3]Interdisciplinary Research Institute on Bio-Nano-Sciences, Babes-Bolyai University, Cluj-Napoca, Romania

Graphene oxide (GO) presents a promising platform for drug delivery, given its versatile surface chemistry and high surface area that enable effective drug loading and controlled release. Our study investigates the capabilities of an in-house produced, highly oxidized GO as a carrier by examining its interactions with two model compounds: methylene blue and methyl orange, as well as two drugs: doxorubicin and gentamicin sulfate. Through spectroscopic investigations (UV-VIS, FT-IR, and Raman), potentiometric titrations, and drug loading and release experiments we successfully identify the functional groups and bond types involved in drug-GO interactions in different pH media, most notably hydrogen bonding, electrostatic interactions, and π-π stacking. Furthermore, by taking into consideration the pKa values between GO acidic groups and the drugs ion-

izable groups, we can estimate both loading and pH-responsive release behavior in simulated physiological pH conditions. These findings highlight the flexibility of GO as a drug carrier, supporting its application in the development of customizable drug delivery systems for various therapeutic needs.

CPP 32.15 Thu 9:30 P3

Electronic Properties of a Naphthalene Diimide (NDI)-based Covalent Organic Framework (COF) — •Johann Olbrich[1], Laura Fuchs[1], Bibhuti Bhusan Rath[2], Bettina V. Lotsch[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, Technische Universität München, Germany — [2]Nanochemistry Department, Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Covalent organic frameworks (COFs) are a versatile class of porous polymers that exhibit exceptional tunability and electronic properties, making them attractive for various applications including water splitting [1], solar batteries [2] or other optoelectronic applications. We investigated the electronic properties of a naphthalene diimide (NDI)-based COF, which demonstrates robust photoinduced charge separation in aqueous environments, by using density functional theory (DFT) calculations. We provide theoretical insights into the stability of the charges in NDI-based COFs under hydrated conditions, highlighting their potential for advanced electronic and material applications. For this, we determined the formation of a stable radical on the NDI unit through the addition of a hydrogen atom. Further modeling of interactions of small water clusters with the COF indicated the emergence of a radical anion on the NDI, accompanied by the stabilization of H+ in an H2O cluster.

[1] K. Gottschling, G. Savasci, H. Vignolo-González, S. Schmidt, C. Ochsenfeld, and B. V. Lotsch, J. Am. Chem. Soc. 2020, 142, 12146.

[2] Y. Wang, Y. T. Chan, T. Oshima, V. Duppel, B. V. Lotsch, J. Am. Chem. Soc. 2024, 146(37), 25467-25476.

CPP 32.16 Thu 9:30 P3

Lithium Distribution Heterogeneity in the Graphite Anode of 21700-Type Cylindrical Li-Ion Cells during Aging — Dominik Petz[1,2], •Peter Müller-Buschbaum[2], and Anatoliy Senyshyn[1] — [1]Heinz Maier-Leibnitz-Zentrum (MLZ), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Electrochemical cycling in lithium-ion batteries involves an active exchange of lithium ions and electrons between the cathode and anode materials. In addition to material properties, this exchange is influenced by cell parameters such as electrode dimensions and geometry, current density, temperature, pressure, reaction rate, and others. These parameters are generally neither uniformly distributed nor static, thereby contributing to the stabilization of heterogeneous states in Li-ion batteries, typically seen in the lithium concentration distribution across the electrodes.

Previous studies have shown that, with cell aging, the distribution of lithium ions in the graphite anode of 18650-type lithium-ion batteries shifts over time. In this study, the heterogeneity of a fresh and an aged 21700-type Li-ion battery was examined using multiple diffraction techniques with both synchrotron and neutron radiation. Laboratory-based techniques such as SEM and incremental capacity analysis were also employed. The findings revealed a notable lithium distribution after cell aging, prompting the question of how cell format impacts cell aging behavior.

CPP 32.17 Thu 9:30 P3

Steering sulfur reduction kinetics of lithium-sulfur batteries by interfacial microenvironment modulation — •Cheng Yuan[1,2], Liang Zhang[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou 215123, China

Catalytic conversion of lithium polysulfides (LiPSs) is considered as an effective avenue to suppress the shuttle effect of lithium-sulfur (Li-S) batteries, for which the interfacial microenvironment constructed by the interaction between electrocatalysts and LiPSs plays a pivotal role in modulating the sulfur reduction kinetics. However, most of previous reports mainly focused on modulating the band structure of electrocatalysts or LiPSs alone to enhance the catalytic activity rather than considering the interfacial microenvironment as a whole. Herein, we propose a binary descriptor composed of the energy difference between d-band of electrocatalysts and p-band of LiPSs ($\Delta\epsilon$M-S) and the antibonding filling degree (ϵABF), which capture the energy band contributions from both electrocatalysts and LiPSs, to reveal the influence of interfacial microenvironment on sulfur reduction kinetics. Among different designed electrocatalysts, NiO presents a moderate LiPSs anchoring capacity and rapid electron transfer kinetics owing to the optimal $\Delta\epsilon$M-S and decreased ϵABF after interacting with LiPSs, which lead to a robust interfacial microenvironment and thus guarantee a continuous catalytic conversion of LiPSs in the long-term cycling.

CPP 32.18 Thu 9:30 P3

Polymer of intrinsic microporosity as the silicon-based anode electrode additive — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, 1219 Zhongguan West Rd, Ningbo, 315201, Zhejiang Province, P. R. China

Silicon-based anodes are promising alternatives due to their high theoretical specific capacity and low voltage platform to traditional graphite anodes for high-energy-density lithium-ion batteries (LIBs). However, their performance is significantly hindered by silicon's substantial volume expansion during cycling, which often leads to electrode degradation. Therefore, it is crucial to design a robust electrode structure and establish a stable solid electrolyte interface (SEI) to address these challenges. Herein, an intrinsic microporosity polymer PIM-COOH is prepared, which has good compatibility with the polyacrylic acid (PAA) binder as a silicon-based anode additive. The microporous structure of the PIM-COOH molecule can effectively improve the transport of lithium ions and improve the electrochemical kinetics. In addition, due to the inherent microporous properties of PIM-COOH additives, the affinity between the electrode and the electrolyte is enhanced. As a result, good lithium-ion transport and mechanical integrity are maintained, resulting in improved long-term stability and high-rate performance.

CPP 32.19 Thu 9:30 P3

In-situ interface film forming on the high-voltage LiCoO2 cathode by a tiny amount of nanoporous polymer additives — •Ruoxuan Qi[1], Ming Yang[1], Tianle Zheng[1], Xingchen Liu[2], Yonggao Xia[2], Ya-Jun Cheng[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]NIMTE, CAS, Zhejiang Province, P. R. China — [3]College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

The LiCoO2 (LCO) cathode has been foreseen for extensive commercial applications owing to its high specific capacity and stability. Therefore, there has been considerable interest in further enhancing its specific capacity by increasing the charging voltage. However, single-crystal LCO suffers from a significant capacity degradation when charged to 4.5 V due to the irreversible phase transition and unstable structure. Herein, an ultra-small amount (0.5 %wt in the electrode) of multi-functional PIM-1 (a polymer with intrinsic microporosity) additive is utilized to prepare a kind of binder-free electrode. PIM-1 modulates the solvation structure of LiPF6 due to its unique structure, which helps to form a stable, robust, and inorganic-rich CEI film on the surface of LCO at a high voltage of 4.5 V. This reduces the irreversible phase transition of LCO, thereby enhancing the cyclic stability and improving the rate performance, providing new perspectives for the electrodes fabrication and improving LCO-based high-energy-density cathodes.

CPP 32.20 Thu 9:30 P3

Ionic transport race between lithium and sodium in non-aqueous electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,3] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]International Graduate School for Battery Chemistry, Characterization, Analysis, Recycling and Application (BACCARA), University of Münster, Corrensstr. 40, 48149 Münster, Germany — [3]Helmholtz Institute Mnster (IEK-12),Forschungszentrum Jülich GmbH, 48149 Münster,Germany;

The need to meet the storage requirements of energy systems safely and efficiently has led to research into electrolytes other than the commonly used lithium-ion batteries. While the lithium-ion battery is the clear market leader, there is increasing interest in sodium-ion batteries, which are cheaper and more abundant. The present work is a comparative study of the transport properties of lithium hexafluorophosphate ($LiPF_6$) and sodium hexafluorophosphate ($NaPF_6$) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Using molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure and how this affects the ionic transport properties such as diffusivity and ionic conductivity of the system. Our results show higher conductivity and diffusivity of Na compared to Li for the analysed systems. Optimal ionic conductivity for Na was achieved above 1 M concentration, in contrast to Li. Overall, we observed differences in the coordination and mobilities of lithium and sodium cations.

CPP 32.21 Thu 9:30 P3

3D Electrodeposition of Porous Cu for long-cycling Lithium-Metal Batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Tianle Zheng[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], Yajun Cheng[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Hohai University, 213022 Changzhou, China

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860) and low voltage (3.04 V vs standard hydrogen electrode) warrant optimal cell energy density. However, these anodes rely on repeated

plating and stripping of Li, which leads to consumption of Li inventory and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems related to the volume change of these anodes, a number of different porous conductive scaffolds have been reported to create high surface area electrodes on which Li can be plated reliably. While impressive results have been reported in literature, current processes typically rely on either expensive or poorly scalable techniques. Herein, we report a scalable fabrication method to create porous Cu anodes using a one-step electrodeposition process. The areal loading, pore structure, and electrode thickness can be tuned by changing the electrodeposition parameters, and we show the in-situ nano WAXS images with lithium growth, which can help to explain the mechanism. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 32.22 Thu 9:30 P3

Operando study on structure-activity relationship between electrolyte components and electrochemical performance for all-solid-state lithium batteries — •Yingying Yan[1], Liangzhen Liu[2], Yuxin Liang[1], Fabian A.C. Apfelbeck[1], Guangjiu Pan[1], Lyuyang Cheng[1], Roland A. Fischer[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, 85748 Garching, Germany

All-solid-state lithium-ion batteries (ASSLIBs) are the most promising power sources for high-safety and high-energy-density energy storage devices. However, the practical application of ASSLBs has been hindered by poor interfacial stability and inferior ionic conductivity. Herein, a layered-double-hydroxide (LDH) reinforced poly(ethylene oxide) (PEO) composite polymer electrolyte is designed, which delivers a wide electrochemical window, high ionic conductivity, and superior Li+ transference number with a low LDH loading. The Li symmetric cells show ultra-long cycling stability at 0.1 mAh/cm2. The all-solid-state Li//LiFePO4 exhibits an excellent cycling stability with a high capacity retention of 90.1% at 0.1 C over 250 cycles. Furthermore, the structure-activity relationship between the component structure of the electrolyte and the electrochemical performance was elucidated by operando nanofocus wide-angle X-ray scattering (nWAXS).

CPP 32.23 Thu 9:30 P3

Organic polyaniline-based cathode materials — •Meriem N. Boudjenane[1], Friederike Ganster[2], Sebastian Mühlbauer[1], and Lucas P. Kreuzer[1] — [1]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic cathode materials feature tuneable structures, abundant active sites, and compatibility with multivalent charge carriers, thereby allowing to overcome challenges typically faced in inorganic cathode systems such as structural instability, and environmental hazards. We focus on the development of polyaniline (PANI) based cathodes. PANI, a conductive polymer, has demonstrated high capacity, excellent rate capability and fast ionic diffusion. Cellulose-based materials such as carboxymethyl cellulose (CMC) are used as binders and enhance the overall stability and electrochemical performance. By tuning parameters such as material composition, ionic strength, water content, and temperature, we elucidate how the conductivity and electrochemical stability of the PANI-based cathode can be optimized. Advanced techniques like X-ray diffraction, scanning and transmission electron microscopy, and electrochemical analysis provide deep insights into the structure-function relationship of the cathode materials while operando Raman spectroscopy will give insights into the charge/discharge mechanism and respective redox reactions, guiding the development of high-performance organic cathodes.

CPP 32.24 Thu 9:30 P3

Consistent Electrostatics in Bottom-Up Modeling of Electrode-Fluid Systems: Determining the Capacity from Ab-Initio to Continuum Models — •Philipp Stärk[1,2], Henrik Stooss[3], Philip Loche[4], and Alexander Schlaich[3] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 — [3]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, 1073 Hamburg, Germany — [4]Laboratory of Computational Science and Modeling, IMX, Ecole Polytechnique Federale de Lausanne,1015 Lausanne, Switzerland

Detailed understanding of electro-catalysis, batteries and supercapacitors, often requires modeling these systems on an atomistic scale. However, at this length scale and level of detail, most continuum assumptions about electrodes are clearly no longer valid. This is problematic for physical models and methods of analysis which rely on concepts from continuum electrostatics. We demonstrate in this work that a realistic Constant Potential Method model based on DFT data for gold can still consistently be described by concepts of continuum electrostatics, provided the electrostatic boundary condition is modeled correctly. Furthermore, we apply this description to determine the dielectric behavior of water in nanoporous gold. We systematically investigate the difference between conducting and inert confinement on the static dielectric response.

CPP 32.25 Thu 9:30 P3

Evaluating the Impact of Electrode Defects on PEMFC Performance and Durability — •Faezeh Mehdizadeh siahroudi[1], Sebastian Prass[1], and Andreas Bett[2] — [1]Division Hydrogen Technologies Department Fuel Cell Fraunhofer Institute for Solar Energy Systems ISE 79110 Freiburg, Germany — [2]Fraunhofer-Institut für Solare Energiesysteme ISE

According to previous research, imperfect membrane electrode assembly (MEA) manufacturing processes can lead to catalyst layer and membrane defects. Therefore, we have decided to investigate the impact of missing areas in cathode and anode electrodes on the performance and durability of polymer electrolyte fuel cell (PEMFC). Missing areas with varied sizes and configurations are used to determine a threshold at which a missing area can be considered as a crucial defect that degrades MEA components. In our work, several in-situ electrochemical techniques were used, including polarization curves, linear sweep voltammetry (LSV), cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) experiments. The structural changes in the electrodes and the membrane are visualized through SEM cross-sectional imaging.

CPP 32.26 Thu 9:30 P3

Hybrid electrolyte LLZO/PEO-systems: Impact of salt concentration and temperature on the structural properties close to the interface — •Laura Hölzer[1], Melania Kozdra[2], Daniel Brandell[2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster, Corrensstr. 28-30, 48149 Münster, Germany — [2]Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 75121 Uppsala, Sweden

Composite electrolytes are an opportunity for creating new and improved materials as ideally they combine the advantages of different types of electrolytes. One example for this being the LLZO/PEO-system. Insights into the properties and dynamics at and around the interface can be gained by looking at the system with atomistic simulations. Previously it could be seen that over the course of a simulation there is a movement of the Li^+ ions into the crystal.[1] Here, we analyse under which conditions equilibration is possible on the simulation time scales. Molecular dynamic simulations are performed. Three different concentrations and temperatures between 400K and 700K are studied. One could see the formation of a well-defined structure around the interface, which includes an additional layer of Li ions on both sides of the crystal that in equilibrium at 700K is independent of concentration, indicating structure formation via strong enthalpic driving forces. Furthermore, interesting insight into the reorganization of the polymer and the salt due to the presence of the LLZO can be gained.

[1] Kozdra, M.; Brandell, D.; Araujo, C. M. G.; Mace, A. Physical Chemistry Chemical Physics 2024, 26, 6216-6227.

CPP 32.27 Thu 9:30 P3

Structural investigation of lithium deficient metal chlorides solid electrolytes — •Francesco Falsina — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The strong demand for new and emerging sustainable energy solutions to address climate change and the requirements for increased high energy and power density have positioned solid-state batteries as a key research area. Lithium metal chlorides (LiMCl) are considered as promising candidates for next-generation batteries due to their high ionic conductivity, thermodynamic stability, and favourable mechanical properties. In this study, we investigated Li(3-3x) M(1+x)Cl6 compounds with M = Dy, Ho, Tb, and Tm using X-ray diffraction (XRD), confirming that all samples crystallize in the space group P3m1, though exhibiting partial crystallinity and high disorder without post-synthesis annealing. The effect of lithium deficiency was explored on the ionic conductivity employing Electrochemical Impedance Spectroscopy (EIS), offering further insights into their potential for solid-state battery applications.

CPP 32.28 Thu 9:30 P3

Morphology and intracrystalline dynamics of semicrystalline polyester Poly(3-hydroxy-2,2-dimethylbutyrate) — •Johann C. Holz[1], Arman Edalat[1], Kay Saalwächter[1], Thomas Thurn-Albrecht[1], and Eugene Chen[2] — [1]Martin-Luther-University, Halle, GER — [2]Colorado State University, Fort Collins, USA

Semicrystalline polymers are classified as crystal-fixed (non-diffusive) or crystal-mobile (diffusive) based on polymer chain mobility within the crystal. Crystal-fixed polymers exhibit lower crystallinity, thinner lamellae ($d_a > d_c$), and less variation in thickness ($\sigma_a > \sigma_c$). Finding a biodegradable alternative for crystal-mobile polyethylene (PE) remains a priority for sustainable research. Poly(3-hydroxybutyrate) (P3HB), a biodegradable polyester, was recently found to be crystal-mobile, but suffers from poor mechanical properties.

We here study Poly(3-hydroxy-2,2-dimethylbutyrate) ($P3H(Me)_2B$), a structurally similar polyester with methyl-groups substituted for the two α-hydrogens, to improve mechanical toughness, thermal stability, and recyclability. Our analysis of $P3H(Me)_2B$ by Small-Angle X-ray Scattering (SAXS) re-

vealed that it crystallizes in a crystal-fixed mode. This finding contrasts with the crystal-mobile behavior observed in P3HB. Wide-Angle X-ray Scattering (WAXS) corroborated the crystal structure that has already been described in literature, while also revealing previously undetected diffraction peaks. Furthermore, Nuclear Magnetic Resonance (NMR) spectroscopy enabled precise quantification of the polymer's crystallinity, facilitating accurate determination of the melting enthalpy H_f for a 100% crystalline sample.

CPP 32.29 Thu 9:30 P3

Optical properties of biosynthesized nanoscaled Eu_2O_3 for red luminescence and potential antidiabetic applications — •Hamza Mohamed — iThemba LABS, Cape Town, South Africa

This contribution reports on the optical properties of biosynthesised Eu_2O_3 nanoparticles bioengineered for the first time by a green and cost effective method using aqueous fruit extracts of Hyphaene thebaica as an effective chelating and capping agent. The morphological, structural, and optical properties of the samples annealed at 500˚C were confirmed by using a high-resolution transmission electron microscope (HR-TEM), x-ray diffrac tion analysis (XRD), UV-Vis spectrocopy, and photoluminescence spectrometer. The XRD results confirmed the characteristic body-centered cubic (bcc) structure of Eu_2O_3 nanoparticles with an average size of 20 nm. HRTEM revealed square type morphology with an average size of ≈6 nm. Electron dispersion energy dispersive x-ray spectroscopy spectrum confirmed the elemental single phase nature of pure Eu_2O_3. Furthuremore, the Fourier transformed infrared spectroscopy revealed the intrinsic characteristic peaks of Eu-O bond stretching vibrations. UV-Vis reflectance proved that Eu_2O_3 absorbs in a wide range of the solar spectrum from the VUV-UV region with a bandgap of 5.1 eV. The luminescence properties of such cubic structures were characterized by an intense red emission centered at 614 nm. It was observed that the biosynthesized Eu_2O_3 nanoparticles exhibit an efficient red-luminescence and hence a potential material as red phosphor.

CPP 32.30 Thu 9:30 P3

Green synthesis of nanocellulose for archaeological wood preservation: a case study of cheops' second solar boat — •Ihab Abdelbaki — Cairo University, Egypt

The preservation of ancient wooden artifacts presents significant challenges due to environmental degradation and biological deterioration. This study addresses these challenges through the development of an eco-friendly nanocellulose-based preservation method, specifically targeting the deterioration observed in the second solar boat of king khufu (cheops), one of egypt's most significant archaeological wooden artifacts. Nanocellulose was synthesized via a green approach using controlled acid hydrolysis of agricultural waste cellulose, followed by mechanical ultrasonication. the degradation assessment of the second solar boat revealed severe biological infestation, structural weakening, and dimensional instability, particularly in areas exposed to fluctuating humidity levels. The prepared nanocellulose, characterized by TEM, FTIR and XRD, exhibited crystallite sizes of 20-30 nm and a crystallinity index of 82%. when applied to degraded wood samples from similar archaeological contexts, the nanocellulose treatment demonstrated significant improvements in mechanical strength (40% increase), dimensional stability (65% reduction in swelling), and biological resistance. Importantly, the treatment maintained the artifact's aesthetic and historical integrity while providing a sustainable, reversible preservation solution. this study presents a promising green approach for the conservation of ancient wooden artifacts, offering implications for cultural heritage preservation worldwide.

CPP 32.31 Thu 9:30 P3

Investigation of photoelectrochemically induced degradation of III-V nanowires — •Chris Y. Bohlemann, Juliane Koch, David Ostheimer, Peter Kleinschmidt, and Thomas Hannappel — Technische Universität Ilmenau, Faculty of Mathematics and Natural Sciences, Fundamentals of Energy Materials, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau

Over the past two decades, nanoscale structures like III-V nanowires (NWs) have become versatile components in electronic and photonic applications [1]. The large surface-to-volume ratio of NWs enhances reaction efficiency by providing more active sites for light-driven processes. To explore NWs' potential in photoelectrochemical solar energy conversion, we investigated their optoelectronic behavior. First, GaAs NWs were grown via Vapor-Liquid-Solid growth mode using Metal-Organic Vapor Phase Epitaxy. We performed Linear Sweep Voltammetry measurements where the III-V sample was brought into direct contact with the electrolyte. However, a major challenge is the degradation in performance due to the limited durability of NWs in electrolytes compared to planar surfaces. To evaluate the corrosion of NWs in electrolytes, we analyzed the NW structures before and after two hours of stability testing measurements by Scanning Electron Microscopy. Our results indicate that under continuous illumination no significant degradation besides surface roughening is observed while samples under chopped illumination, are nearly completely etched, with few or no NWs remaining intact.

[1] J. Koch et al., Adv. Mater. Interfaces 9, 2200948, 2022.

CPP 32.32 Thu 9:30 P3

Fabrication of Gas Sensors with High Sensitivity to NO_2 Based on Photoactivation of Porous Carbon Materials — •Laura Pascual[1], Berta Pérez-Román[2], Jesús López-Sánchez[2], M. Alejandra Mazo[2], Álvaro Peña[3], David G. Calatayud[4], Daniel Matatagui[3], and Fernando Rubio-Marcos[2] — [1]Instituto de Catálisis y Petroleoquímica (ICP-CSIC), Madrid, España — [2]Instituto de Cerámica y Vidrio (ICV-CSIC), Madrid, España — [3]Instituto de Magnetismo Aplicado, (IMA-UCM-ADIF), Madrid, España — [4]Departamento de Química Inorgánica, Universidad Autónoma de Madrid (UAM), Madrid, España

The rise in gas emissions harms public health, with nitrogen dioxide (NO_2) being particularly dangerous due to its impact on the lungs and respiratory conditions. This emphasizes the need for highly selective gas sensors capable of detecting concentrations below 1 ppm in real time, while being miniaturised and operable at room temperature (RT).

Carbon-derived materials from carbides (CDC) are created through high-temperature chlorination, achieving surface areas over 2000 m^2/g. These materials feature hierarchical porosity (micro- to mesopores) and abundant active sites that support redox reactions for NO_2 detection. Incorporating heteroatoms improves charge transfer and electron-hole trap formation. The results show exceptional selectivity and sensitivity to NO_2, with detection below 1 ppm and room temperature operation using UV excitation (275 nm).

CPP 32.33 Thu 9:30 P3

Bimetallic Core-Shell-Nanoparticles for enhanced Raman spectroscopy — •Moritz Willems[1], Steffi Stumpf[1,2], and Stephanie Hoeppener[1,2] — [1]Jena Center for Soft Matter (JCSM) — [2]Institute of Organic and Macromolecular Chemistry (IOMC)

Bimetallic Core-Shell-Nanoparticles have emerged as a versatile tool for advanced sensing applications, particularly in surface-enhanced Raman spectroscopy and tip-enhanced Raman spectroscopy. The combination of two metals in a Core-Shell configuration enhances the plasmonic properties and allows for extended plasmonic bandwidths, as well as superior electromagnetic field amplification in comparison to the monometallic nanoparticles. Silver nanoparticles have been demonstrated to offer effective enhancements for Raman spectroscopy. However, they do present certain challenges, including a narrow spectral range, poor chemical stability, and a relatively short lifespan. The coating of silver nanoparticles with a thin gold shell promises precise control over localised surface plasmon resonance, expanding spectral ranges for Raman spectroscopy measurements, especially between the peaks of gold and silver, by changing the relative thickness of the shell. Furthermore, the gold coating allows for measurements in water, while also providing a prolonged lifespan. The synthesis of these nanoparticles utilizes chemical reduction by microwave irradiation, providing fast, energy efficient and uniform heating. Various methods have been tested to overcome the problems of synthesising a gold shell on silver, and detailed transmission electron microscopy and UV-Vis spectroscopy analysis complement the Raman spectroscopy results.

CPP 32.34 Thu 9:30 P3

Classical simulation studies of dissociation equilibria in nanoconfined systems — •Kira Fischer, Henrik Stooss, and Alexander Schlaich — Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Germany

Dissociation equilibria in nanoconfinement are relevant to the chemistry of nanostructured catalysts, aerosols and protein pockets. Experiments indicate that nanoconfinement affects the dissociation of water, however to date a comprehensive understanding is still lacking. Here, we investigate dissociation equilibria in nanoconfinement from a classically. Using molecular dynamics and free energy methods we study hydrochloric acid in diamond nanoconfinement in the dilute limit at ambient conditions.

Our studies reveal a depletion of hydrochloric acid in nanoconfinement, with a negative excess by up to a factor of 100. The negative excess is attributed to the balance between hydronium adsorption and chloride depletion at the interface. Additionally, we propose that hydronium is adsorbed to the diamond interface by dipole orientation within a local electric field. Notably, in the smallest pore, the pK_a is increased by 1. We also introduce useful concepts for analysing dissociation equilibria in confinement. This includes the chemical potential in confinement, which enables quantification of ionic excess in the dilute limit. Furthermore, we demonstrate how to derive the chemical potential from the potential of mean force, thereby decomposing the different energetic contributions to the excess chemical potential.

CPP 32.35 Thu 9:30 P3

Gas quenching under ambient conditions for efficient and stable inverted perovskite solar cells with surface treatment — •Zhaonan Jin, Xiongzhuo Jiang, Zerui Li, Xiaojing Ci, Guangjiu Pan, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Inverted perovskite solar cells have gained significant attention due to their potential for high efficiency and stability. In the process, the active layer fabri-

cation plays a key role in determining the performance of the solar cells. Gas quenching is an important technique in the preparation of perovskite solar cells as it enhances the film quality and solar cell performance by precisely controlling the crystal growth and minimizing defects. As for the post-treatment of the active layer, surface passivation plays a crucial role in enhancing the performance of perovskite solar cells by reducing surface defects of perovskite interfaces. This study explores the influence of different passivation materials on the morphology of perovskite films and the performance of gas-quenching assisted FA0.8Cs0.2Pb(I0.6Br0.4)3 solar cells. This work provides a practical solution for the production of low-cost and high-performance inverted perovskite solar cells while maintaining operational stability in real-world environments.

CPP 32.36 Thu 9:30 P3

Facet-dependent photovoltaic efficiency and stability variations in mixed Sn-Pb perovskite solar cells — •Xiaojing Ci, Xiongzhuo Jiang, Guangjiu Pan, Jinsheng Zhang, Zerui Li, Kun Sun, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Since the first breakthrough of perovskite solar cells using a solid-state structure, the solar cell power conversion efficiency has increased from 9.7% to 26%. These exciting improvements are mainly attributed to achieving a pinhole-free thin film at the beginning and an increased understanding of microstructures on perovskite thin films. In addition, the rapid PCE improvement has been accompanied by an increased understanding of microstructures on perovskite thin films. The photovoltaic performance of PSCs has been found to correlate strongly with their facet orientations. For example, the charge carrier lifetime, open-circuit voltage deficit and device hysteresis of PSCs are related to the structure and density in (111) crystal facets of perovskite. Besides, different crystal facets have different atomic arrangements and coordination, which lead to different atomic potential landscapes and, subsequently, to different electronic, physical, and chemical properties. Nevertheless, the deep understanding of perovskite thin films, especially the crystal facets of the thin film, still lags behind that of single-crystal samples or other inorganic thin films. In this work, we prepare the mixed tin-lead perovskite film with different orientations according to the facet engineering. We research the role of the different perovskite crystal facets in stability and optoelectronic properties.

CPP 32.37 Thu 9:30 P3

Processing-property relationships in printed hybrid halide perovskites — •Manuel Lippert[1], Meike Kuhn[1], Maximilian Spies[2], Anna Köhler[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Optoelektronik weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

Solution processable hybrid halide perovskites solar cells have been extensively studied over the last ten years and great advances in efficiency have been achieved. An important factor for the performance of the final solar cell is the morphology of the perovskite layer. Therefore, control of structure formation mechanisms is highly desirable. [1] We investigate systematically the processing of the active layer to determine processing parameters that are decisive for structure formation. To reliably study the effect of time relevant processing steps on the perovskite layer, we use automated processing. Applying photoluminescence, optical microscopy and grazing incidence wide angle X-ray scattering (GIWAXS) allows us to determine the morphology on the nano and micron scale and detect the correlations between processing and efficiency.

[1] Meike Kuhn, Felix A. Wenzel, Christopher Greve, Klaus Kreger, Matthias Schwartzkopf, Hans-Werner Schmidt, Helen Grüninger, Eva M. Herzig, Tailored Supramolecular Additives to Control the Crystallization Process and Morphology of MAPbI3, *submitted*

CPP 32.38 Thu 9:30 P3

Simulating light induced phase separation in $MAPbBr_{1.8}I_{1.2}$ perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekaterina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By changing the ratio of halides within mixed organic halide perovskites, such as $MAPbBr_{1.8}I_{1.2}$ (MA -methylammonium), one can adjust the band gap. This is quite desirable for solar cell applications where precisely tunable bandgaps enable the creation of high efficiency solar cells. However, when illuminated with visible light, these materials undergo a phase separation into Br-rich and I-rich phases, which destroys the tuned band gap. To better understand; and hopefully control this process, we utilize phenomenological approaches, such as Cahn-Hilliard and Monte Carlo models, to simulate the light-induced phase separation. We compared the results of our simulations with the experimental diffraction data. Cahn-Hilliard simulations presented quite a few difficulties in replicating the observations. The Monte Carlo simulations on the other hand allow us to investigate the influence of various material parameters on the phase separation, such as iodine-to-bromine ratio, charge carrier density and intensity of illumination. In general, we found that Monte Carlo simulations with the right choice of model parameters are quite capable of reproducing the experimental observations.

CPP 32.39 Thu 9:30 P3

Enhanced Stability of Perovskite Solar Cells via Double-End Coupling Silane — •Xinwei Tian, Xiongzhuo Jiang, and Peter Müller-Buschbaum — TUM School of Natural Science, Chair for Functional Materials, 85748 Garching, Germany

Containing reactive triethoxysilyl groups, 1,4-bis(triethoxysilyl)benzol (BTEB) has high thermal stability by forming robust siloxane networks through hydrolysis and condensation reaction. Besides, BTEB has good hydrophobicity, so it can function as a protective barrier to prevent moisture ingression into the sample, which ensures long-term operation of the perovskite solar cells (PSCs). BTEB can also passivate the interface defect, thus reducing non-radiative recombination. On the other hand, because of the surface passivation effect of BTEB, a smoother and more uniform film layer can be obtained, which can enhance light absorption and reduce scattering loss effectively. In this way, the power conversion efficiency (PCE) can also be improved. In our work, we aim to apply BTEB as the interface modification material, ethyl acetate as antisolvent, to construct inverted perovskite solar cells with higher efficiency and stability.

CPP 32.40 Thu 9:30 P3

Morphology Control and Optical Modelling of $CsPbBr_3$ Nanocrystal Films for Emission Orientation Studies — •Lea Kolb, Roshini Jayabalan, and Wolfgang Brütting — Universität Augsburg, 86135 Augsburg, Germany

The remarkable properties of $CsPbBr_3$ perovskite nanocrystals, exhibiting a high photoluminescence quantum yield (PLQY) and a narrow emission linewidth with size- and composition-tunable bandgap, render them promising for the application as emitters in light-emitting diodes (LEDs). While PLQY and charge carrier transport for perovskite LEDs have been in the focus of extensive studies, the orientation of the emissive transition dipole moment (TDM) has not been investigated thoroughly yet. However, for TDM analysis, determining the complex refractive index of the nanocrystal films is crucial. In this work, variable angle spectroscopic ellipsometry (VASE) was used to obtain the optical constants of various samples containing $CsPbBr_3$ nanocrystals. To avoid scattering effects, VASE measurements require homogeneous films with minimal roughness. For this reason, the substrates on which the nanocrystal films were spin-coated had to be modified and the sample fabrication process was optimized. In order to describe the measured data accurately with optical fit models, the morphology and thickness of the films were studied comprehensively by atomic force microscopy (AFM). Finally, angular dependent photoluminescence (ADPL) measurements have been performed and modelled in order to obtain information about the TDM-orientation.

CPP 32.41 Thu 9:30 P3

PIN-type perovskite solar cells for space applications — •Ruodong Yang, Simon A. Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Perovskite solar cells have advantages such as low costs and high power-to-weight ratio, which render them to be promising candidates for space applications, where the mass is crucial for launch costs. In this study PIN-type solar cells are investigated. With its inverted p- and n-type structure, it has great research potential. However, solar cells in space also face challenges, such as vacuum, extreme temperature fluctuations during each orbit, and high radiation levels. The purpose of this study is to optimize the manufacturing procedure of PIN-type perovskite solar cells to address these challenges. We investigate the power conversion efficiency of the solar cells under similar environmental conditions to the low Earth orbit with illumination from an AM0 light source and thermal cycling by using optical microscopy to observe the structural changes during the operation. With the results of the measurements, the manufacturing procedure will be optimized, to determine the key factors to improve the performance and efficiency of PIN-type cells under space conditions.

CPP 32.42 Thu 9:30 P3

Perovskite solar cells temperature dependence under space-like conditions — •Anthony Vizcaino, Simon Alexander Wegener, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair of Functional Materials, 85748 Garching, Germany

In recent years, perovskites have attracted the scientific community's attention due to their properties and possible applications, making their use in solar cells one of the most relevant. Their high-power conversion efficiency, power-to-weight ratio, and manufacturing compared to the to-date used multi-junction devices make them a promising device for space applications, where it is possible to take advantage of all the intensity of sunlight that at the Earth*s surface is lost by absorption or scattering by the atmosphere. However, in this scenario, radiation and high temperatures would affect the solar cell. This study focuses on one of these problems and tries to understand how extreme temperatures and thermocycling through large periods of heating and cooling encountered in low Earth*s orbit affect perovskite solar cell performance and degradation.

Operando studies allow to simulate thermal cycling conditions and measure the transmittance of solar cells, which combined with electrical characteristics from I-V measurements and active layer morphology from GIWAXS give us a robust knowledge of the temperature dependence of perovskite-based solar cells.

CPP 32.43 Thu 9:30 P3

In-situ Monitoring for Optimizing Perovskite Solar Cell Fabrication: Correlating Process Parameters with Power Conversion Efficiency — •Yuxin Liu, Alexander Tarasov, Maxim Simmonds, and Eva Unger — Department Solution Processing of Hybrid Materials and Devices, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Halide perovskite solar cells need dependable, reproducible production to reach commercialization. For stable perovskite photovoltaic manufacture and research, deposition processes must be monitored. In-situ photoluminescence (PL) monitoring compares the PL during spin-coating and annealing with absolute PL measurements obtained after annealing of the sample. Examples demonstrating how process conditions and variables like anti-solvent type and drip timing significantly influence PL signatures. We demonstrate that insight during processing can serve as feedback to stabilize the perovskite solar cell fabrication. In-situ PL monitoring shows two distinct peaks within one second of anti-solvent treatment, revealing perovskite nucleation and growth mechanism. All Helmholtz association perovskite PV research uses a standard operating procedure (SOP) for solar cell samples. Absolute PL measurements for thin-film samples quantify Quasi-Fermi Level Splitting, reflecting the opto-electronic quality of the absorber and losses at selective contacts. The absolute PL is correlated to the in-situ PL to establish how far in-situ PL during processing can predict solar cell performance. This study highlights the potential of optical process monitoring to enhance material and interface quality.

CPP 32.44 Thu 9:30 P3

The Construction of Temperature Gradient during Annealing to Guide Crystallization Direction — •Yiran Shi — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Perovskite solar cells have gained significant attention as promising candidates for next-generation photovoltaics due to their outstanding advantages. The quality of the perovskite layer is a crucial determinant of the efficiency and stability of photovoltaic devices. As a polycrystalline thin film, the size and compactness of crystals are key quality metrics, closely linked to the annealing process. Conventional annealing typically involves placing the thin film, post-nucleation, on a fixed-temperature heating platform for crystal growth. Without external guidance, crystallization usually progresses top-down, preferentially completing at the upper surface. This sequence often traps solvents within the film, hindering evaporation and leading to void formation, which negatively affects film quality and device performance. To address this issue, we propose an improved annealing strategy by introducing a vertical thermal gradient to guide a bottom-up crystallization process. This approach aims to delay top-surface crystallization, allowing solvents to escape more effectively and reducing void formation. From the results about SEM and GIWAX, it is improved film quality, with enhanced structural integrity and reduced defects, offering a pathway to optimize perovskite photovoltaic performance.

CPP 32.45 Thu 9:30 P3

Optimizing RbCsFAMA perovskite solar cells with piperazine-inspired passivation technique — •Bashudev Bhandari[1,2,3], Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena — [2]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany — [3]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany

Perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology, with extraordinary optoelectronic properties. However, stability and defects are the challenges of perovskite solar cells. This work explores the role of piperazine as a novel passivating agent to address these limitations. Piperazine's bifunctional structure enables effective defect passivation at the grain boundaries and interfaces of RbCsFAMA perovskite films, significantly reducing non-radiative recombination losses. Different characterization and imaging techniques photoluminescence spectroscopy, X-ray diffraction and scanning electron microscopy demonstrate improved crystallinity and electronic properties of the RbCsFAMA perovskite films after passivation. This improvement is shown to be transferred into solar cell devices.

CPP 33: Modeling and Simulation of Soft Matter IV

Time: Thursday 11:45–13:00 Location: H34

CPP 33.1 Thu 11:45 H34

Understanding COF/Electrode interfaces for electrocatalysis using DFT and molecular simulations — •Henrik Stooss[1], Philip Stärk[1,2], and Alexander Schlaich[1] — [1]Institute for Atomistic Modeling of Materials in Aqueous Media, Hamburg University of Technology, Hamburg — [2]SC SimTech, University of Stuttgart, Stuttgart

This study explores the complex dynamics at electrode/electrolyte interfaces under constant potential, crucial for advancing electrocatalysis and designing efficient energy systems, by combining advanced computational techniques to gain insights into mechanisms at these interfaces. We perform Density Functional Theory (DFT) simulations while maintaining a constant electrode potential. Despite challenges and computational costs, the DFT simulations provide insights into the electronic structure and behavior of electrode surfaces. We then parameterize a classical model based on the DFT data, enabling simulations of larger systems over longer timescales for comprehensive comparison with experimental ATR-SEIRAS data. This approach offers a detailed understanding of adsorption and transport phenomena at the electrode interface, potentially leading to better electrolyte compositions and improved electrode designs. This work advances the connection between first-principles calculations and experimental observations for material design.

CPP 33.2 Thu 12:00 H34

Porous microstructure of fibrous sheets in two transport regimes — Alexandra Serebrennikova[1], Phillip Gräfensteiner[2], Matthias Neumann[1], Volker Schmidt[2], Andoni Rodriguez[3], Peter Leitl[3], Werner Napetschnig[1], Ekaterina Baikova[1], Maximilian Fuchs[1], and •Karin Zojer[1] — [1]Graz University of Technology, Graz, Austria — [2]Ulm University, Ulm, Germany — [3]bionic surface technologies, Graz, Austria

In many applications, a porous material serves multiple functions. For example, paper sheets in packaging bags should allow excess air to escape quickly while minimizing moisture migration. Although the underlying physics are different, both transport processes depend on porosity. However, each function it is likely to be supported by additional, possibly different, microstructural properties. Can these microstructural properties be optimized for all functions or is this not possible due to inherently dependent properties? To answer this question for Stokes flow and reactive diffusive transport through paper, we simulate flow through μ-CT-determined microstructures using physics-informed neural networks, computational fluid dynamics, and pore network modeling. We combine these simulations with statistical morphological analysis including dependency quantification to provide the relevance and dependence of structural properties in both transport processes. Our study suggests that the two transport scenarios do not rely on the same set of structural properties, even when fiber swelling due to moisture transport is considered.

CPP 33.3 Thu 12:15 H34

Nuclear Quantum Effects in Clays — Sam Shepherd, Pawan Kurapothula, Nataly Realpe, Gareth Tribello, and •David Wilkins — Queen's University Belfast, Belfast, United Kingdom

Clay materials consist of layers, whose structure is heavily influenced by hydrogen-bonding interactions. Given the importance of nuclear quantum effects such as zero-point energy in water, a hydrogen-bonded liquid, a natural question to ask is how important these effects are in clays themselves.

I describe some work done by my group to understand the importance of nuclear quantum effects in clays and clay-water systems, and to interpret these effects in the same terms used to understand water. I also demonstrate a fully quantum-mechanical description of the interactions and dynamics in kaolinite clay.

CPP 33.4 Thu 12:30 H34

Protonated water clusters by stochastic approaches: probing machine learning resilience against quantum Monte Carlo noise — •Matteo Peria, Antonino Marco Saitta, and Michele Casula — Sorbonne Université, 4 place Jussieu Paris, France

A complete understanding of the hydrogen bond and proton transfer mechanism in water is still lacking, since it requires an accurate potential energy surface (PES) and very expensive quantum mechanical simulations of the nuclear part. Reproducing this high-dimensional surface with current high-level computational chemistry methods is infeasible for the largest clusters. We test gradient-based kernel ridge regression methods and neural networks to reproduce the PES starting from a dataset of energies and forces of the protonated water clusters obtained via simulations combining classical molecular dynamics (MD) for the nuclei and quantum Monte Carlo (QMC) for the electrons. The QMC+MD

approach yields very accurate results for the classical dynamics, which are however affected by the intrinsic noise inherent in the stochastic sampling of both nuclear and electronic phase space. We prove that QMC multivariate noise is not necessarily detrimental to the learning of energies and forces and we determine under which conditions one can derive accurate and reliable MLIPs from QMC data.

CPP 33.5 Thu 12:45 H34

Effect of solid fillers on the thermodynamics and electrical properties of diblock copolymers and polymer blends. — •Alexander Chervanyov — University of Münster, Münster, Germany.

By making use of the developed theory we study the effect of solid fillers on the thermodynamics, phase behaviour and electrical properties of diblock copolymers (DBC) and polymer blends (PB). The theory relies on the combination of the liquid state approach, phase-field model for polymers, Monte-Carlo simulations, and the resistor random network model for fillers. Using the developed approach, we prove that the correlations imposed by the variations of the composition of PB cause a significant non-osmotic contribution to the polymer mediated interaction between fillers immersed in this blend. The effect of fillers on the stability and miscibility of compressible PB is studied in detail. We show that the presence of non-adsorbing fillers can be used to enhance the stability of a PB that shows low critical solution temperature (LCST) behavior. Finally, as an important practical application of the developed theory, we study the electrical response of an insulating DBC filled with conduictive fillers. In particular, the order-disorder transition in the host DBC system is found to be accompanied by the conductor-insulator transition in the filler network. The order-order transition between the lamella and cylindrical microphases of DBC proves to co-occur with a spike of the composite conductivity caused by restructuring of the conductive filler network.

CPP 34: Focus Session: Interactions Between Water and Cellulose I

Time: Thursday 15:00–16:00 Location: H34

Invited Talk CPP 34.1 Thu 15:00 H34

Understanding Nanocellulose-Water Interactions to Engineer Advanced Functional Materials — •Valentina Guccini — Uppsala University, Lägerhyddsvägen 1, Uppsala, Sweden

Water interactions are a central topic in the field of nanocellulose due to their pivotal role in nanocellulose's chemical reactivity, processability and physical properties. Yet, a key challenge that remains is bridging the fundamental understanding of nanocellulose-water interactions with the design and engineering of advanced functional materials. This presentation will address this challenge by summarizing the main characteristics of water-nanocellulose interactions and how these can be leveraged to engineer nanocellulose-based materials, in which water has both a structural and functional role. We will analyze the structure-property relationship in nanocellulose-based hydrogels, films and membranes for biotechnological and fossil-free energy applications (e.g. fuel cells and lithium-ion batteries). This presentation offers a new perspective on using nanocellulose-water interactions as a tool to enhance and tailor material performance and functionalities.

CPP 34.2 Thu 15:30 H34

Using Nanocellulose Hygroscopicity for Conductive 3D Paper Structures — •Marie Betker[1,2], Tim Erichlandwehr[3], Benedikt Sochor[1,4], Elisabeth Erbes[1,5], Yamit Alon[2], Alisher Kurmanbay[2], Yanan Li[6], Irene Fernandez-Cuesta[3], Peter Müller-Buschbaum[6], Simone Techert[1,5], Daniel Söderberg[2,7], and Stephan Roth[1,2,7] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 56, 10044 Stockholm, Sweden — [3]Hamburg Advanced Research Centre for Bioorganic Chemistry, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, CA 94720, USA — [5]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Göttingen, Germany — [6]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [7]Wallenberg Wood Science Center, Teknikringen 52, 10044 Stockholm, Sweden

We report the fabrication of the, to this date, thinnest sprayed nanopaper foils. For that, we spray aqueous nanocellulose dispersions layer-by-layer on a hot substrate. The foils are only 2 um thin with an average basic weight of 1.9 g/square metre. We specifically exploit the hygroscopicity of paper-based materials to rearrange our water-soaked foils into three-dimensional, free-standing shapes. We further demonstrate the applicability of our foils by making them conductive via integration of silver nanowires. This approach is a step towards more sustainable, 3D organic electronics.

CPP 34.3 Thu 15:45 H34

A simulation study of the structure and mechanical properties of cellulose and callose hydrogels — •Robinson Cortes-Huerto[1], Nancy C. Forero-Martinez[2], and Pietro Ballone[1] — [1]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, DE — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudinger 9, 55128 Mainz, DE

The cell wall of plants is a complex, self-organized and continuously evolving structure playing important roles in the life cycle of individual cells and the plant as a whole. It consists primarily of cellulose, which is the main responsible for its mechanical properties. Under environmental stress, a crucial role is played by callose, a polysaccharide closely related to cellulose and a minority component of the cell wall. A recent study (*Plant Signal. Behav.* **2019**, *14*, e1548878) suggested that the enhancement of mechanical properties by callose is due to its ability to order neighbouring water molecules, giving origin to solid-like water-callose domains. This hypothesis is tested by atomistic MD simulations using models representing cellulose and callose hydrogels. The results highlight systematic differences in the coordination and H-bonding of callose and cellulose by water, reflected in different dynamical properties of water in callose or cellulose hydrogels, partly validating the hypothesis. However, mechanical properties, characterized by the Young's modulus of the polysaccharide / water gels, are the same in callose/ and cellulose/water samples, suggesting that callose's ability to link cellulose nanofibres into networks is the main responsible for the strengthening of the plant cell wall.

CPP 35: Microswimmers and Microfluidics (joint session DY/BP/CPP)

Time: Thursday 15:00–17:45 Location: H37

Invited Talk CPP 35.1 Thu 15:00 H37

Light-Driven Manipulation of Passive and Active Microparticles — •Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Germany

Chemical gradient near a solid/liquid can result in lateral long-range fluid transport termed diffusioosmotic (DO) flow. For instance, when photosensitive surfactant is irradiated with light converting the majority of the molecules in one of the possible isomers, emerging concentration gradient of isomers generates an osmotic pressure gradient tangent to the wall actuating the surrounding liquid to flow. [1-3] In my talk I will show how one can manipulate microparticles and even induce their self-propulsion by light urtilizing light driven diffusioosmotic (LDDO) phenomenon. Depending on the applied wave length one can either disperse/remove or gather particles. We will discuss how to establish light-driven hydrodynamics as a useful and versatile tool for investigating collective motion of self-propelled particles and aggregation

[1] Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S. Scientific Reports, 6 (2016) 36443. [2] Santer, S. J. Phys. D: Applied Physics, 51 (2017) 013002. [3] Arya, P.; Umlandt, M.; Jelken, J.; Feldmann, D.; Lomadze, N.; Asmolov , E. S.; Vinogradova, O. I.; Santer, S. A. The European Physical Journal E, 44(50) (2021), 1-10.

CPP 35.2 Thu 15:30 H37

Regulated polarization of active particles in local osmotic flow fields — •Lisa Rohde, Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Regulation in living systems is a fundamental principle for achieving robust functionality and maintaining specific non-equilibrium states. The control of certain properties and functionalities of systems on the microscale presents particular challenge since thermal fluctuations and environmental perturbations dominate. While synthetic active matter has demonstrated remarkable self-organization capabilities, examples of autonomous regulation processes at the single-particle level remain scarce. Here, we show experimentally that the interplay of two non-equilibrium processes leads to a regulated polarization state of

active particles in local osmotic flow fields. Based on thermophoretic repulsive and attractive forces that are generated by a single heat source at the boundary, the active particles encircle the heat source at a stable distance depending on the heat source temperature. The balance of these temperature-induced processes causes a polarization of the active particles that is independent of the heat source temperature. The individual control of heat source and active particles in the experiment allows detailed investigation of the self-regulated polarization effect in which we find hydrodynamic interactions to dominate. As the effects rely on osmotic flows and phoretic interactions, we expect that the observed phenomena can be generalized to other active systems and flow fields.

CPP 35.3 Thu 15:45 H37

Active particle steering in three dimensions — •Gordei Anchutkin and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Synthetic active particles serve as a model system that mimic the self-propulsion of living matter to explore fundamental aspects of non-equilibrium physics. Various collective phenomena of active agents have been studied, but mostly in the presence of hydrodynamic and physicochemical boundary effects. While theoretical works predict different collective dynamics in 3D, experimental investigations remain limited due the lack of experimental control over active swimmers in three dimensions.

Here we introduce three-dimensional control to the study of synthetic active matter. We demonstrate simultaneous control of thermophoretic microswimmers in 3D using single-particle tracking through digital holography and dark-field pattern tracking, with real-time wavefront shaping for steering. With the help of these experiments, we explore the interplay of thermophoretic propulsion, gravity, and optical forces for the active particles. By creating a three-dimensional active ensemble, we reveal how bulk interactions and boundary effects shape the collective behavior of active particles.

CPP 35.4 Thu 16:00 H37

***Trypanosoma brucei* in microchannels: the role of constrictions** — •Zihan Tan, Julian I. U. Peters, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Trypanosoma brucei (*T. brucei*), a single-celled parasite and natural microswimmer, is responsible for the fatal sleeping sickness in infected mammals, including humans. Understanding how *T. brucei* interacts with fluid environments and navigates through confinements is crucial for elucidating its movement through blood vessels and tissues, and across the blood-brain barrier.

Using a hybrid multiparticle collision dynamics (MPCD)–molecular dynamics (MD) approach, we investigate the locomotion of an in-silico *T. brucei* in three types of fluid environments: bulk fluid, straight cylindrical microchannels, and microchannels with constrictions. We observe that the helical swimming trajectory of the in-silico *T. brucei* becomes rectified in straight cylindrical channels compared to bulk fluid. The swimming speed for different channel widths is governed by the diameter of the helical trajectory. The speed first slightly increases as the channel narrows and then decreases when the helix diameter is compressed. An optimal swimming speed is achieved when the channel width is approximately twice the bulk helix diameter. Furthermore, *T. brucei* notably slows down when entering the narrow constriction in a microchannel and strongly speeds up upon exiting due to a release of deformation energy of the straightened cell body.

CPP 35.5 Thu 16:15 H37

Helical motion of microorganisms can be more persistent than straight motion — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[2], Freddy Frischknecht[2], and Ulrich S. Schwarz[1] — [1]BioQuant & Institute for Theoretical Physics, Heidelberg University — [2]Center for Integrative Infectious Disease Research, Heidelberg University

The movement of microorganisms has been extensively modeled by stochastic active particle models. In three dimensions, both swimming microorganisms, like sperm cells and some bacteria, and gliding microorganisms, like malaria sporozoites in the skin, often exhibit helical trajectories. If the internal driving force is the primary source of noise in the system, it induces random, yet time-correlated variations in the torque. To investigate this effect, we introduce a three-dimensional active rotational Ornstein-Uhlenbeck particle model. We find that the presence of a rotational component and the resulting helical path can mitigate the effect of intrinsic noise in the drive, allowing for larger long-time mean square displacements than straight movement at the same speed. The model not only provides qualitative insights into the constraints faced by microbes that may have led to the evolutionary selection of certain motility patterns, but also presents an analytical, quantitative tool for extracting information from these movements. We present and analyze corresponding data for malaria parasites gliding through hydrogels.

15 min. break

CPP 35.6 Thu 16:45 H37

Corrugated channels can filter ciliated microorganisms based on the metachronal wavelength — •Gonçalo Antunes and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Many microorganisms (e.g. Paramecium) move by a carpet of cyclically beating cilia that cover their surface. These cilia often beat in an organized fashion, such that the beating phases form a traveling wave, referred to as a metachronal wave. In this study, we investigate the swimming of such microorganisms in corrugated microchannels. We model the motion of the cilia via a time-varying effective slip velocity applied on the microorganism's surface, which we approximate as an infinite slab. By employing the lubrication approximation, we show analytically that the swimming speed of ciliated microorganisms placed inside a corrugated channel is sensitive to the corrugation height, provided that the wavelength of the corrugation matches that of the metachronal wave. Indeed, the direction of motion itself may invert with respect to swimming in bulk fluid, with the channel acting as a virtual barrier which blocks microorganisms under specific conditions for corrugation and slip-velocity modulations, but allow others to pass through. We also show that the interplay between the corrugation and the slip velocity profile allows for the swimming of microorganisms with zero time-averaged slip velocity, which thus cannot swim in bulk fluid. Finally, we complement our theory with preliminary results from hydrodynamic simulations for radially-symmetric microorganisms of finite length in radially-symmetric corrugated channels.

CPP 35.7 Thu 17:00 H37

Motion of a single particle partially exposed in a simple shear flow — •Dominik Geyer[1,2], Aouane Othmane[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), FZ Jülich — [2]Department of Physcis, FAU Erlangen-Nürnberg

Sand immersed in the water can be imagined as a wet granular matter. Besides sedimentation, friction, and surface roughness are two relevant physical phonemes within this system. Many body systems in a turbulent regime have been studied using discrete elements methods for a long time, but a single particle in the Stokes flow regime is particularly interesting for biological systems and microfluidic devices.

A layer of quadratic-arranged spheres models the rough surface. The question arises of how to describe the motion of a single traveling particle over this substrate.

We choose a combined numerical and analytical approach. The Stokes equation is solved analytically for the sphere near a rough wall. Lattice Boltzmann simulations with momentum-exchange particle coupling are performed for different wall roughness and friction coefficients.

Although, the Stokes equation assumes that the particle Reynolds number is zero. Surprisingly, the numerical results match our theoretical description until a particle Reynolds number of two. In this regime, friction between the moving particle and the substrate significantly influences the angular velocity but has a minor influence on the traveling velocity in the flow direction.

CPP 35.8 Thu 17:15 H37

Rational Design of Smart Microfluidics in Responsive Channels — •Arwin Marbini — Albert-Ludwigs Universität Freiburg

Responsive microfluidics offers exciting potential for self-regulating biomimetic systems. This study explores bifurcating microchannel networks with pressure-sensitive resistances, combining experiments with simulations based on the Hagen-Poiseuille equation and a linear model. These methods extract critical, experimentally inaccessible parameters under steady-state and dynamic conditions. Our findings enable the design of adaptable microfluidic networks, unlocking precise flow control for future applications in biology, soft robotics, and advanced material systems.

CPP 35.9 Thu 17:30 H37

Blue Water: A passive, reusable microfiltration device for water purification — •Tim R. Baumann, Ioannis Gkekas, Martina Viefhues, and Dario Anselmetti — Experimental Biophysics, Bielefeld University

Water is the most vital resource for life on Earth. Due to pollution of freshwater and oceans, this valuable resource has become globally endangered. The effects of microplastic pollution are widely discussed in scientific, political, and socioeconomic contexts. Despite regulations on single-use plastics and microplastic output, efforts should also focus on reintegrating microplastics to achieve a sustainable circular economy. Furthermore, microplastic-sized particles can migrate through organic tissue and can therefore be classified as contaminants of emerging concern. However, filtering plastics of this size is a challenging task.

Thus, this work examines and extends the findings of Divi et al. regarding the suspension feeding mechanisms of various ray species. We studied the filtration performance and efficiency for different geometric ratios of channel widths in simulations and laboratory environments. First, we have the main inner channel connected to the pressure inlet. From this, two rows of tilted lamellae structures branch off laterally to the outer secondary channels.

By applying sufficiently high pressure ($> 6 \cdot 10^5\ Pa$) to the inlet and achieving flow and particle velocities of $> 35\ \frac{m}{s}$, we can purify 82 % of half of the initial fluid. To prevent rupturing of our microfluidic chip under this pressure, we further investigated using glass fiber reinforced PDMS and lowering the operating pressure.

CPP 36: Organic Electronics and Photovoltaics IV

Time: Thursday 15:00–16:00 Location: H38

CPP 36.1 Thu 15:00 H38

How to Capture and Release Fullerene from an Azobenzene-Bithiophene Nanolayer? — Dmitry A. Ryndyk and •Olga Guskova — IPF Dresden, Hohe Str. 6 01069 Dresden

Optimizing organic photovoltaic devices involves the strategic use of well-defined monolayers of azobenzene-bithiophene (Azo-BT) switches. These monolayers serve as a bridge between inorganic and organic components, allowing precise nanoscale control over electrode morphology [1]. Previous studies have demonstrated that cis- and trans-Azo-BT switches chemisorbed on a gold surface exhibit distinct geometrical, electronic, and charge transport properties. We further investigate the behavior of cis- and trans-Azo-BT monolayers, with a particular focus on "nanotraps" nanometer-sized nanopores formed within the monolayers and their ability to capture&release fullerene. Our findings confirm that the photoswitchable "closed" and "open" configurations of Azo-BT nanotraps remain stable at room temperature under experimentally relevant surface densities. Energy calculations reveal that C60 molecules preferentially stabilize inside the open nanotrap near the pore surface, effectively capturing the fullerene. Additionally, a local energy minimum for C60 near the electron-donating BT block suggests charge transfer from the BT fragment to the fullerene, enhancing the interaction between the trap and the captured molecule. To expel the fullerene from the monolayer, we applied an alternating voltage electric field and determined the optimal parameters required to displace the nanoparticle, demonstrating the feasibility of controlled capture and release. [1] Savchenko, V. et al., Processes, 11 (2023) 2625.

CPP 36.2 Thu 15:15 H38

Deciphering vibronic interactions in NDI-T2 based donor-acceptor type oligomers with theoretical and experimental spectroscopy — •Maximilian F.X. Dorfner[1], Marko Medugorac[1], Ajeet Kumar[2], Jürgen Hauer[1], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — [2]Department of Chemistry, Lund University, Naturvetarvägen 14 222 62 Lund, Sweden

In this study, we investigate the alternating Naphthalendiimide-bithiophene co-oligomer (T2-NDI2OD-T2), a fundamental building block of the high charge-mobility polymer-semiconductor PNDI(2OD)2T. This class of materials has garnered significant attention for its exceptional charge transport properties, making it a promising candidate for applications in field-effect transistors and as non-fullerene acceptors in organic photovoltaics. We use Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) to examine the ground and singlet excited state properties to understand the electronic structure and vibrational excitations. Additionally, we analyze the coupling between electronic and vibrational degrees of freedom by means of a Linear Exciton-Vibrational Coupling Model parameterized by DFT. We compare the computed optical observables to the experiment and discuss the role of molecular vibrations in this system.

CPP 36.3 Thu 15:30 H38

Grain Boundaries and Charge Mobility in Organic Semiconductors: A Non-Adiabatic Molecular Dynamics Approach — •Sonali Garg[1], Farhad Ghalami[1], Sebastian Schellhammer[2], and Marcus Elstner[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Technische Universität Dresden, Germany

Organic semiconductors have emerged as crucial materials in the development of electronic and optoelectronic devices due to their exceptional mechanical flexibility, lightweight nature, and cost-effectiveness. However, the presence of grain boundaries (GBs) can significantly impede device performance by introducing traps or potential barriers that reduce charge carrier mobility. This study investigates the influence of the GB characteristics, including misorientation angles and GB width, on charge carrier mobility and compares the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing Fewest Switches Surface Hopping (FSSH) approach[1,2,3], were used to model charge transport dynamics. The charge transfer Hamiltonian was constructed using a fragment orbital approach, with its elements computed via the Density Functional Tight Binding (DFTB) method[4,5]. These insights provide a deeper understanding of the effects of GB on charge carrier mobility in organic semiconductors.

[1]Spencer. J et al. J. Chem. Phys. (2016) [2]Roosta. S J. Chem. Theory Comput. (2022) [3]Xie. W et al. J. Chem Theory Comput. (2020) [4]Elstner. M et al. Phys. Rev. B (1998) [5]Kubař. T et al. J. Phys. Chem. B (2010)

CPP 36.4 Thu 15:45 H38

Single-particle spectra of pentacene from exact simulations of Green's functions in the time-domain — •Michel Panhans[1], Frank Ortmann[1], and Hiroyuki Yoshida[2] — [1]TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — [2]Graduate School of Engineering, Chiba University, 1-33 Yayoicho, Inage-ku, Chiba, 263-0043, Japan

The investigation of single-particle spectra using experimental techniques such as photo-electron spectroscopy and inverse-photoelectron spectroscopy reveal the nature of the charge carriers close to the Fermi energy. In particular for organic crystals such as pentacene, the single-particle spectra are strongly affected by the electron-phonon coupling (EPC) and crucially deviate from the theoretical spectra based on ab initio band-structure calculations associated with the HOMO and the LUMO of the pristine crystal.

To model these experiments more accurately, Green's-function approaches including the EPC are a suitable methodology to describe what is seen in experiments. In our present study, we calculated the HOMO and the LUMO spectra of pentacene single-crystals and compared them to experimental results. We find that the quantum mechanical treatment of the EPC has a crucial impact on the fine structure of the spectra and explains the band features of the experimental spectra for HOMO and LUMO of pentacene.

CPP 37: Focus Session: Interactions Between Water and Cellulose II

Time: Thursday 16:15–17:15 Location: H34

Invited Talk CPP 37.1 Thu 16:15 H34

Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level — Marie Hartwig-Nair, Sara Florisson, Kristofer Gamstedt, and •Malin Wohlert — Dep of Materials Science and Engineering, Uppsala University

Softwood branches develop compression wood (CW) in the lower and opposite wood (OW) in the upper part exhibiting different hygro-mechanical properties and differ in structure at several length scales. Distinctive differences are found at cell level, cell wall level and at the level of chemical composition of the lignin and hemicellulose matrix.

The effect each of these respective differences have on tissue level of wood hygromechanical properties is not yet clear. Here, a hierarchical multiscale modelling approach is employed, where the impact composition, MFA and lignin chemical difference have on wood hygro-expansion is studied by the means of hierarchical modelling as support to tissue level experimental investigation of CW and OW hygro-expansion [1]. With atomistic models and Molecular Dynamics simulations of lignin at different levels of hydration, swelling coefficients for the different lignin matrices are obtained [2] and implemented in a Finite Element (FE) model of the cell wall. The FE model also accounted for differences in MFA and composition.

The results of the FE model will be discussed and connected to the MD and tissue level results.

[1] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, 58, 887-906.
[2] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, in press.

CPP 37.2 Thu 16:45 H34

Exploring Hygroexpansion of Cellulose Based Fibers via μCT — •Maximilian Fuchs[1,2], Raimund Teubler[2,3], Alexandra Serebrennikova[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper — [3]Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Austria

Understanding the swelling of cellulose-lignin-based fibers is crucial for describing the processes involved in the uptake of water or other volatile organic compounds in paper. Microcomputed tomography (μCT) promises to monitor the

hygroexpansion on a paper sheet level. However, extracting and analyzing individual fibers from the interwoven fiber network in these μCT images is challenging. We present a new approach to identify, extract, and analyze hollow fibers by focusing on the fiber lumen as the structural backbone. Using this approach, we quantify changes in fiber shape as the paper sheet absorbs water and another polar solvent, dimethyl sulfoxide (DMSO), from the vapor phase. We continue to observe these changes long after saturation, when no further mass is absorbed in the fibers. With both water and DMSO, the fiber wall thickness continues to increase even after reaching saturation. Furthermore, when exposed to water, the fibers tend to become rounder during swelling, suggesting fiber decollapse. In contrast, the data for DMSO indicates that the outermost fiber layer gets damaged, leading to unrestricted swelling once saturation is exceeded.

CPP 37.3 Thu 17:00 H34

Structure and dynamics of water adsorbed to amorphous cellulose: a comparison of experimental and simulated neutron scattering data — •Veronika Reich[1], Martin Müller[1,2,3], and Sebastian Busch[1] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum hereon GmbH, Garching, Germany — [2]Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel

Neutron scattering experiments provide valuable insights into the nanoscopic properties of matter, a scale that is also accessible through Molecular Dynamics (MD) simulations. If the simulations reproduce the experiments, they can give greater insight into the material properties on the nanoscopic scale than traditional data analysis methods. In our work we establish a connection between published experimental data about water absorbed to amorphous cellulose from neutron experiments [1] and MD simulations. Special focus was put on the comparison of the structure factor of non-crystalline water and the dynamics as a function of temperature. The MD simulations were designed to be close to the experimental data from literature to achieve a meaningful comparison.

[1]Czihak, Christoph: Cellulose: Structure and dynamics of a naturally occurring composite material as investigated by inelastic neutron scattering, PhD thesis in material science, University of Vienna (Austria) and Institute Laue-Langevin (France), 2000

CPP 38: Interfaces and Thin Films II

Time: Thursday 16:15–17:45 Location: H38

Invited Talk CPP 38.1 Thu 16:15 H38

Adsorption and Interaction of Amino Acids on Titanium Oxide Photocatalyst — Miguel Blanco-Garcia[1], Mona Kohantorabi[1], Benedikt Socher[2], Ulrike Protzer[3], Stephan V. Roth[2], Cristiana Di Valentin[4], Andreas Stierle[1], and •Heshmat Noei[1] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Institute of Virology, Technical University of Munich/Helmholtz Munich, 81675 Munich, Germany — [4]Department of Materials Science, University of Milano-Bicocca, Via R. Cozzi 55, I-20125, Milano, Italy

We investigated the adsorption behavior of amino acids and SARS-CoV-2 virus on rutile (110) and anatase (101) TiO2 surfaces through a combined experimental and theoretical approach and explored the molecular configurations and bonding mechanisms involved in interaction of cysteine and SARS-CoV-2 with TiO2. Clarification of the interaction of the virus with the surface of semiconducting oxides will aid in obtaining a deeper understanding of the chemical processes involved in photo-inactivation of microorganisms which is important for developing advanced photocatalytic materials for environmental and biomedical applications. [1] M. Kohantorabi, et al., ACS Appl. Mater. Interfaces 16, 28 (2024) 37275. [2] M. Kohantorabi, et al., ACS Appl. Mater. Interfaces 15, 6 (2023) 8770.

CPP 38.2 Thu 16:45 H38

PNIPAM Microgel-Stabilized Foam Films: Effect of Crosslinker Content and Purification State — •Luca Mirau, Joanne Zimmer, Kevin Gräff, Matthias Kühnhammer, and Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Aqueous foams find widespread application in fields such as cosmetics, food industry, oil recovery and fire-fighting. Their stabilization requires the presence of surface-active molecules or colloidal particles. In this study, thermoresponsive microgels (MGs) composed of poly(N-isopropylacrylamide) (PNIPAM) with varying crosslinker contents are applied as foam stabilizers, resulting in temperature-sensitive foams. Foam films serve as the fundamental building blocks of foams. The structuring of MGs within these films is analyzed using the Thin Film Pressure Balance (TFPB) technique. Foam films are formed within a pressure chamber, and their thickness is determined through interferometric methods under a light microscope. The foam films display an inhomogeneous structure comprising significant pattern formation, i.e. a network-like, several 100nm thick region containing MGs, interspersed with thin MG-depleted zones less than 100nm thick. The findings indicate that the crosslinking content plays a crucial role in MG layering within these thick network regions, influencing the film thickness. Additionally, the purification state of the MGs, monitored through interfacial tension measurements, governs the formation of thin zones in the foam films, which strongly affects their stability.

CPP 38.3 Thu 17:00 H38

Ion Specific Effects and Photo-Switching of Surfactants at Interfaces — •Dana Glikman and Björn Braunschweig — Institute of Physical Chemistry and Center for Soft Nanoscience, University of Münster, Busso-Peus-Str. 10, 48149 Münster (Germany)

Understanding surface charging and molecular structure changes at oil/water (O/W) interfaces in nanoemulsions is critical for enhancing colloidal properties. In previous work, we demonstrated that photo-switchable surfactants could modulate interfacial behavior. Specifically, we studied an arylazopyrazole (AAP) derivative that undergoes photoisomerization between E and less surface-active Z isomers. In nanoemulsions with droplets showing an average radius of 90 nm, no significant changes in drop size or ζ-potential were observed upon E/Z photoisomerization. However, second-harmonic scattering (SHS) revealed substantial changes in surfactant coverage which were attributed to ion condensation at the interface [1]. In this contribution, we now focus on the role of specific ion effects and the structural influence of the surfactants' head group. By systematically varying between Li, Na, and Cs cations and by using surfactants with different head group architectures, we aim to dissect the interplay between ionic specificity and head group structure. To study the adsorption of the surfactants at the interface, we are analyzing SHS profiles combined with measurements of the ζ-potential at the shear plane, in order to reveal a detailed mechanisms of ion-specific effects and ion condensation in these nanoemulsions. [1] Glikman et al. J. Am. Chem. Soc. 146, 8362 (2024).

CPP 38.4 Thu 17:15 H38

Anomalous Screening Behavior of Superchaotropic Ions — •Thomas Tilger, Esther Ohnesorge, Michalis Tsintsaris, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Due to their special properties, which make them suitable for many applications such as wastewater treatment, separation of nuclear waste and the stabilization of foams, the interest in superchaotropic nano ions grew during the last years. Especially for the last application, it is crucial to understand how the presence of these ions modifies the interaction between interfaces.

To directly measure the forces between well-defined interfaces, colloidal probe atomic force microscopy (CP-AFM) has proven to be a powerful tool. As model system for nano ions we chose Keggin ions as well as dodecaborate clusters and investigated their influence on the interaction between colloidal silica beads in aqueous solutions.

It turned out that - despite the large ion size of up to one nanometer - the interaction between the silica beads can still be described by the classical DLVO-theory of electrolyte solutions, consisting of a van der Waals attraction and an electrostatic double layer repulsion. However, the obtained screening lengths exhibit a significant deviation from the ones expected according to the nominal ionic strength of the solutions. This might be a hint for an ion aggregation. The magnitude of the deviation depends on the type of nano ion as well as the concentration of the solution.

CPP 38.5 Thu 17:30 H38

The Physics of Water-based Inkjet Printing: Fundamentals in a Nutshell — Helder Savaldor[1,2] and •Nicolae Tomozeiu[1,2] — [1]Canon Production Printing, P.O Box 101, Van der Grintenstraat 1, 5914HH Venlo, The Netherlands — [2]Fluids & Flows Group, Department of Applied Physics, Eindhoven University of Technology, The Netherlands

The printing industry is rapidly evolving, driven by advances in understanding physical-chemical processes and societal needs. Digital inkjet printing, especially with water-based inks, has become a cornerstone of sustainable and cost-effective printing, with Canon Production Printing (CPP) leading innovations in this field. The interaction between ink droplets and porous paper is crucial to achieving high-quality prints, and understanding these processes is essential for improving print performance and durability.

This work explores key scientific domains involved in CPP water-based inkjet technology. We focus on: (i) ink formulation through chemical and polymer

physics for optimal droplet formation and film creation; (ii) the dynamics of thin films, including ink spreading, evaporation, and imbibition in porous paper; (iii) surface science's role in ink absorption and spreading. We will show the use of Optical Spectroscopy, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR) and uGISAXS to provide deeper insights into ink film formation at the micro- and nano-level. These findings optimize print quality, durability, and color properties, advancing both industrial development and academic knowledge in inkjet technology.

CPP 39: Members' Assembly

Time: Thursday 18:00–19:00 Location: H38

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 40: Energy Storage and Batteries II

Time: Friday 9:30–11:15 Location: H34

CPP 40.1 Fri 9:30 H34

Nanoscale Agglomeration Mechanisms of BF-DPB:BPyMPM Donor-Acceptor Systems for Organic Optoelectronic Devices — •Milena Merkel[1], Philipp Wiesener[1], Robert Schmidt[1], Rishi Shivhare[2,3], Rudolf Bratschitsch[1], Saeed Amirjalayer[4], Koen Vandewal[2,3], and Harry Mönig[1] — [1]Physikalisches Institut, Münster University, Münster, Germany — [2]Institute for Materials Research (imo-imomec), Hasselt University, Hasselt, Belgium — [3]imec, imo-imomec, Diepenbeek, Belgium — [4]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany

The molecular order of photo-active molecules of organic optoelectronic devices has major impact on their performance. However, it is usually investigated only by indirect measurements or simulations. Here we use low-temperature scanning probe microscopy to image the molecular assembly and interfaces of the donor and acceptor molecules BF-DPB and BPyMPM with submolecular resolution. We illustrate the crucial effect of the substrate and the position of the nitrogen atoms in the BPyMPM molecules on the formation of intermolecular C-H..N hydrogen bonds, metal coordination bonds and corresponding self-assemblies. Using scanning tunneling spectroscopy, we are able to correlate the increasing disorder at the BF-DPB:BPyMPM interface with an increase in the HOMO-LUMO gap of BF-DPB. Photoluminescence measurements on BF-DPB indicate a significant increase in intersystem crossing due to molecule-substrate interactions. Our results provide new insights for a tailored design of active molecules and contact layers for organic optoelectronic devices.

CPP 40.2 Fri 9:45 H34

Multi-layered electrodes for flexible solid-state super capacitors with polymer-based gel electrolyte — •Reyhaneh Bahramian[1,2,3] and Yaser Abdi[3] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran — [3]Nanophysics Research Laboratory, Department of Physics, University of Tehran, Tehran 14395-547, Iran

Flexible solid-state supercapacitors are gaining popularity due to their advantages, including flexibility, lightweight design, high power density, rapid charge and discharge rates, broad operating temperature ranges, long cycle life, safety, and ease of fabrication. The use of gel polymer electrolytes enhances ionic conductivity while addressing safety concerns associated with liquid electrolytes.

This research focuses on developing nanocomposite electrodes using Ag-decorated zinc oxide, synthesized through a chemical deposition method on carbon paper, and ferrite applied via a drop-casting technique. The goal is to create electrodes that can operate across a wide voltage range in a non-aqueous electrolyte.

Advanced characterization techniques, such as atomic force microscopy, X-ray diffraction, field emission scanning electron microscopy, and Raman spectroscopy, are employed to analyze the structural properties of the electrodes. The findings reveal an effective specific capacitance of approximately 70 milliFarads per square centimeter.

CPP 40.3 Fri 10:00 H34

Dual-cation pre-intercalated hydrated vanadium oxide achieves 20,000 cycles in aqueous zinc-ion batteries — •Yan Ran and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Aqueous zinc-ion batteries (AZIBs) have broad application prospects in energy storage due to their low cost and high safety. However, cathode materials still face challenges such as low specific capacity and decreased long-cycle performance. In this work, hydrated vanadium oxide with pre-intercalated K and Mn ions (K0.07Mn0.13V2O5*1.47H2O) was synthesized via a one-step hydrothermal method, demonstrating an excellent specific capacity of 524.7 mA h g-1 at 0.1 A g-1, and outstanding stability with 82.47% capacity retention after 20,000 cycles at 5 A g-1. The co-intercalation of dual cations increases the interlayer spacing while stabilizing the material structure, expanding the ion transport channels, and improving both the specific capacity and long-cycle stability. Moreover, the Zn2+/H+ co-intercalation mechanism was confirmed by ex-situ characterization. This work will provide insights for the development of competitive cathodes in high-performance aqueous batteries.

CPP 40.4 Fri 10:15 H34

Temperature-resolved Crystal Structure of Ethylene Carbonate — •Lea Westphal[1,2], Vladislav Kochetov[2], Volodymyr Baran[3], Maxim Avdeev[4,5], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]MLZ, TUM, 85748 Garching, Germany — [3]DESY, 22607 Hamburg, Germany — [4]ANSTO, NSW 2234, Sydney, Australia — [5]School of Chemistry, University of Sydney, NSW 2006, Sydney, Australia

Lithium-ion batteries (LIBs) have been a dominant power source for portable electronics for over three decades and are of interest for applications in electric vehicles and large-scale energy storage systems. Despite significant advancements in LIB design, the main solvents used in the liquid electrolytes, responsible for the charge transfer between the electrodes, have largely remained the same. A key class of these solvents are linear and cyclic carbonates, which, when two or more solvents are combined with lithium salts and additives, exhibit favorable physical/chemical properties. Ethylene carbonate (EC) is a common solvent in commercial batteries due to its high dielectric constant and its ability to form the protective solid-electrolyte interphase (SEI) layer. However, it has to be mixed with other solvents because of its high melting point. Following the determination of EC's crystal structure from single crystals, this study presents temperature dependent Neutron and Synchrotron Powder Diffraction data, studying the sample from 3 K up to its melting point and investigations by Synchrotron Total Scattering and Pair Distribution Function analysis.

CPP 40.5 Fri 10:30 H34

Polymer-nano-tufts: A hairy story of limited conductivity — •Martin Tress, Alaa Yussef Hassan, Nico Junkers, and Wing Kit Or — Peter-Debye-Institute for Soft Matter Research, Leipzig University, Leipzig, Germany

Here we present an approach to study conductivity in small polymer aggregates of as few as ten chains using dielectric spectroscopy [Macromol Chem Phys, 224 (2023) 2200452]. For that, a nano-structured electrode arrangement is combined with several physico-chemical surface modifications to deposit a regular pattern of gold nanoparticles onto which end-functionalized polymer chains are grafted to create tuft-like ensembles of individualized chain aggregates. For polyethylene, pronounced changes in conductivity are observed in tufts compared to bulk with details indicating an alteration of the type of charge transport. This might signal a switch from fast inter-chain ion hopping, dominating in bulk, to slower intra-chain ion hopping in the tufts attributed to the chain configurations and orientation forced by the grafting. Consequently, this could be a more general phenomenon of polymer-solid interfaces that may explain significantly increased electrode polarization and interfacial resistance in ion-conducting polymers, potentially diminishing their performance. Hence, the hypothesis, that bottle-brush architectures could reduce these unwanted effects, was developed. Supported by preliminary results, this might be a step to improve polymeric electrolytes for various fields ranging from solid-state electrolyte batteries to ion-conducting fuel cell membranes.

CPP 40.6 Fri 10:45 H34

Interpretation of the Impedance Signal of Composite Materials using a 3D Electrical Network Model — •Felix Schug[1,2], Sascha Kremer[2,3], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, 35392 Giessen, Germany

All solid-state batteries (aSSBs) are promising candidates for next-generation energy storage systems, offering high energy and power densities as well as improved device safety compared to the established lithium-ion batteries. Electrochemical impedance spectroscopy (EIS) is one of the key methods to determine charge transport characteristics of the material components in an aSSB. Many of these components are composed of multiple phases, with various transport processes affecting the impedance response signal. Furthermore, the microstructure of the material manifests as a signal within the impedance spectrum. The interpretation of an impedance spectrum is therefore not straightforward, as many signals overlap or are indistinguishable from each other. We therefore employ a microstructure-resolved 3D electrical network to modulate charge transport on microscopic length scales. This approach reveals how microstructure affects the impedance response, as well as the potential and current distributions within a system. It is used to investigate the impedance of composite materials and to develop guidelines for its interpretation.

CPP 40.7 Fri 11:00 H34

Measuring Local Electrochemical Properties with Scanning Probe Microscopy — •Alexander Klasen and Andrea Cerreta — Park Systems Europe GmbH, Mannheim, Germany

Electrochemical (EC) applications, ranging from novel energy storage systems to advanced catalysts, are defined on an ever-decreasing length scale. Investigating these systems requires to map key functional features with sufficient resolution, such as the local structure, electronic properties and electrochemical response. Scanning probe microscopy-based techniques are well established to investigate surface parameters using the physical interaction with a nanometer-sized probe allows studying properties such as the topography, work function, or adhesion at high resolution. One such technique, Scanning Electrochemical Cell microscopy (SECCM), was first introduced by E. Daviddi, P.R. Unwin, et al. and uses a pipette-based SPM approach to probe local EC features. When brought in close proximity to the sample, the electrolyte-filled pipette pipette creates a small electrolyte meniscus between the pipette aperture and the surface of interest . This confined volume of solution constitutes a small electrochemical cell that allows for local measurements of electrochemical characteristics. In this talk, we discuss the basics of SECCM, present recent examples from literature, discuss the limitations of the technique and outline potential pathways to overcome those.

CPP 41: Charged Soft Matter, Polyelectrolytes and Ionic Liquids I

Time: Friday 9:30–11:15 Location: H38

Invited Talk CPP 41.1 Fri 9:30 H38

Simulations of reaction equilibria in macromolecular systems — •Peter Košovan — Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czechia

Most molecular simulations are performed assuming a fixed chemical composition, focusing on structural and conformational changes and intermolecular interactions, while neglecting the possible chemical changes which may occur simultaneously. In this lecture, we present an overview of our modeling work, addressing how reversible chemical reactions affect the properties of macromolecular solutions and gels. In particular, we discuss the effect of acid-base equilibria on the net charge of peptides, synthetic polyelectrolytes, polyelectrolyte hydrogels, and proteins. By comparing with experiments, we show that our models can quantitatively predict how this net charge depends on pH of the solution. Next, we show that a change in the pH can trigger attraction between macromolecules, resulting in the formation of condensates, precipitation or gelation. Finally, we show how changes in the pH can be used to control the uptake of charged proteins into coacervates, and how the pH affects the properties of protein solutions during purification processes used by the pharmaceutical industry: dialysis and ultra- or dia-filtration.

CPP 41.2 Fri 10:00 H38

Surface Charged Polymeric Micelles - A Tunable Model System Studied by SANS — Lingsam Tea[1], Luis Willner[1], Christin Waldorf[1], Olga Matsarskaia[2], Ralf Schweins[2], Stephan Förster[1], Lutz Willner[1], and •Jörg Stellbrink[1] — [1]JCNS-1, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut Laue-Langevin, 38042 CEDEX 9 Grenoble, France

We investigate surface charged micelles in aqueous solution formed by carboxy terminated n-octacosyl-poly(ethylene oxide) block copolymers, C-PEO5-COOH with 5 the PEO molar mass in kg/mol, by small angle neutron scattering (SANS), zeta-potential measurements and rheology. The -COOH end group was introduced by selective oxidation of the CH_3OH end group of a C-PEO5-OH precursor using Bobbitt's salt. Micellar solutions of different concentrations in the dilute and semidilute range were investigated at pH 2, 6 and 12 to vary ionic strength and the number of effective surface charges Z. Z was further varied by using mixtures of C-PEO5-COOH and C-PEO5-OH at different mixing ratios. SANS measurements reveal that the intramicellar form factor is identical at the different pH-values which implies that the individual micellar structure is unaffected by the number of surface charges. On the contrary, the intermicellar structure factor and the phase behavior show a strong dependence on Z. In particular, we observe a distinct shift of the liquid - fcc crystal phase boundary. A quantitative analysis in terms of a screened Hard Sphere Yukawa potential reveals a very good agreement between experiment and theory.

Macromolecules 2024, 57, 5818-5830

CPP 41.3 Fri 10:15 H38

Orientation analysis in polyelectrolyte multilayer and brush coatings by dichroic ATR-FTIR spectroscopy — •Martin Müller, Mirjam Hofmaier, Patricia Flemming, Olga Guskova, Alexander Münch, and Petra Uhlmann — Leibniz-Institut für Polymerforschung Dresden e.V.

Dichroic ATR-FTIR spectroscopic data on two types of thin oriented polyelectrolyte (PEL) coatings relevant for life science are presented. Trapezoidal silicon multiple internal reflection elements, sealed in-situ cell in ATR mirror attachment with polarizer and commercial FTIR spectrometer were used. (i) At first dichroic ATR-FTIR data on thin PEL multilayer (PEM) coatings composed of a-helical poly(L-lysine) and various polyanions (PLL/PA) at unidirectionally texturized silicon substrates are presented. Based on experimental dichroic ratios RATR, the known angles theta between transition dipole moment (TDM) of Amide I and Amide II vibration and a-helix axis (38°, 73°) and on calculated electrical field components Ex,y,z high in-plane y-axial orientation of PEM was identified. (ii) Secondly, thin cationic PEL brushes with three different grafting densities at silicon substrates were characterized by dichroic ATR-FTIR. Using concept of (i) and angle theta between TDM of n(C=O) vibration of PDMAEMA and molecular main axis (69°), which was determined by atomistic simulations, high out-of-plane z-axial orientation was identified. Swelling in water increased the orientation if compared to dry state. Both PEL coating types may be used as bioactive platforms towards proteins and microorganisms.

CPP 41.4 Fri 10:30 H38

Vertical Polyelectrolyte and Site Diffusion of PSS in PSS/PDADMA Multilayers — Annekatrin Sill, •Per-Ole Hilken, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

The spontaneous formation of polyelectrolyte multilayers or polyelectrolyte complexes depends on the (inter)diffusion of polyelectrolytes. We investigate the transport of extrinsic sites - charged polyelectrolyte repeat units balanced by counterions - and their relationship to polymer diffusion. We determine the vertical diffusion coefficient D_{PSS} of polystyrene sulfonate (PSS) repeat units in polyelectrolyte multilayer films from poly (diallyldimethylammonium) (PDADMA) and PSS using a quartz crystal microbalance with dissipation (QCM-D) and analyze the observed film growth. Varying the NaCl concentration c_{NaCl} results in $D_{PSS} = 3.2{\cdot}10^{-20}\ \mathrm{m^2/s}{\cdot}e^{\alpha \cdot c_{NaCl}}$. As known from the free volume model, the prefactor is constant for each system. For site diffusion, the exponent is also constant ($\alpha \approx 4.9\ \mathrm{M^{-1}}$). For polymer diffusion, however, α increases linearly with M_{PSS}, the molecular weight of PSS. The results for site diffusion quantitatively agree with those of Fares and Schlenoff (JACS (2017) 139; 14656). Polymer diffusion occurs when $M_{PSS} < 65$ kDa (for $M_{PDADMA} = 117$ kDa). For these low PSS molecular weights, the diffusion coefficient is $D_{PSS} = B \cdot M_{PSS}^{-\gamma}$. The dependence of B on c_{NaCl} is a power law, while γ increases linearly with c_{NaCl}.

CPP 41.5 Fri 10:45 H38

Understanding the Mechanisms of pH-Sensitive Collapse of Hydrophobic Polymers — •Varun Mandalaparthy and Nico F. A. van der Vegt — Technical University, Darmstadt

The hydrophobic effect is a important contributor to the stability of proteins and may be influenced by many factors including the pH of the solution. To simplify the study of pH effects on proteins, we parameterize biologically motivated titratable monomers which we insert into the sequence of a hydrophobic polymer and study via constant pH molecular dynamics (MD) simulations. We calculate the potential of mean force of the polymer at different pH values and observe that the collapsed state of the polymer is destabilized when the titratable monomer is more charged (high pH for an acid and low pH for a base). Further, the extent of the destabilization is influenced by the position of the titratable monomer along the polymer sequence. The pK_a value of the titratable monomer is also observed to be sensitive to polymer conformation, in agreement with studies of proteins. We further study a zwitterionic polymer with an acidic and a basic monomer in the same sequence which presents a pH-dependent hairpin formation. Our

model provides a simplified yet powerful framework to study pH effects on the hydrophobic effect, providing insights into mechanisms governing the behavior of intrinsically disordered proteins (IDPs) and pH-sensitive drug delivery, among other applications.

CPP 41.6 Fri 11:00 H38

Machine learning potentials for redox chemistry in solution — •Redouan El Haouari[1,2], Emir Kocer[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Machine-Learning Potentials (MLPs), which can offer the accuracy of quantum mechanics at a fraction of the costs, have been applied with great success in atomistic simulations of many systems. Still, most MLPs rely on environment-dependent atomic energies, and are thus unable to distinguish different oxidation states of simple ions in solution. Here, we show for the example of ferrous (Fe2+) and ferric (Fe3+) chloride in aqueous solution that this limitation can be overcome with 4th-Generation High-Dimensional Neural Network Potentials (4G-HDNNPs), in which the local atomic energies are complemented with global charges from a charge equilibration scheme. We find that the iron oxidation states match the total number of chloride ions in the system irrespective of their positions. Furthermore, the model captures charge transfers between ferrous and ferric ions, enabling the general simulation of redox chemistry in solution involving different oxidation states.

CPP 42: Active Matter IV (joint session BP/CPP/DY)

Time: Friday 9:30–13:00 Location: H44

Invited Talk CPP 42.1 Fri 9:30 H44

Wave propagation in systems of active filaments — •Kirsty Y. Wan — Living Systems Institute, University of Exeter, UK

Active hair-like protrusions called cilia are found in many eukaryotes where they produce physiological flows for a variety of functions. Cilia assume a myriad of configurations both external to an organism for the purposes of feeding or swimming motility, but also internally where they mediate mucociliary clearance in vertebrate tissues. Single cilia can propagate large-amplitude non-decaying bending waves, even in the absence of a cell body. These waves assume a variety of stereotyped forms and frequencies, depending on the species. Multiple cilia also interact to produce different types of local and global coordination patterns, including robust metachronal waves. Do these dynamic states of coordination arise spontaneously, or do they require some form of internal control by the cell or animal? We propose new and emerging organisms to address these questions.

CPP 42.2 Fri 10:00 H44

Metabolic activity controls the emergence of coherent flows in microbial suspensions — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to the spatio-temporal variations of environmental parameters within their habitat. In the absence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment may be deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we study the effect of motility and cell density of *C. reinhardtii* in a confined system, on the emergence of bioconvection [2]. This collective phenomenon can be reversibly switched by light and arises due to the natural tendency of the bottom-heavy cells to move against gravity. We show that the rate at which the system evolves, as well as the dominant wavelength of the instability can both be directly controlled by the number density of cells. Further, we provide insights on the internal flow fields and density profiles of single bioconvection plumes for different parameters.

[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).
[2] A.A. Fragkopoulos et al., *arXiv*:2407.09884 (2024)

CPP 42.3 Fri 10:15 H44

Tumbling *E.coli* in bulk and close to surfaces — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian institute of science education and research (IISER), Tirupati, India

Escherichia coli (*E. coli*) swims by rotating multiple flagella which are connected to the cell body forming a thick bundle. To change direction, *E. coli* performs tumble events by reversing the rotation of one or more flagella. The involved filaments undergo a series of polymorphic transformations, altering both their helicity and handedness. This complex phenomenon involves the interplay of semiflexible filaments and hydrodynamic flow fields.

Here, we have developed a detailed numerical framework to simulate *E. coli*, capturing the full dynamics of flexible flagella, including their polymorphism and their hydrodynamic interactions. The filaments and the cell body are embedded in a viscous fluid, which we model using multi-particle collision dynamics. We analyzed a large number of tumble events, with fixed tumble time or taken from a gamma distribution, exploring the roles of hook and flagellar flexibility as well as flagellar polymorphism. We find that they strongly influence the distribution of tumble angles. Finally, we also show that close to a flat surface the mean tumble angle is strongly shifted to smaller values. This indicates that tumble events may not be recognized, which could give the impression of suppressed tumbling near surfaces.

CPP 42.4 Fri 10:30 H44

***Trypanosoma brucei* (un)chained - effects of confinement on a parasitic microswimmer** — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth — [2]Laboratory of Molecular Parasitology, University of Bayreuth

Trypanosoma brucei is a parasitic unicellular microswimmer that causes the African sleeping sickness. An active spiral movement of the parasite, mediated by a microtubule-driven flagellum that wraps around the cell body, is mandatory to evade the host's immune system while exploring tissues and blood vessels. In addition, the nematic subpellicular micotubule array plays a pivotal role in the elasticity, propulsion, and navigation of the parasite. To study the features and mechanisms behind the cell's motion in such complex environments, we have mimicked spatial confinement in microfluidic devices with different geometries. Our data show that spatial constraints in narrow channels and channel networks can improve cell locomotion of wild-type trypanosomes, supposedly due to the interaction of the elastic cell body and nearby walls. The addition of microtubule-disrupting drugs or the use of mutant strains with altered post-translational modifications of microtubules resulted in significantly altered swimming velocities and marked changes in the intermittent switching between run and tumble phases. Shape analyses of individual cells suggest that microtubules in the sub-pellicular array, the corset that keeps trypanosomes in their native spindle-like shape, are most affected in these cases.

CPP 42.5 Fri 10:45 H44

Micro-swimmer motility in presence of signaling factors — Agniva Datta, Robert Grossmann, and •Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

The navigation of bacteria through aqueous environments, driven by the rotation of helical flagella, has been a significant region of interest in the biophysics community for the last few decades. In this study, we focus on the motility of our model organism, Pseudomonas putida, which exhibits persistent mobile episodes (Active Brownian motion) interrupted by stochastic reorientation events (turns), driven by flagellar self-propulsion, thereby leading to a run-and-turn motility.

Key motility parameters including tumbling rates, run lengths, trajectory persistence (rotational diffusion coefficient), and the characteristics of the self-propulsion force*are hypothesized to depend on the density of quorum-sensing autoinducer molecules, produced by the bacteria themselves as signaling factors. To test this hypothesis, we expose swimming bacteria to aqueous environments with controlled autoinducer concentrations and analyze the resulting changes in motility patterns. Through a combination of experimental data and theoretical modeling, we aim to elucidate the principles of micro-swimmer motility in presence of signaling molecules.

CPP 42.6 Fri 11:00 H44

Collective dynamics of active dumbbells near a circular obstacle — •Chandranshu Tiwari[1] and Sunil Singh[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India. — [2]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

We present the collective dynamics of active dumbbells in the presence of a static circular obstacle using Brownian dynamics simulation. The active dumbbells aggregate on the surface of a circular obstacle beyond a critical radius, and the aggregate size increases with the activity and the curvature radius. The dense aggregate of active dumbbells displays persistent rotational motion with a certain angular speed, which linearly increases with activity. Furthermore, we show a strong polar ordering of the active dumbbells within the aggregate. The polar ordering exhibits long-range correlation, with the correlation length corresponding to the aggregate size. Additionally, we show that the residence time of an active dumbbell on the obstacle surface increases rapidly with area fraction due to

many-body interactions that lead to a slowdown of the rotational diffusion. This article further considers the dynamical behavior of a tracer particle in the solution of active dumbbells. Interestingly, the speed of the passive tracer particle displays a crossover from monotonically decreasing to increasing with the size of the tracer particle upon increasing the dumbbells' speed. Furthermore, the effective diffusion of the tracer particle displays non-monotonic behavior with the area fraction; the initial increase in diffusivity is followed by a decrease for a larger area fraction.

CPP 42.7 Fri 11:15 H44

Free growth under tension — •Chenyun Yao and Jens Elgeti — Forschungszentrum Jülich GmbH, Jülich, Germany

Ever since the ground breaking work of Trepat et al. in 2009, we know that cell colonies growing on a substrate can be under tensile mechanical stress. The origin of tension has so far been attributed to cellular motility forces being oriented outward of the colony. Works in the field mainly revolve around how this orientation of the forces can be explained, ranging from velocity alignment, self-sorting due to self-propulsion, to kenotaxis.

In this work, we demonstrate that tension in growing colonies can also be explained without cellular motility forces! Using a combination of well established tissue growth simulation technique and analytical modelling, we show how tension can arise as a consequence of simple mechanics of growing tissues. Combining these models with a minimalistic motility model shows how colonies can expand while under even larger tension. Furthermore, our results and analytical models provide novel analysis procedures to identify the underlying mechanics.

15 min. break

CPP 42.8 Fri 11:45 H44

A route to active turbulence in circular activity spots — •Arghavan Partovifard and Holger Stark — Institute of Theoretical Physics, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany.

Active nematics exhibit distinctive behavior such as active turbulence and regular flow patterns under spatially varying activity [1]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investigate active nematics confined to a circular spot by switching off activity outside the spot. The open boundary allows topological defects to enter and leave the spot.

We calculate the total topological defect charge inside the spot using three approaches: counting all defects, measuring the rotation of the director field along the rim of the spot, and integrating the diffusive charge density. All methods agree that for spot radii just larger than the nematic coherence length, the system has a total topological charge of +1, where two +1/2 defects perform a regular swirling motion. As the radius increases, more defects enter and their motion becomes more and more chaotic. Ultimately, the charge per unit area saturates at the value characteristic of bulk active turbulence. For the range of radii where the total charge in the spot is +1, the nematic director exhibits shear-induced anchoring at an angle of 45° with respect to the tangent at the spot rim. With increasing radius, when more defects enter, the anchoring angle deviates from 45° but its distribution still peaks around this value.

[1] A. Partovifard *et. al.*, Soft Matter **20**, 1800 (2024)

CPP 42.9 Fri 12:00 H44

Cognitive flocks: order-disorder transitions and threat evasion — •Priyanka Iyer[1], Cecilia Soroco[2], and Gerhard Gompper[1] — [1]Forschungszentrum Jülich — [2]University of British Columbia, Canada

Directed self-propulsion is ubiquitous in living organisms. From E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379.
[2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

CPP 42.10 Fri 12:15 H44

Myosin-independent amoeboid cell motility — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell motility is essential for many physiological and pathological processes, such as the immune system, embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode which allows them to move rapidly in a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. We introduce a model for an amoeboid cell where the cortex is described as a thin shell along the cell surface. The cell shape evolves due to polymerization of actin filaments and the forces acting on the cortex. We find analytically and numerically that the state of a resting, non-polarized cell can become unstable for sufficiently large actin polymerization velocities, resulting in the spontaneous onset of cell polarity, migration, and dynamical shape changes. Notably, this transition only relies on actin polymerization and does not necessitate molecular motors, such as myosin. These findings yield a deeper understanding of the fundamental mechanisms of cell movement and simultaneously provide a simple mechanism for cell motility in diverse configurations.

CPP 42.11 Fri 12:30 H44

Active membrane deformations of a synthetic cell-mimicking system — Alfredo Sciortino[1], •Dmitry Fedosov[2], Gerhard Gompper[2], and Andreas Bausch[1] — [1]Physik Department, Technische Universität München, Garching bei München, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

CPP 42.12 Fri 12:45 H44

Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles — Eike Eberhard, •Ludwig Burger, Cesar Pastrana, Giovanni Giunta, and Ulrich Gerland — Physik komplexer Biosysteme, Technische Universität München, Deutschland

Recent experiments show that the diffusion coefficient of some metabolic enzymes increases with the concentration of their cognate substrate, a phenomenon known as enhanced diffusion. In the presence of substrate gradients, enhanced diffusion induces enzymatic drift, resulting in a non-homogeneous enzyme distribution. In this work, we study the behavior of enzyme-loaded vesicles exposed to external substrate gradients using a combination of computer simulations and analytical modeling. We observe that the spatially inhomogeneous enzyme profiles generated by enhanced diffusion result in a pressure gradient across the vesicle, which leads to macroscopically observable effects, such as deformation and self-propulsion of the vesicle. Our analytical model allows us to characterize dependence of the velocity of propulsion on experimentally tunable parameters. The effects predicted by our work provide an avenue for further validation of enhanced diffusion, and might be leveraged for the design of novel synthetic cargo transporters, such as targeted drug delivery systems.

CPP 43: Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:45 Location: H47

Invited Talk CPP 43.1 Fri 9:30 H47

From Cavitation in Soft Matter to Erosion on Hard Matter — •Claus-Dieter Ohl — Institute of Physics, Otto-von-Guericke University, Magdeburg, Germany

Cavitation is the technical term for the formation of empty spaces in a liquid. These unstable voids eventually implode and focus energy on small volumes. Shock wave emission, light emission, erosion, and even nuclear reactions are the consequence of this near singular energy focusing. Here, I will present recent research related to cavitation not only in liquids but also in elastic solids and particularly at the interface of both materials. Singularities developing on the axis of symmetry in non-spherical collapses near boundaries are able to amplify shock waves through self focusing. We think that this mechanism is the primary cause for erosion. In contrast, the non-spherical collapse and shock wave focusing near a tissue allows for the penetration of the tissue with liquid jets at 1000m/s and above. The mechanism at play may be relevant in sports and battle zones, as they could lead to traumatic brain injuries.

CPP 43.2 Fri 10:00 H47

Shape switching and tunable oscillations in adaptive droplets — •Tim Dullweber[1,2], Roman Belousov[1], Camilla Autorino[1,4], Nicoletta Petridou[1], and Anna Erzberger[1,3] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]University Heidelberg, Heidelberg, Germany — [3]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [4]Faculty of Biosciences, Heidelberg University, Heidelberg, Germany

Soft materials can undergo irreversible shape changes when driven out of equilibrium. When shape changes are triggered by processes at the surface, geometry-dependent feedback can arise. Motivated by the mechanochemical feedback observed in multicellular systems, we study incompressible droplets that adjust their interfacial tensions in response to shape-dependent signals. We derive a minimal set of equations governing the mesoscopic droplet states, controlled by just two dimensionless feedback parameters. We find that interacting droplets exhibit bistability, symmetry-breaking, excitability and tunable shape oscillations ranging from near-sinusoidal to relaxation-type. We apply our framework to model shape measurements in zebrafish embryos and identify a shape-switching mechanism promoting boundary formation. The underlying critical points reveal novel mechanisms for physical signal processing through shape adaptation in soft active materials, and suggest new modes of self-organization at the collective scale.

CPP 43.3 Fri 10:15 H47

Impact of the history force on the motion of droplets in shaken liquids — •Frederik Gareis and Walter Zimmermann — Theoretical Physics, University of Bayreuth

The Basset-Boussinesq history (BBH) force acts on droplets and solid particles in flows, alongside stationary viscous friction, inertia, and gravitational forces. This force arises from vortex shedding around objects undergoing unsteady acceleration. In this study, we analytically calculate the BBH force for spherical, sedimenting heavy particles in horizontally shaken (periodically accelerated) fluids at low Reynolds numbers and identify the parameter ranges where BBH effects are significant. Our results reveal that BBH can increase particle displacement amplitude by over 60 percent, particularly in the transition region between the low-frequency viscous Stokes regime and the high-frequency inertia-dominated regime. Additionally, we derive a power law for the oscillatory displacement amplitude of a particle around its mean position in a horizontally shaken fluid, facilitating clear experimental identification of BBH effects.

CPP 43.4 Fri 10:30 H47

Bubble Dynamics and Transport in Porous Structures: Insights from Mesoscale Simulations — •Qingguang Xie[1], Othmane Aouane[1], and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg (IET-2), Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Bubble formation, detachment, and transport within porous structures are critical phenomena in various applications, including electrolyzers and chemical reactors. We numerically investigate the dynamics of bubble growth and detachment at a catalytic surface using the lattice Boltzmann method. The departure radius of a bubble, growing with either a pinned or moving contact line, shows good agreement with theoretical predictions. Beyond detachment, we examine the subsequent transport of bubbles through a porous transport layer, systematically evaluating transport efficiency by considering factors such as pressure gradients, reaction rates, and pore wettability. Our findings provide valuable insights for optimizing the design of porous structures, potentially resulting in enhanced performance in electrolyzers and other gas-evolving devices.

CPP 43.5 Fri 10:45 H47

Displacements in thin fluid and elastic films — •Andreas M. Menzel — Otto von Guericke University Magdeburg, Germany

We address the displacements of comparatively small objects in flat thin fluid films under low-Reynolds-number conditions or in flat thin elastic sheets under linear elasticity.

It is well-known that the fundamental solution of the corresponding continuum equations for forced in-plane displacements diverges logarithmically in strictly two-dimensional systems, the so-called Stokes paradox. We provide an illustrative way of interpretation and demonstrate how the divergence cancels under pairwise interactions and confinement [1,2]. Interestingly, logarithmic spatial dependencies prevail under rectangular clamping of elastic membranes [3]. Moreover, the divergence is still present in free-standing sheets of finite thickness, unless they are stabilized, for instance, by substrates [4,5].

We are confident that our analytical results will prove useful in corresponding quantitative experimental evaluations.

[1] S. K. Richter, A. M. Menzel, Phys. Rev. E **105**, 014609 (2022).
[2] T. Lutz, S. K. Richter, A. M. Menzel, Phys. Rev. E **106**, 054609 (2022).
[3] A. R. Sprenger, H. Reinken, T. Richter, A. M. Menzel, EPL (Europhys. Lett.) **147**, 17002 (2024).
[4] T. Lutz, A. M. Menzel, A. Daddi-Moussa-Ider, Phys. Rev. E **109**, 054802 (2024).
[5] A. Daddi-Moussa-Ider, E. Tjhung, T. Richter, A. M. Menzel, J. Phys.: Condens. Matter **36**, 445101 (2024).

CPP 43.6 Fri 11:00 H47

Magnetic dynamics in ferromagnetic liquid crystal emulsions — •Christoph Klopp[1], Hajnalka Nádasi[1], Darja Lisjak[2], and Alexey Eremin[1] — [1]Otto von Guericke University, Institute of Physics, 39106 Magdeburg, Germany — [2]Jozef Stefan Institute, Department for Materials Synthesis, 1000 Ljubljana, Slovenia

We explore magnetic liquid crystal (LC) emulsions for applications as manipulatable chemical sensors in giant cells of Characean algae. Such emulsions can be controlled by magnetic fields and provide targeted drug delivery or sensing [1]. The investigated emulsions consist of a ferromagnetic liquid crystal [2] dispersed in an aqueous solution. We investigate the dynamic magnetic response using AC-susceptometry [3] as a function of the carrier medium viscosity and the particle or droplet size distribution. The emulsions' magnetic spectra differ drastically from those in the bulk of the hybrid liquid crystal mixture. We demonstrate the influence of the liquid crystal director configuration at the water-droplet interface by analyzing the effect of different surfactants (mainly SDS and PVA) in the aqueous phase.

[1] F. von Rüling et al., Liquid Crystals, 2024, 51, 1546
[2] A. Mertelj, et al., Nature, 2013, 504, 237-241
[3] M. Küster et al., J. Magn. Magn. Mater., 2023, 588, 171368

This study was supported by DFG with projects ER 467/14-1 and NA1668/1-3.

15 min. break

CPP 43.7 Fri 11:30 H47

Drying effects in soft colloidal monolayers — •Kai Luca Spanheimer[1], Matthias Karg[2], Nicolas Vogel[3], Liesbeth Janssen[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [3]Lehrstuhl für Partikelsynthese Friedrich-Alexander-Universität,91058 Erlangen, Germany — [4]Soft Matter and Biological Physics Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

Langmuir-Blodgett deposition is a staple of colloidal monolayer research. It is used in sample preparation for imaging techniques, that spatially resolve colloid patterns. Recent experimental observations have shown that drying can strongly rearrange micron sized microgel patterns after their deposition. The usual dictum that these drying effects do not play a role for colloidal deposition can thus not be held up as a general rule. While capillary effects are well known to be strong at microscopic length scales and play a significant role in drying processes they have been mostly neglected concerning Langmuir-Blodgett deposition. In order to better understand the mechanism of drying we propose a model based on capillary attraction as well as hard core and soft shell repulsion. This model reproduces colloid patterns observed at interfaces as well as ones that occur after drying in the corresponding parameter regimes. From here we are able to derive parameter ranges where drying can play a role in rearranging patterns of colloids and where it can't.

CPP 43.8 Fri 11:45 H47

Interplay of Elasticity and Capillarity in Droplets on Flexible Sheets — •Salik Sultan and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Droplets resting on flexible sheets deform into lens-like shapes, offering promising applications in areas like tunable liquid lenses. We have extended and employ our fully three-dimensional Boundary Element Method (BEM) simulation framework [1] to investigate dynamic wetting on thin flexible sheets. Our study focuses on the intricate interplay between the mechanical properties of the sheet and droplet behavior, particularly emphasizing contact angle and droplet shape. By varying the tension and mechanical properties of the sheet, our model demonstrates how we can control and tune the shape of the droplet. Additionally, by introducing stiffness gradients, we aim to explore the potential to steer droplets along the sheet via durotaxis. The versatility of our model suggests potential extensions to other soft material and droplet interactions, such as capillary origami. This work sheds light on the complex interactions between soft substrates and liquid interfaces, leading the way for advancements in material science and interfacial biology.

[1] J. Grawitter and H. Stark, Steering droplets on substrates with plane-wave wettability patterns and deformations, Soft Matter 20, 3161 (2024).

CPP 43.9 Fri 12:00 H47

Cluster quasicrystals composed of ultrasoft particles vs. soft quasicrystals built of colloids with hard cores — Robert F.B. Weigel and •Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study and compare two different approaches for the stabilization of quasicrystals:

First, we consider a Phase Field Crystal model of complex patterns that self-assemble in systems consisting of ultrasoft colloids. Quasicrystals can be either stabilized by interactions with multiple length scales [1,2] or by preferred binding angles as in patchy colloids [3].

Second, we study a system with patchy colloids with a hard core with a Density Functional Theory. The hard-core is implemented by using a variant of the Fundamental Meassure Theory [4] that probably is the best mean field approach to hard particles.

While the ultrasoft particles assemble in cluster quasicrystals where the particles can completely overlap, in case of hard cores we observe structures that are rather dominated by the tiles that occur on a local level. Our results explain the differences between quasicrystlas that occur in different systems.

[1] Lifshitz, Petrich, PRL 79, 1261 (1997).
[2] Achim et al., PRL 112, 255501 (2014).
[3] Weigel, Schmiedeberg, Modelling Simul. Mater. Sci. Eng. 30, 074003 (2022).
[4] Rosenfeld, PRL 63, 980 (1989).

CPP 43.10 Fri 12:15 H47

Beyond rings and chains: exploring porous crystals and flexible networks with magnetic colloids — •Carina Karner — Technische Universität Wien

We report on the self-assembly of magnetic colloids engineered with two distinct magnetic patches positioned at their poles, an advancement from traditional Janus particles with a single magnetic dipole. While Janus particles are known to form a variety of superstructures including chains, rings, and close-packed arrangements [1], the two-patch design significantly expands the range of achievable structures. Our simulation study reveals the formation of porous networks with adjustable flexibility, variable pore sizes, and controllable crystalline order. Notably, we observe the formation of a porous Kagome lattice, reminiscent of the experimental Kagome lattice observed colloids with two hydrophobic patches, the well known Janus-triblock system [2]. This enhanced self-assembly behavior in two-patch magnetic particles opens up further possibilities for creating fully tunable, field-responsive ferrofluids. Such systems could useful for applications requiring externally modulated viscosity, such as adaptive damping systems in automotive and aerospace engineering. [1] Vega-Bellido, G. I., DeLaCruz-Araujo, R. A., Kretzschmar, I., & Córdova-Figueroa, U. M. (2019). Self-assembly of magnetic colloids with shifted dipoles. Soft Matter, 15(20), 4078-4086. [2] Chen, Q., Bae, S. C., & Granick, S. (2011). Directed self-assembly of a colloidal kagome lattice.Nature,469(7330), 381-384.

CPP 43.11 Fri 12:30 H47

Effect of geometrical confinement on friction in soft solids — •Aashna Chawla and Deepak Kumar — Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India

Soft and biological materials come in a variety of shapes and geometries. When two soft surfaces with mismatched Gaussian curvatures are forced to fit together, beautiful patterns emerge at the interface due to geometry-induced stress. In this study, we explore the effect of geometrically incompatible confinement of a thin sheet on a soft hydrogel substrate on friction. We use a novel experimental setup to measure the friction between a thin flat elastic sheet placed on a low-friction hydrogel substrate. We show that the frictional force at the interface strongly depends on the geometry and is significantly larger for the geometrically incompatible configuration of a flat sheet on a spherical substrate compared to the other two geometrically compatible configurations: flat sheet on a flat substrate and flat sheet on a cylindrical substrate. Furthermore, for the incompatible configuration of the flat sheet on a spherical substrate, we observe that the frictional force increases monotonically with the sheet radius, with a transition in the behavior at an intermediate radius. We show that these effects arise from the coupling of the stress developed in the sheet due to its geometrically incompatible confinement with the curvature of the interface, resulting in an increased normal force, thereby increasing friction. The insights gained from this study could have significant implications for our understanding of friction in various biological, nanoscale, and other soft systems.

CPP 44: 2D Materials

Time: Friday 11:30–12:30 Location: H34

CPP 44.1 Fri 11:30 H34

Sensors based on graphene field-effect transistors functionalized with molecularly imprinted polymers — •David Kaiser[1], Hamid Rasouli[1], Michael Ringleb[2,3], Ludwig Büttner[2], Martin Hager[2,4], Guobin Jia[5], Jonathan Plentz[5], Christian Beringer[4], Patrick Bräutigam[4], Uwe Hübner[5], Patrick Endres[2], Christof Neumann[1], Steffi Stumpf[2,3], Benjamin Dietzek-Ivanšić[1,4,5], Ulrich S. Schubert[2,3,4] und Andrey Turchanin[1,3,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena — [3]Jena Center for Soft Matter, Friedrich Schiller University Jena — [4]Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena — [5]Leibniz Institute of Photonic Technology (Leibniz IPHT)

Monitoring of micropollutants has become a regulatory requirement due to their environmental and health impacts. However, their on-site detection remains challenging, as current methods require transporting samples to centralized laboratories. Here, we present a method for the direct identification of the pharmaceutical carbamazepine (CBZ) utilizing solution-gated graphene field-effect transistors (SG-GFETs) that is appropriate for on-site use. We integrate molecularly imprinted nanoparticles (MIPs) with a diameter of 20 nm onto graphene via their self-assembly, creating highly stable films that specifically bind CBZ, and demonstrate a detection sensitivity reaching as low as 1 pM in buffer solutions and 10 pM in samples of environmental water.

CPP 44.2 Fri 11:45 H34

Efficient DFT Band Gap Correction for 2D-Covalent Organic Frameworks Towards Hybrid Functional Level — •Laura Fuchs and Frank Ortmann — Technische Universität München, TUM School of Natural Sciences

Density functional theory (DFT) is the workhorse computational tool for predicting the structure and physical properties of inorganic and organic molecules as well as semiconductors. Unfortunately, the optical and fundamental band gaps are not well described by semi-local DFT approaches. In particular, common DFT methods like the local density approximation (LDA) and the generalized gradient approximation (GGA) severely underestimate the fundamental band gaps, which is commonly referred to as the "band gap problem". However, the correct band gap is of utmost importance for evaluating the suitability of materials such as organic semiconductors for applications like photocatalysis or green energy harvesting. Besides highly expensive many-body perturbation theory, hybrid functionals can address the band gap problem. However, these functionals still involve high computational costs and, for large two-dimensional covalent organic frameworks (2D-COFs), these efforts are not always feasible. Here, we study the relation between semi-local PBE and hybrid HSE06 functionals and present a simple and computationally cheap scheme to extrapolate the PBE band gaps in 2D-COFs to a more precise band gap at HSE06 level.

CPP 44.3 Fri 12:00 H34

Towards the Computational Design of Molecular Olfactory Receptors for Digital Odor Detection — •Li Chen[1], Leonardo Medrano Sandonas[1], Arezoo Dianat[1], Nina Tverdokhleb[1], Rafael Gutierrez[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena

We present the MORE-Q dataset using quantum-mechanical (QM) simulations for dimer systems composed of body odor volatilome (BOV) and olfactory re-

ceptors. The dataset contains abundant QM properties of diverse BOV-receptor systems, both in the gas phase and when deposited on a graphene surface. After analyzing the property space spanned by MORE-Q, we observed flexibility when searching for a dimer configuration with a desired set of electronic binding features. To gain insights into the complex interplay between these sensing properties, an ensemble learning method (XGBoost) was constructed for the fast evaluation of BOV adsorption behavior using only the dimer configurations properties. The results show a significant increase in model performance by adding multiple conformers to the training procedure, and SHAP analysis identifies the most relevant descriptors for predicting the binding features. Our work provides valuable insights into the the sensing mechanism of BOV molecules and paves the way for the computational design of receptors with targeted sensitivity and selectivity.

CPP 44.4 Fri 12:15 H34

Effective EMI shielding solutions: the role of 2D materials and their performance across frequency ranges — •Reyhaneh Bahramian[1,2] and Mohammad Nezafati[2] — [1]Department of Cognitive Sciences, Faculty of Psychology and Education, University of Tehran, Tehran, Iran — [2]Condensed Matter National Laboratory, Institute for Research in Fundamental Sciences, Tehran 19395-5531, Iran

The rise in electronic device usage has led to increased electromagnetic interference (EMI), creating a pressing need for effective shielding materials that are flexible, lightweight, cost-efficient, and high-performing. Two-dimensional (2D) materials are emerging as strong candidates for next-generation EMI shielding solutions. This review examines the origins of electromagnetic responses and shielding mechanisms, focusing on photon-matter interactions, and evaluates the instruments and standards for measuring shielding effectiveness.

Recent advancements in 2D materials for EMI shielding are analyzed, comparing their performance across different frequency ranges with other composite materials. Although 2D material-based composites show significant promise, challenges remain in expanding their applications, particularly in the sub-gigahertz range.

CPP 45: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Friday 11:30–12:45 Location: H38

CPP 45.1 Fri 11:30 H38

Binding of small molecules to polyelectrolytes driven by electrostatics — •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

The interaction of small molecules or ligands to macromolecules (polyelectrolytes or proteins) in solution is plays an important role in biological and medical applications. Pulsed-field-gradient (PFG) nuclear magnetic resonance (NMR) has been applied to measure translational motion of molecules and complexes in aqueous solution, that may be diffusion orelectrophoretic motion. Two-dimensional NMR experiments correlating chemical shift that is used to assign different species with either the diffusion coefficient or the electrophoretic mobility enable determining the mobility of diffusion coefficient respectively in mixtures for the individual components. From the combination of diffusion and electrophoresis NMR the effective charge of the species under investigation is derived. Weak interaction of the ligand to the macromolecule means that the ligand binds for a fraction of time to the macromolecule and is free in the solution for another fraction. From the thus observed weighted average the bound fraction is calculated for every condition no titration experiment is required. The strong polyelectrolyte PDADMAC has been studied interacting with glutamic acid as a function of pH. The bound fraction of glutamic acid increases with increasing pH and thus increasing negative charge of glutamic acid showing that the interaction is driven by electrostatic interaction rather than other possible interactions. The bound fraction as a function of pH coincides with the charge.

CPP 45.2 Fri 11:45 H38

How charge regulation affects adsorption of proteins into polyelectrolyte brushes: A simulation study — •Keerthi Radhakrishnan and Christian Holm — Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany

In recent years, polyelectrolyte (PE) brushes have drawn significant attention for their industrial and biomedical applications, particularly their ability to immobilize proteins via electrostatic interactions, even beyond the isoelectric point where both brush and protein share a similar charge. This counterintuitive phenomenon is normally attributed to "charge patch" effects from protein surface heterogeneity or "charge regulation" involving reionization and charge reversal near charged entities.

Using coarse-grained simulations, we investigate weak PE brushes interacting with pH-responsive ampholytic nanoparticles exhibiting patchy and non-patchy charge distributions. Building on prior single-ion models, we incorporate realistic protein models with asymmetric charge group distributions to explore higher-order and charge patch-induced effects. Our findings reveal the critical role of charge regulation stemming from anisotropic nanoparticle surface charge, brush potential, and brush-induced pH modulation in driving protein adsorption beyond the isoelectric point.

[1] K. Radhakrishnan, D. Beyer, and C. Holm, How Charge Regulation Affects pH-Responsive Ampholyte Uptake in Weak Polyelectrolyte Brushes, https://doi.org/10.26434/chemrxiv-2024-b10lj-v2., Macromolecules, in print.

CPP 45.3 Fri 12:00 H38

Molecular Dynamics Simulations of Structural and Dynamical Properties of Polymerized Ionic Liquids — •Arshid Ahmad and Michael Vogel — Institute for Condensed Matter Physics, Technische Universität Darmstadt, Darmstadt, Germany

Ionic liquids consist of cations and anions and have melting points less than 100°C. Their key features include negligible vapor pressure, high thermal stability, and favorable solvation properties, rendering them valuable materials for applications, e.g., in green chemistry and electro-chemistry. In addition to these simple ionic liquids (SILs), polymerized ionic liquids (PILs) receive considerable attention because they add the favorable mechanical properties of polymers to these systems. We present MD simulations of a SIL and a corresponding PIL. The latter comprises BF4 anions and polymerized cations, which feature imidazolium rings connected by 6 methylene groups along the backbone. We use MD simulations to determine both structural and dynamical prop- erties of this PIL. In particular, we relate the temperature-dependent local and diffusive dynamics of the anions and polymerized cations and we analyze dynamical couplings of both components. For the anions, the analysis includes the mechanism and f the motion. For the polymerized cations, we investigate not only the segmental motion but we also tackle the question to which degree the Rouse model is capable of describing the dynamics of highly charged polymer chains, which strongly interact with counter-ions. A detailed comparison of the results for the SIL and PIL reveals the effects of cation polymerization on structural and dynamical properties.

CPP 45.4 Fri 12:15 H38

Condensate size control by charge asymmetry — •Chengjie Luo[1], Nathaniel Hess[2], Dilimulati Aierken[2], Yicheng Qiang[1], Jerelle A. Joseph[2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Princeton University

Biomolecular condensates are complex droplets composed of various types of biomolecules, including nucleic acids and proteins. These condensates form mainly due to liquid-liquid phase separation, which is driven by short-range attraction between biomolecules. Typical biomolecules carry various net charges, so that long-ranged electrostatic interactions could affect phase separation. We study this situation using a simple model of two short-ranged attractive polymers with opposite charges and their counterions. We find that the charged polymers segregate from the solvent, and thus form two macrophases, when their charges are symmetric. In contrast, many droplets of equal size coexist when charge asymmetry is sufficiently strong. Such patterned phases form because the short-range attraction concentrates polymers within droplets, leading to net charges, which prevents droplet growth. Our molecular dynamics simulation and a continuous field theory demonstrate that droplet size decreases with charge asymmetry. Overall, we present a mechanism controlling droplet size via a trade-off between short-ranged attraction driving phase separation and long-ranged electrostatic repulsion if droplets accumulate net charges. Our results are relevant for understanding biomolecular condensates and creating synthetic patterns in chemical engineering.

CPP 45.5 Fri 12:30 H38

Structural transitions of a Semi-Flexible Polyampholyte — •Rakesh Palariya and Sunil P Singh — Indian Institute Of Science Education and Research, Bhopal , India

Polyampholytes (PA) are charged polymers composed of positively and negatively charged monomers. The sequence of the charged monomers and the bending of the chain significantly influence the conformation and dynamical behavior of the PA. Using coarse-grained molecular dynamics simulations, we comprehensively study the structural and dynamical properties of flexible and semi-flexible PA's. The simulation results demonstrate a flexible PA chain, displaying a transition from a coil to a globule in the parameter space of the charge sequence. Additionally, the behavior of the mean-square displacement (MSD), denoted as $< (\Delta r(t))^2 >$, reveals distinct dynamics, specifically for the alternat-

ing and charge-segregated sequences. The MSD follows a power-law behavior, where $< (\Delta r(t))^2 > \sim t^{\beta}$, with $\beta \approx 3/5$ and $\beta \approx 1/2$ for the alternating sequence and charge-segregated sequence in the absence of hydrodynamic interactions, respectively. However, when hydrodynamic interactions are incorporated, the exponent β shifts to approximately 3/5 for the charge-segregated sequence and 2/3 for the well-mixed alternating sequence. For a semi-flexible PA chain, varying the bending rigidity and electrostatic interaction strength (Γ_e) leads to distinct, fascinating conformational states, including globule, bundle, and torus-like conformations. The transition between various conformations is identified in terms of the shape factor estimated from the ratios of eigenvalues of the gyration tensor.

CPP 46: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H2

Invited Talk CPP 46.1 Fri 13:15 H2

Active control of forces, movement and shape: from biological to non-living systems — •Ulrich S. Schwarz — Heidelberg University, Heidelberg, Germany

Animal cells are highly dynamic and continuously generate force, for example for division, migration and mechanosensing. Their main force generators are myosin II molecular motors, whose activity is precisely controlled by biochemical circuitry. We first discuss how this system can be hijacked by optogenetics, thus that cellular force generation can be controlled in time and space using light. Next, we use active gel theory combined with van der Waals theory for myosin II molecules to demonstrate that cell contractility is sufficient to explain cell migration and that optogenetics can be used to initiate and revert migration. For two myosin II species, we predict the possibility of oscillations. We then move up in scale and analyze force generation in intestinal organoids, which are epithelia with the topology of a sphere. Combining experimental data, image processing and the bubbly vertex model, we show how apico-basal asymmetries can lead to cell extrusion and budding. We finally discuss how force generation and shape changes can be achieved in non-living systems, in particular for nematic elastomers, in which the direction of contraction is imprinted during polymerization and actuation is achieved by temperature control.

Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture halls H3 and H14; Poster P1)

Invited Talks

DS 4.1	Tue	9:30–10:00	H3	**Graphene-based epitaxial 2D heterosystems: making graphene great again** — •Christoph Tegenkamp
DS 7.1	Wed	9:30–10:00	H14	**Enhancing Organic Spin Valves Through Spinterface Engineering** — •Shuaishuai Ding, Wenping Hu
DS 9.1	Thu	9:30–10:00	H3	**Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces** — •Sebastian Heidenreich, Nando Hegemann, Victor Soltwisch, Markus Bär
DS 9.2	Thu	10:00–10:30	H3	**Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces** — •Bernd Bodermann, Matthias Wurm, Manuela Schiek, Jana Grundmann, Tim Käseberg
DS 12.1	Thu	16:15–16:45	H3	**Probing the Electronic Structure of Halide Perovskites** — •Selina Olthof
DS 12.2	Thu	16:45–17:15	H3	**Quantum Science with Single Atoms and Molecules on Surfaces** — •Philip Willke
DS 12.3	Thu	17:30–18:00	H3	**Gallium Nitride Technology - the second pillar of microelectronics** — •Andreas Waag
DS 12.4	Thu	18:00–18:30	H3	**Ultrafast X-ray photoelectron spectroscopy and photoelectron diffraction** — •Philip Hofmann
DS 15.1	Fri	9:30–10:00	H3	**Structure formation and growth at the metal-organic interface** — •Peter Zeppenfeld

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole

SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Sessions

DS 1.1–1.10	Mon	9:30–12:30	H3	**Thin Film Properties**
DS 2.1–2.5	Mon	9:30–10:45	H14	**Layer Deposition**
DS 3.1–3.10	Mon	15:00–17:45	H3	**2D Materials and their Heterostructures I (joint session DS/HL)**
DS 4.1–4.11	Tue	9:30–13:00	H3	**2D Materials and their Heterostructures II (joint session DS/HL)**
DS 5.1–5.5	Tue	14:00–15:15	H3	**Thin Oxides and Oxide Layers**
DS 6.1–6.8	Wed	9:30–11:45	H3	**Thin Film Application**
DS 7.1–7.7	Wed	9:30–11:45	H14	**Spins in Molecular Systems: Strategies and Effects of Hyperpolarization**
DS 8.1–8.4	Wed	12:00–13:00	H3	**Optical Analysis of Thin Films I**
DS 9.1–9.9	Thu	9:30–12:45	H3	**Optical Analysis of Thin Films II**
DS 10.1–10.4	Thu	11:30–12:30	H14	**Transport Properties**
DS 11.1–11.4	Thu	15:00–16:00	H3	**Thermoelectric and Phase Change Materials**
DS 12.1–12.4	Thu	16:15–18:30	H3	**Gaede-Jubiläumssitzung**
DS 13.1–13.64	Thu	18:00–20:00	P1	**Poster**
DS 14	Thu	18:30–20:00	H3	**Members' Assembly**
DS 15.1–15.7	Fri	9:30–11:45	H3	**Organic Thin Films, Organic-Inorganic Interfaces**

Members' Assembly of the Thin Films Division

Thursday 18:30–20:00 H3

- Report of activities in 2024
- Election of deputy speaker DS

Sessions

– Invited Talks, Contributed Talks, and Posters –

DS 1: Thin Film Properties

Time: Monday 9:30–12:30 Location: H3

DS 1.1 Mon 9:30 H3

From ferromagnetic semiconductor to anti-ferromagnetic metal in epitaxial CrxTey monolayers — •Naina Kushwaha[1,2], Olivia Armitage[1], Brendan Edwards[1], Liam Trzaska[1], Jennifer Rigden[2], Peter Bencok[3], Deepnarayan Biswas[3], Tien-Lin Lee[3], Charlotte Sanders[2], Gerrit van der Laan[3], Peter Wahl[1,4], Phil D. C. King[1], and Akhil Rajan[1] — [1]University of St Andrews, UK — [2]Central Laser Facility, UK — [3]Diamond Light Source, UK — [4]Physikalisches Institut, University of Bonn , Germany

Two-dimensional (2D) materials can exhibit markedly distinct electronic and magnetic properties compared to their bulk counterparts [1]. Among these, the Cr-Te compounds are of particular interest. 1T-CrTe2, in particular, is a room-temperature ferromagnet in the bulk, but is only metastable, readily decomposing into self-intercalated compounds like Cr2Te3 [2]. Utilizing a nucleation-assisted molecular-beam epitaxy growth method [3], we achieve the growth of phase selective monolayer Cr2Te3 and 1T-CrTe2 with enhanced growth rates and uniformity. Characterization using X-ray magnetic circular dichroism, scanning tunneling microscopy, and angle-resolved photoemission spectroscopy reveals metallic antiferromagnetic behavior in 1T-CrTe2 and semiconducting ferromagnetic properties in Cr2Te3. These findings advance new understanding of the magnetic order in Cr-Te monolayers, and demonstrate routes to control this, of potential future interest for advancing 2D spintronics [1].

[1]Gibertini, et al., Nat. Nanotech. (2019), [2]Lasek, et al., ACS Nano (2020), [3]Rajan, et al. Adv. Mater. (2024).

DS 1.2 Mon 9:45 H3

In-situ and operando characterization of atomic layer deposited SnO_2 and SnO_2/CeO_2 heterostructures for gas sensing applications — •Rudi Tschammer, Carlos Morales, Karsten Henkel, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology, Cottbus, Germany

The amorphous and defective nature of atomic layer deposited (ALD) thin films results in material properties deviating from those of well-ordered and crystalline samples. For instance, we recently reported that ALD cerium oxide (CeO_2) ultrathin (<10nm) layers could be reduced under H_2/O_2 mixtures at room temperature without decoration with noble metals, thus opening the door to design miniaturized resistive sensors based on ALD-CeO_2 active layers. However, the remaining challenges include high electrical resistance (GΩ) and relatively long response and recovery times, which may be solved by combination with conductive oxides. In particular, tin oxide (SnO_2) has been shown to improve the sensing properties of CeO_2, tentatively explained by interface effects. Here, we present in-situ X-ray photoelectron spectroscopy (XPS) and operando spectroscopic ellipsometry measurements of ultra-thin ALD-SnO_2 layers, highlighting a linear growth rate, an evolution of the Sn Auger parameter related to distinct chemical envioroments rather than different oxidation states, and changes in C and N residues with the ALD number of cycles. Lastly, preliminary results from structural and chemical characterization, as well as sensing capabilities, of ALD-SnO_2/CeO_x heterostructures are discussed.

DS 1.3 Mon 10:00 H3

RF sputtered growth of β-Ga_2O_3 on Ru(0001) films — •Aman Baunthiyal, Marco Schowalter, Martin Williams, Jon-Olaf Krisponeit, Thorsten Mehrtens, Alexander Karg, Andreas Rosenauer, Martin Eickhoff, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Gallium oxide (Ga_2O_3) is a leading candidate for high-power, high-frequency electronics due to its wide bandgap and high breakdown voltage. While its growth on insulating substrates like AlN and Al_2O_3 has been well-studied, research on metal substrates remains limited. This study investigates RF-sputtered growth of Ga_2O_3 thin films on Ru(0001) surfaces with varying roughness at temperatures from room temperature (RT) up to 600°C [1].

AFM measurements showed that surface roughness peaks at intermediate growth temperatures, then decrease at 600°C, suggesting a shift toward two-dimensional growth or increased surface diffusion. XRD revealed the amorphous nature of RT-grown Ga_2O_3 films but polycrystallinity in higher-temperature grown films. Films grown at 600°C exhibited minimal change on annealing due to pre-existing polycrystallinity. TEM confirms polycrystalline β-Ga_2O_3, with crystallite sizes of ≈ 10 nm for RT samples and ≈ 80 nm for samples grown at 600°C after annealing. These results highlight the impact of substrate morphology, growth temperature, and annealing on optimizing Ga_2O_3 films, supporting developments in Ga_2O_3-based vertical devices.

[1] Baunthiyal *et al.*, Appl. Phys. Lett. **123**, 213504 (2023).

DS 1.4 Mon 10:15 H3

Molecule adsorption at Sc(x)Ga(1-x)N surfaces investigated by photo electron spectroscopy — •Fabian Ullmann[1,2] and Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

ScGaN can occur in various crystal orientations. The most important are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition between these orientations can be found. ScGaN surfaces with different scandium concentrations and orientations were grown by molecular beam epitaxy (MBE) to investigate the near-surface electronic structure. The interaction of gas molecules (oxygen and water) in vacuum were analyzed by X-ray (XPS) and ultraviolet photoelectron spectroscopy (UPS).

session break

DS 1.5 Mon 10:45 H3

Low temperature solid state dewetting of gold thin films on polystyrene nano structures — •Felix Lohmeyer and Jörg K.N. Lindner — Universität Paderborn, Department Physik, Warburgerstraße 100, 33098 Paderborn

Solid-state dewetting describes the breakup of a thin film into isolated objects due to surface energy minimization below the material's melting point. While well-studied for hard substrates, little research has been done on the dewetting of metal thin films on polymer substrates. This study shows that gold thin films can undergo dewetting at temperatures that preserve the underlying polymer substrate, with dewetting kinetics increasing with annealing temperature. Gold thin films (7 nm) were deposited on planar and nanostructured polystyrene (PS) substrates and thermally annealed at 100 to 120 °C, near the polymer's glass transition temperature ($T_{g,PS}$=100°C). Homogeneous spin coated PS films and nanostructured PS lamellae, created via block copolymer self-assembly, served as substrates. Dewetting was characterized using SEM, AFM, and TEM. On planar PS, dewetting was observed at any temperature and proceeded without incubation time, triggered by the initial non-uniformity of the gold film. On nanostructured PS, gold formed nanorods aligned with the polymer lamellae, breaking into particles while preserving the substrate pattern. These findings demonstrate the role of substrate morphology and temperature in dewetting and suggest a route to fabricating sub-10 nm gold structures for applications in sensing, catalysis, and nanoelectronics using BCP-based polymer templates.

DS 1.6 Mon 11:00 H3

Morphological characterization of Sub-10 nm surface patterns created by block-copolymer self-assembly — •Harikrishnan Venugopal, Janna X. Friebel, Julius Bürger, and Jörg K.N. Lindner — Universität Paderborn, Department Physik, Warburgerstraße 100

The microphase separation in block copolymers (BCPs) is a self-assembly process allowing to create ordered patterns on large substrate surfaces in short times and at low costs. Numerous applications of such patterns have been identified in the area of micro- and optoelectronics, data storage, catalysis, nanoporous membranes, and biomedical materials. If BCP self-assembly is used to create lithographic masks by removing one of the polymers selectively, for any targeted application it is important to characterise the morphology of polymer domains precisely at each processing step. In this work, we report on the morphology of silicon oxide nano structures fabricated by BCP self-assembly on Si substrates. A polystyrene-polydimethylsiloxane block copolymer (PS-b-PDMS) with a molar mass of 15 kg/mol and a PS volume fraction of 68.75 % was dissolved and spin coated onto silicon substrate. Microphase separation was initiated by solvent vapor annealing and results in the formation of fingerprint like surface patterns. A high-power oxygen plasma treatment is done to selectively remove the PS domains while converting the PDMS to silicon oxide. TEM, SEM and AFM analyses were performed to understand why after the plasma treatment half-cylinder patterns are observed.

DS 1.7 Mon 11:15 H3

Sub-10 nm Nanostructures in Thin Films of a Cylinder-Forming PS-b-PDMS Block Copolymer — •Janna X. Friebel, Harikrishnan Venugopal, Julius Bürger, and Jörg K. N. Lindner — Universität Paderborn, Germany

Block copolymers (BCPs) with a combined Flory-Huggins parameter $\chi N > 10$ form ordered domains even at low degrees of polymerization (N), enabling sub-10 nm nanostructures suitable for e.g. nanomasks in microelectronics. However, interfacial energy effects in thin films complicate the direct application of the bulk phase diagram by Bates et al. [1].

This study investigates the morphology of thin PS-b-PDMS high-χ BCP films with $N_B/N_A \approx 0.25$, spin-coated onto silicon, titanium, and chromium substrates (all with their native oxides). The films were top coated with PVA, solvent vapor annealed, PVA stripped, and the PS phase was selectively etched. Cross-sectional TEM reveals hemispherical structures instead of the expected hexagonal arrangement of cylinders, as suspected from SEM and AFM investigation. The energetic reasons for this geometry are discussed.

[1] F. S. Bates et al., Physics Today 52 (1999) 32-38.

session break

DS 1.8 Mon 11:45 H3

Ultrathin-Film Y6 at Air-Water Interface via the Langmuir-Blodgett Technique for Optoelectronic Application — •Yisak Tsegazab Gerase[1,2] and Martin Presselt[1,2] — [1]Institute of Physical Chemistry, Jena, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

Supramolecular structures are critical to the optoelectronic properties of films. The Langmuir-Blodgett (LB) technique provides precise molecular assembly, enabling control and homogenization of the morphology of Y6 Langmuir films, which is essential for scalable fabrication and commercial production. Y6, a non-fullerene acceptor, has significantly improved the power conversion efficiency of organic solar cells. We monitored the in-situ formation of Y6 Langmuir films using Brewster angle microscopy, surface pressure isotherms, and fluorescence spectroscopy. Isotherms revealed high packing densities, while compression-expansion cycles showed increased stiffness due to intermolecular rearrangements. BAM images confirmed smooth, well-defined quasi-2D films, and in-situ fluorescence spectroscopy identified the existence of Y6 fluorophore at the air-water interface and with lateral compression growth in supramolecular structure were observed. In agreement with in-situ observations, these well-ordered morphologies were further characterized after deposition on solid supports. Y6 films used in organic thin-film transistors showed a mobility of about 0.007 cm2 /Vs as cast film, comparable to other deposition techniques.

DS 1.9 Mon 12:00 H3

Femtosecond Laser Ablation (fs-LA) - A New Approach to XPS Depth Profiling — •samir mammadov — Thermo Fisher Scientific, 1 The Feldbridge Centre, Imberhorne Lane, East Grinstead, West Sussex, RH19 1XP, UK

XPS depth profiling is a widely employed analytical technique to determine the chemical composition of thin films, coatings and multi-layered structures, due to its ease of quantification, good sensitivity and chemical state information. Since the introduction of XPS as a surface analytical technique more than 50 years ago, depth profiles have been performed using ion beam sputtering. However, many organic and inorganic materials suffer from ion beam damage, resulting in incorrect chemical compositions to be recorded during the depth profile. This problem has been resolved for most polymers by using argon gas cluster ion beams (GCIBs), but the use of GCIBs does not solve the issue for inorganics. A prototype XPS depth profiling instrument has been constructed that employs a femtosecond laser rather than an ion beam for XPS depth profiling purposes. This novel technique has shown the capability of eradicating chemical damage during XPS depth profiling for all initial inorganic, compound semiconductor and organic materials examined. The technique is also capable of profiling to much greater depths (several 10s microns) and is much faster than traditional ion beam sputter depth profiling. fs-LA XPS depth profile results will be shown for selected thin films, coatings, multilayers and oxidised surfaces and the outlook for this new technique discussed.

DS 1.10 Mon 12:15 H3

Optimizing erbium luminescence for integrated photonics via ytterbium co-doping and thermal annealing — •Sören Lerner[1], Felix Mania[1], Jiale Sun[2], Zheru Qiu[2], Xinru Ji[2], Yang Liu[2], Tobias Kippenberg[2], and Carsten Ronning[1] — [1]Friedrich-Schiller Universität, Helmholtzweg 3, 07743 Jena, Germany — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Erbium ions are promising candidates for enabling efficient optical amplification of signals in photonic integrated circuits, but their practicality is hindered by insufficient output power. To address this, we utilize ion implantation into ultralow-loss silicon nitride (Si_3N_4) thin films and investigate co-doping with ytterbium ions to enhance absorption and emission through resonant energy transfer. We systematically investigate the effects of doping concentration and subsequent thermal annealing parameters using photoluminescence measurements. These findings provide insights into optimizing erbium-based light emitters for integrated photonics.

DS 2: Layer Deposition

Time: Monday 9:30–10:45 Location: H14

DS 2.1 Mon 9:30 H14

Bidirectional Growth of Functional Oxides by Molecular Beam Epitaxy — •Nicolas Bonmassar[1], Georg Christiani[2], and Gennady Logvenov[2] — [1]University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Here I present some recent results on the use of offcut substrates by enabling atomic precision layer-by-layer growth in both in-plane and out-of-plane directions. This is achieved by in situ monitoring of the oscillations of the reflected high-energy electron diffraction (RHEED) patterns. The potential of this method is demonstrated using a bidirectionally grown superlattice of alternating $LaMnO_3$ and $SrMnO_3$ layers, showing interfacial ferromagnetism. This superlattice serves as a model system to showcase the method's versatility through detailed structural and functional characterization by using various scanning transmission electron microscopy techniques, sheet resistance measurements, and magnetometry. Next, the approach is applied to the growth of superconducting $La_{1.84}Sr_{0.16}CuO_4$ thin films grown in ozone atmosphere on various offcut substrates, where the anisotropic critical current is found to arise from two distinct mechanisms induced by the substrate geometry.

Furthermore, I will present the issues we faced when we first started this project and how we had overcome well-known problems like the loss over the in situ RHEED oscillations, terrace broadening, step bunching, 3D defect formation and the concomitant loss of functionalities like superconductivity.

DS 2.2 Mon 9:45 H14

Enabling vacuum process monitoring with time-of-flight spectroscopy — •Marco John, Kristian Kirsch, Andreas Trützschler, Christoph Bartlitz, Marcel Herrmann, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, Großlöbichau, Germany

A crucial aspect to manage industrial vacuum processes is the importance of fast in-situ monitoring and control of process parameters such as pressure and residual gas composition. Improving process control in this way minimizes production errors, avoids damage to process equipment and ensures longer operating times. The capabilities of hot cathodes and quadrupole mass spectrometers are limited for this complex task, as they can only measure either the total pressure or the gas composition. One answer to this challenge is our novel ion source NOVION*, which combines the well-known technology of time-of-flight spectroscopy with our patented ion trap to an industrially available gas analyzing application.

In this talk we present the fundamental physical principles of the novel ion source and explain the compact combination of time-of-flight spectroscopy with our own patented ion trap. We discuss the advantages and limits in different applications as well as best practices in the field and show the capability to push the principle to its limits at high pressures without compromising the performance or lifetime of the filaments.

DS 2.3 Mon 10:00 H14

Selective Area Atomic Layer Deposition via Photoexcitation — •Paul Butler[1,2], Stefan A. Maier[3], and Ian D. Sharp[1,2] — [1]Walter Schottky Institut, Technische Universität München, 85748, Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technical Universität München, 85748, Garching, Germany — [3]School of Physics and Astronomy, Monash University, 3800, Melbourne, Australia

While atomic layer deposition (ALD) is a powerful technique for uniformly coating complex surfaces with thin films, achieving lateral control of ALD layers remains a primary challenge. In this work, we examine a selective-area ALD (S-ALD) process via photoexcitation of the growth surface. We demonstrate that optical laser excitation enhances ALD-growth of TiO_2 films on gold surfaces deposited onto Si and SiO_2. These surfaces were exposed to titanium isopropoxide (TTIP) and ozone as reactants for the ALD process, during which some of the samples were exposed to laser illumination. In-situ ellipsometry was used to monitor the growth rate of the TiO_2 films during ALD, and ex-situ ellipsometry was used to map the height profile of the resulting TiO_2 films deposited. The results show intensity-dependent enhanced growth on surfaces that were excited with laser illumination. We also show that a shadow mask can be used to make patterned depositions.

DS 2.4 Mon 10:15 H14

Enabling FAIR Data Practices in MBE Growth and Characterization — •Andrea Albino[1], Hampus Näsström[1], Sarthak Kapoor[1], Altuğ Yildirim[2], Oliver Bierwagen[2], Martin Albrecht[3], and Sebastian Brückner[1,3] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Data-driven materials science is transforming materials design by moving beyond traditional trial-and-error methods. Molecular beam epitaxy (MBE) experiments highlight the challenge of navigating complex parameter spaces [1], often exceeding human cognitive limits, particularly when integrating diverse datasets. This complexity is compounded by the absence of standardized models for capturing detailed experimental workflows and instrument diversity. Addressing these issues requires metadata aligned with FAIR (Findable, Accessible, Interoperable, Reusable) principles [2].

Within the NOMAD ecosystem (nomad-lab.eu) [3], we digitize the data lifecycle for MBE growth, including in-situ and ex-situ characterization. Key tools, like Electronic Laboratory Notebooks (ELNs), systematically document growth procedures, enabling streamlined data management and AI-driven analytics to optimize MBE processes.

[1] O. Bierwagen et al., J. Phys. Condens. Matter 28, 22 (2016) [2] M. Wilkinson et al., Sci. Data 3, 160018 (2016) [3] M. Scheidgen et al., J. Open Source Software 8, 5388 (2023)

DS 2.5 Mon 10:30 H14

Role of point defects on the superconducting transition temperature in NbTIN thin films with positron annihilation spectroscopy — •Sebastian Klug[1], Maik Butterling[1], Maciej Oskar Liedke[1], Eric Hirschmann[1], Andreas Wagner[1], Bharath Reddy Lakki Reddy Venkata[2], Aleksandr Zubtsovskii[2], and Xin Jiang[2] — [1]Institute of Radiation Physics, HZDR, Germany — [2]Chair of Surface and Materials Technology, University of Siegen, Germany

Positron annihilation spectroscopy (PAS) is a non-destructive method for studying point defects in materials with high sensitivity. It can sense defect densities in the range of 10^{15} to $10^{19} cm^{-3}$. The time for positrons to annihilate with electrons depends on the local electron density. Therefore, positrons can be trapped in neutral and negatively charged open-volume defects. Positrons are implanted into the studied material with a defined implantation energy. Changing of this energy allows for depth-resolved characterization. The user facility ELBE of HZDR provides the two main PAS techniques Doppler broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS) which allows for evaluation of the atomic environment of defects as well as defect size and density.

In this contribution the most recent results of magnetron sputtered NbTiN thin films as promising candidate for improving the characteristics of superconducting radio-frequency cavities (SRF cavities) will be discussed. The correlation between defect size and their concentration and the superconducting transition temperature will be highlighted.

DS 3: 2D Materials and their Heterostructures I (joint session DS/HL)

Time: Monday 15:00–17:45 Location: H3

DS 3.1 Mon 15:00 H3

Nanoscale NMR of two-dimensional solids using NV centers in diamond — •Marcel Martin[1], Mokessh Kannah Ciwan[1], Yejin Lee[2], Jakob Nachtigal[1], Nicola Poccia[3,4], Uri Vool[2], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [4]Department of Physics, University of Naples Federico II, Naples, Italy

Nuclear magnetic resonance (NMR) is a powerful method to investigate electronic properties of condensed matter but is inherently limited by its low sensitivity. Nitrogen-vacancy (NV) centers in diamond are quantum sensors that allow extending NMR to thin films and μm-scale exfoliated flakes of 2D materials which exhibit electronic phases such as charge density waves (CDW) and superconductivity. For the latter, NMR is especially powerful as it can elucidate the pairing symmetry of the charge carriers.

In this talk, we first discuss solid-state nano-NMR with NV centers of CaF_2, a testbed material for this method. The ultimate goal, however, is to study the CDW and Ising superconductivity phases of few-layer NbSe2 with nano-NMR. In this context, we present initial optical studies of $NbSe_2$ flakes which have been exfoliated and transferred onto a diamond. In addition to this, we will present results of conventional NMR on bulk $NbSe_2$ which serve as a reference.

DS 3.2 Mon 15:15 H3

Twist-tunable spin control in twisted bilayer bismuthene — •Ludovica Zullo[1,2,3,4], Domenico Ninno[4,5], and Giovanni Cantele[5] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France — [4]Dipartimento di Fisica E. Pancini, Università degli Studi di Napoli *Federico II*, Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy — [5]CNR-SPIN, c/o Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy

The role of spin-orbit coupling (SOC) in twisted bilayers has gained increasing attention due to its potential for spintronics, opening a quest for new layers with substantial SOC. In this work [1], by means of first principles calculations, we investigate how the interplay between SOC and twist angle impacts the band structure and spin textures of twisted bilayer bismuthene. We find that the twist angle can be deemed a control knob to switch from a small-gap semiconductor to a metallic behavior. Most crucially, the accurate analysis of the energy bands close to Fermi energy reveals a twist-tunable splitting in the mexican-hat shape of the bands that can otherwise be obtained only by applying enormous electric fields, providing insight into innovative technologies for future spintronic devices. [1] Ludovica Zullo, Domenico Ninno, Giovanni Cantele, Phys. Rev. B, 110, 165411 (2024)

DS 3.3 Mon 15:30 H3

Iron Diffusion in Thermally Stable $Ti_3C_2Cl_2$ MXenes under UHV Conditions — •Moritz Vanselow[1], Maksim Riabov[2], Hanna Pazniak[2], Thierry Ouisse[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

MXenes are 2D materials derived from a MAX phase precursor. Molten salt etching of $Ti_3C_2Cl_2$ results in hydrophobic $Ti_3C_2T_X$ MXenes with T_X = -Cl as a termination species [1]. $Ti_3C_2Cl_2$ MXenes are deposited on Si(100)/SiO_2 and we in situ study its chemical stability by mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum. Compared with standard hydrophilic $Ti_3C_2T_X$ MXenes, where T_X = -F, =O, and -OH, fluorine and hydroxyl groups can be removed by annealing at temperatures up to 1000 K, the thermal stability of $Ti_3C_2Cl_2$ MXenes is significantly enhanced. Moreover, intercalated water changing the MXene sheet separation, is not present in hydrophobic $Ti_3C_2Cl_2$ as proven by ex situ X-ray diffraction, wide-angle X-ray scattering (WAXS) and X-ray photoelectron spectroscopy (XPS). After optimizing the annealing procedure, we in situ intercalate Fe by e-beam assisted deposition on top of MXene thin films and subsequent Fe diffusion by soft annealing at 600 K. This work is funded by a joint ANR-DFG-Project under ANR-23-CE09-0031-01 and DFG ID 530103526. [1] T. Zhang et al., Chem. Mater. 36, 1998 (2024).

DS 3.4 Mon 15:45 H3

Interactions Between Two-Dimensional Crystals and Molecules via Density Functional Theory — •Stefan Wolff[1], Xin Chen[2], Tobias Dierke[1], and Janina Maultzsch[1] — [1]Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

The unique properties of two-dimensional (2D) materials can be modified through chemical functionalization, driven by their interactions with functional groups or molecules. Density functional theory (DFT) calculations are employed to investigate non-covalent functionalization of bilayer graphene with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) molecules. The interactions between the graphene layers and the HATCN molecules play a significant role in determining the functionalization behavior, which depends on the stacking arrangement. Locally stacked regions within the moiré lattice of twisted bilayer graphene (tBLG) play a crucial role for functionalization. Consequently, the moiré pattern of tBLG can serve as a template to control the degree of functionalization. Furthermore, laser-triggered covalent functionalization of molybdenum disulfide (MoS_2) enables the fabrication of patterned 2D heterostructures with phenyl-based interface linkers. Through DFT calculations, various potential binding motifs and their associated optical properties are predicted. Calculations of reaction energies and Raman modes provide insights into the likelihood of different reaction pathways and the structures they yield.

DS 3.5 Mon 16:00 H3

Toward high-sensitivity and low-power consumption gas sensor devices based on 2D-transistors. — •Aurelio García Valenzuela[1], Zahra Fekri[1], Madhuri Chennur[1], Nikol Lambeva[1], Jens Zscharschuch[1], Victoria Constance Köst[2], Krysztof Nieweglowski[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Electronic Packaging Technology, AVT, TU-Dresden, Germany

Two-dimensional (2D) materials exhibit excellent properties compared to their bulk counterparts and are promising for applications like gas sensors. Their high surface-to-volume ratio and surface-active sites enhance gas absorption and sensitivity, addressing challenges in detecting low concentrations and reducing power consumption.

This work presents the fabrication and testing of 2D materials-based field-effect transistor (FET) gas sensors. Mechanically exfoliated 2D materials are stacked into heterostructures to create back-gated FETs, with device patterning achieved via electron beam lithography.

The devices were exposed to NH3 and NO2 gases at various temperatures. Gas interactions caused systematic changes in p- and n-type currents and shifts in the transfer curve, depending on gas concentration and type (donor or acceptor). These results demonstrate the suitability of 2D materials-based FETs as efficient and sensitive gas sensors.

short break

DS 3.6 Mon 16:30 H3

Pressure-dependent Effective Hamiltonian and Topological Transitions for Twisted Bilayer Transition Metal Dichalcogenides — •Miftah Hadi Syahputra Anfa[1], Sabri Elatresh[1,2], Hocine Bahlouli[1,3], and Michael Vogl[1,2] — [1]Physics Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia — [2]Interdisciplinary Research Center (IRC) for Intelligent Secure Systems, KFUPM, Dhahran, Saudi Arabia — [3]Interdisciplinary Research Center (IRC) for Advanced Materials, KFUPM, Dhahran, Saudi Arabia

Recent studies have shown the existence of nontrivial topological moire bands in twisted bilayer transition metal dichalcogenides (TMDs), which depend on the twist angle. Motivated by this, we present a study of such a system under applied vertical pressure. The study begins by first considering the untwisted bilayer case without pressure. We find that the system can be described by an effective low-energy Hamiltonian that behaves approximately quadratic and includes layer-shift dependent terms that we were able to determine by symmetry. The structure is then relaxed under pressure in the 0.0 - 3.5 GPa range using ab initio density functional theory (DFT). The DFT band structures for each corresponding pressure are fitted to the effective Hamiltonian to obtain the pressure-dependent parameters. Consecutively, the explicit expression for the twisted pressure-dependent Hamiltonian is obtained by treating the twist as a position-dependent shift between layers. We then present changes in Chern number results for the important energy bands due to pressure.

DS 3.7 Mon 16:45 H3

Effect of spin-dependent tunneling in a $MoSe_2/Cr_2Ge_2Te_6$ van der Waals heterostructure on exciton and trion emission — •Annika Bergmann[1], Swarup Deb[1,2], Veronika Schneidt[1], Mustafa Hemaid[1], Kenji Watanabe[3], Takashi Taniguchi[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, Rostock University, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]Research Center for Electronic and Optical Materials, Tsukuba, Japan — [4]Research Center for Materials Nanoarchitectonics, Tsukuba, Japan

In recent years, thin films of magnetic van der Waals materials have gained increasing interest due to their potential applications in spintronics. For instance, heterostructures (HS) consisting of ferromagnetic CRI_3 and a WSe_2 monolayer have demonstrated the existence of magnetic proximity effects, manifesting in the lifting of WSe_2 valley degeneracy as well as helicity-dependent photoluminescence (PL) emission of the WSe_2 monolayer in proximity to the 2D ferromagnet [1,2]. Here, we study HS consisting of monolayer $MoSe_2$ and few-layer ferromagnetic $Cr_2Ge_2Te_6$ (CGT). Under circularly polarized excitation, PL measurements show that the $MoSe_2$ exciton-trion emission ratio depends on the relative orientation of excitation helicity and CGT magnetization, even though the PL emission itself is unpolarized. This hints at an ultrafast, spin-dependent interlayer charge transfer that competes with exciton and trion formation and recombination.

[1] D. Zhong et al., Science Advances, 3 (2017)

[2] D. Zhong et al., Nat. Nanotechnol. 15 (2020)

DS 3.8 Mon 17:00 H3

Magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Tauqir Shinwari[1], Kacho I. A. Khan[1], Jens Herfort[1], Michael Hanke[1], Chen Chen[2], Joan M. Redwing[2], Achim Trampert[1], Mehak Loyal[3], Gerhard Jakob[3], Mathias Kläui[3], Roman Engel-Herbert[1], and João Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]2D Crystal Consortium Materials Innovation Platform, Materials Research Institute, The Pennsylvania State University, PA, United States — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

Van der Waals (vdW) heterostructures consisting of two-dimensional (2D) ferromagnetic and nonmagnetic materials hold great promises for tailoring their magnetic and transport properties. Here we report on the magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2$ (FGT, with $x \approx 0.2$)/WSe_2 heterostructures tailored via the FGT thickness. Magnetic characterizations and anomalous Hall effect measurements with both out-of-plane and in-plane magnetic fields reveal an enhanced perpendicular magnetic anisotropy (PMA) in thinner FGT and a ferromagnetic order up to room temperature. The pronounced unconventional Hall effect (UHE) suggests the possible formation of skyrmions. The thickness-dependent asymmetric magnetoresistance reveals a unique magnetization switching process. Our results demonstrate the high potential of all-epitaxial FGT/WSe_2 heterostructures for the advancement of future 2D spintronic applications.

DS 3.9 Mon 17:15 H3

Effect of Ni-doping on the structural/magnetic properties of large area epitaxial 2D-ferromganet Fe_3GeTe_2 — •Kacho Imtiyaz Ali Khan[1], Tauqir Shinwari[1], Hua Lv[1], Frans Munnik[2], Jens Herfort[1], Michael Hanke[1], and Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Helmholtz-Zentrum Dresden- Rossendorf e.V. Dresden, Germany

2D ferromagnets with strong perpendicular magnetic anisotropy exhibit magnetic order down to the monolayer thickness and have the potential to overcome long-term challenges faced by 3D ferromagnets to build up advanced energy-efficient spintronic devices. In this work, we show the large-area epitaxial growth of Ni-doped Fe_3GeTe_2 films via molecular beam epitaxy. X-ray diffraction measurements demonstrate high-quality epitaxy of pure Fe_3GeTe_2 phase on graphene/SiC(0001) substrates. Magneto-transport measurement unveils the ferromagnetic nature of the film, with strong perpendicular magnetic anisotropy for pure Fe_3GeTe_2 and Ni-doped films. However, the Ni-doped Fe_3GeTe_2 shows a decrease in Curie temperature T_C with an increase in Ni-doping. We believe that the Ni doping modifies the lattice parameters and structure (e.g., Ni intercalation), which results in the dilution of magnetic properties of Fe_3GeTe_2 by reducing the T_C down to 50 K. Our findings show the role of Ni incorporation on the ferromagnetic behavior of Fe_3GeTe_2 films, which is crucial for the development of future spintronic devices.

DS 3.10 Mon 17:30 H3

The epitaxial growth of Gallium Selenide — Michele Bissolo, Marco Dembecki, Florian Rauscher, Jan Schabesberger, Abhilash Uhle, Jonathan J. Finley, Gregor Koblmüller, and •Eugenio Zallo — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Garching, Germany

Group III-VI post-transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are van der Waals semiconductors with layer-dependent electronic, thermoelectric and optical properties, strong photoresponsivity, and a Caldera type valence band [1]. However, the limited scalability and risk of contamination of the standard mechanical exfoliation technique are detrimental to developing devices at an industrial scale. Here, we demonstrate the molecular beam epitaxy growth of PTMC [2] GaSe on 2-inch sapphire wafers. To study the pristine properties of this air-sensitive material in situ, we perform Raman spectroscopy in a UHV chamber directly connected to the growth chamber. Film composition and morphology are investigated by tuning the growth temperature and group VI/III flux ratio and by correlating them with the known spatial gradients across the whole substrate. The combination of these findings with ex-situ surface morphology characterization allows us to construct the phase diagram and identify the 2D layered region [3]. Perspectives on the growth of PTMC on 2D substrates and the epitaxial registry will be discussed. [1] H. Cai, et al., Appl. Phys. Rev. 6, 041312 (2019).[2] E. Zallo, et al., npj 2D Mater. & Appl. 7, 19 (2023).[3] M. Bissolo, et al., [to be submitted].

DS 4: 2D Materials and their Heterostructures II (joint session DS/HL)

Time: Tuesday 9:30–13:00 Location: H3

Invited Talk DS 4.1 Tue 9:30 H3

Graphene-based epitaxial 2D heterosystems: making graphene great again — •Christoph Tegenkamp — Institut für Physik, TU Chemnitz

2D materials and their heterostructures are at the forefront of research, anticipated to serve as fundamental building blocks for new quantum materials. Proximity coupling is a key concept in this domain, enabling diverse and novel functionalities. Epitaxial graphene (EG) grown on SiC(0001) resembles a truly 2D electron gas system, celebrated for its manifold and flexible functionalization schemes at both its vacuum and interface sites. These functionalization strategies enable extreme doping scenarios in graphene, tuning spin-orbit coupling, realizing interface states, or introducing mini-bands through zone folding. The controlled transition from linear to flat bands in EG, along with the coupling of functionalized epitaxial graphene to 2D electron gases (2DEGs), opens avenues for exploring electronic correlation effects and mesoscopic phenomena in epitaxial 2D heterostructures. In this presentation, I will showcase some recent findings achieved through the adsorption and intercalation of elements such as Pb and Sn, demonstrating their potential to further tune the properties of graphene.

DS 4.2 Tue 10:00 H3

Proximity-induced spin-orbit coupling in bilayer graphene quantum wires — •Michael Laumer and Angelika Knothe — Universität Regensburg, 93053 Regensburg, Germany

The gate-tuneable band gap and the possibility to tailor its band structure by proximitizing with other 2D materials [1] make bilayer graphene (BLG) an excellent platform for future quantum technologies. By applying spatially modulated displacement fields, one may confine BLG's charge carriers into electrostatically induced nanostructures [2, 3]. Proximitizing the BLG with a transition metal dichalcogenide (TMDC) strongly enhances the SOC of the adjoining graphene layer [1]. Fascinated by the concept of proximity-tailoring BLG nanostructures, we convey the idea of proximity-inducing SOC to a gate-confined BLG quantum wire. We theoretically study the resulting quantized subband structure for different SOC strengths and as a function of the wire geometry. Our results help us understand how proximity-induced SOC manifests in confined geometries and identify different regimes of the wires' electronic properties.

[1] K. Zollner, M. Gmitra, and J. Fabian. Swapping exchange and spin-orbit coupling in 2d van der waals heterostructures. Phys. Rev. Lett., 125:196402, (2020). [2] A. Knothe and V. Fal'ko. Influence of minivalleys and berry curvature on electrostatically induced quantum wires in gapped bilayer graphene. Phys. Rev. B, 98:155435, (2018). [3] H. Overweg et al. Topologically nontrivial valley states in bilayer graphene quantum point contacts. Phys. Rev. Lett., 121:257702, (2018).

DS 4.3 Tue 10:15 H3

Above room temperature ferromagnetism in large-area Fe_3GaTe_2/graphene van der Waals heterostructures — •Tauqir Shinwari[1], Kacho Imtiyaz Ali Khan[1], Hua Lv[1], Atekelta Abebe Kassa[1], Frans Munnik[2], Achim Trampert[1], Michael Hanke[1], Jens Herfort[1], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V. Dresden, Germany

Two-dimensional (2D) magnetic materials and van der Waals (vdW) heterostructures offer new possibilities for the realization of advanced spintronic devices. Fe_3GaTe_2, a 2D ferromagnetic metal with a high Curie temperature (~ 360K) and strong perpendicular magnetic anisotropy, has emerged as a promising candidate for energy-efficient magnetic devices. However, all investigations conducted in Fe_3GaTe_2 so far have been performed using millimeter-sized bulk crystals and flakes exfoliated from them, both not suitable for integration in device processing. Hence, it is crucial to develop controlled large-scale growth of this material and investigate its properties. In this contribution, we present a breakthrough in the high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films on epitaxial graphene/SiC(0001) substrates using molecular beam epitaxy. These results are highly relevant for the future development of high-performance spintronic devices based on 2D heterostructures potentially revolutionizing data storage, processing, and quantum computing applications.

DS 4.4 Tue 10:30 H3

Modeling carbon nanomembranes through molecular dynamics simulations — •Levin Mihlan and Jürgen Schnack — University of Bielefeld

Carbon nanomembranes (CNMs) are nanometer-thin materials synthesized via electron-induced crosslinking of aromatic self-assembled monolayers. CNMs can be functionalized for various applications, initially serving as molecular filters. Due to their presumed irregular internal structure, these membranes pose challenges for standard spectroscopic efforts, often being insufficiently informative [1]. Ehrens et al. initially conducted molecular dynamics simulations to investigate CNM formation, replicating crosslinking and pore formation via momentum transfers in carbon-only systems [2]. Here, we extend the approach by incorporating hydrogen atoms, which may play a critical role in the crosslinking process, even though they largely disappear in the final CNM products. This additionally reduces the number of theoretical assumptions. We examine whether and in what way pores form and analyze properties such as aromaticity, sp content, and Young's modulus to compare with previous simulations and experiments.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" Chem. Phys. Chem 21, 1006 (2020)
[2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416 (2021)

session break

DS 4.5 Tue 11:00 H3

Photo-electrochemical oxidation and thinning of transition metal dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Franz Gröbmeyer[2], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Walter Schottky Institute, Physics Department and TUM School of Natural Science, Technical University of Munich — [2]Nanoinstitute Munich and Faculty of Physics, Ludwig-Maximilians-Universität — [3]Naval Research Laboratory, Washington, D.C

Two-dimensional transition metal dichalcogenides (TMDs) exhibit unique optoelectronic and mechanical properties. For their integration in functional devices and for catalytic applications, it is crucial to understand and control their behavior in the reactive environments. Here, we investigate the stability of thin MoS_2, WS_2, $MoSe_2$ and WSe_2 films in acidic, neutral, and basic solutions using a three-electrode photoelectrochemical cell, which enables experiments under both illumination and in the dark. Under anodic conditions, sulfides and selenides undergo different protonic reactions, depending on the pH of the electrolyte, resulting in different resistances to oxidation. Additional exposure to light from a solar simulator creates photo-excited holes, which drive a self-limiting electrochemical thinning procedure that enables the top-down fabrication of large-area TMDs with a thickness of only a few layers. The degradation, initiated at the edges or defects, propagates through the flakes and can be monitored in-situ using an optical microscope. Under laser excitation, multilayer TMDs can be thinned in predefined patterns, paving a new route for processing and integration of 2D materials into functional devices.

DS 4.6 Tue 11:15 H3

Rapid MOCVD synthesis of stratified MoS2 and WS2 2D heterostructures — •Nikolas Dominik, Sebastian Klenk, Cormac Ó Coileáin, and Georg S. Duesberg — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, München, Deutschland

The two-dimensional (2D) structure of layered materials such as the transition metal dichalcogenides MoS2 and WS2, imparts exceptional electrical, mechanical and optical properties. This makes them particularly interesting for electronic, photovoltaic and sensing application. Van der Waals heterostacks, composed of assembled 2D materials, expand on the possible range of properties, and so have attracted extensive attention due to factors such as ultrafast carrier transport and high bandgap tunability.

Here we present metal-organic chemical vapour deposition (MOCVD) synthesis of MoS2/WS2 combination heterostructures using a highly controllable industrial-scale multi-precursor system, thus avoiding the laborious need for manual stacking. We show how this synthesis method allows the creation of clearly defined and highly ordered stacks by producing a 7-layer combination structure below 10 nm. We explore the characteristics of these films using Raman spectroscopy and XPS, EDX, TOF-SIMS and microscopy techniques.

DS 4.7 Tue 11:30 H3

Unveiling the mechanism of monolayer selective large-area exfoliation of 2D materials — •Jakob Ziewer[1], Abyay Ghosh[1], Michaela Hanušová[2], Luka Pirker[2], Otakar Frank[2], Matěj Velický[2], Myrta Grüning[1], and Fumin Huang[1] — [1]Queen's University Belfast, Belfast, U.K. — [2]J. Heyrovský Institute of Physical Chemistry

Metal assisted exfoliation has made it possible to selectively isolate single crystal monolayers of 2D materials at sizes up to a centimetre [1][2]. This represents a million fold increase compared to standard tape exfoliation.

In this presentation the mechanism of enhanced yield is discussed. Through spectroscopic measurements and observation of macroscopic bubbles it is discovered that the Au substrate decouples attached MoS_2 monolayers from the remaining crystal. The interfacial weakening is dependant on the thickness of the crystal and is maximised for thick crystals.

These findings are used to explain the mechanism behind metal assisted exfoliation and are expected to extend to other Au-2D heterostructures.

[1] Velický, M.; et. al. Mechanism of Gold-Assisted Exfoliation of Centimeter-Sized Transition-Metal Dichalcogenide Monolayers. ACS Nano 2018, 12, 10463*10472. [2] Huang, Y.; et. al. Universal Mechanical Exfoliation of Large-Area 2D Crystals. Nat. Commun. 2020, 11:2453.

session break

DS 4.8 Tue 12:00 H3

Probing the electronic band structure of the 2D magnetic materials MPS3 (M=Fe,Ni) across magnetic phase transitions — •Jeff Strasdas[1], Benjamin Pestka[1], Biplab Bhattacharyya[1], Adam K. Budniak[2], Marcus Liebmann[1], Niklas Leuth[1], Honey Boban[3], Lutz Waldecker[1], Bernd Beschoten[1], Christoph Stampfer[1], Lukasz Plucinski[3], Efrat Lifshitz[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH, Aachen, Germany — [2]Schulich Chem. Fac., Solid State Inst., Russell Berrie Nanotech. Inst., Helen Diller Quantum Center, Technion - Israel Inst. of Technology, Haifa, Israel — [3]Forschungszentrum Jülich, Peter Grünberg Inst. (PGI-6), Jülich, Germany

We investigate the band structure of the van der Waals materials FePS3 [1] and NiPS3, both 2D antiferromagnetic insulators, using μm-scale Angular Resolved Photoelectron Spectroscopy (ARPES), above and below their Néel temperatures (TN). The data is compared with DFT+U calculations and simplified selection rules to deduce the orbital character of changing bands. In FePS3, we observe three distinct band structure changes across TN, involving bands with Fe 3d, S 3p, and pure P 3p character, reflecting the intricate competition of direct exchange between Fe atoms and superexchange via S and P atoms. In NiPS3, we identify one band shift near Γ across TN, containing a band of mixed Ni and S character. Here, pronounced deviations from the DFT+U calculations indicate more complex electronic correlations. Moreover, we refine the photoelectron selection rules using ARPES data from CrPS4. [1] B. Pestka et al. doi:10.1021/acsnano.4c12520

DS 4.9 Tue 12:15 H3

Investigation of 1T-TaS2 phase transition and charge transfer phenomena at interfaces with perovskites — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Centre of Scientific Research Demokritos, 15341 Athens, Greece — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Athens, Greece

1T-TaS2 is a distinguished 2D-layered transition metal dichalcogenide with a rich phase diagram upon cooling including charge density wave (CDW) states and a Mott insulating phase. On the other hand, halide perovskites (HPs) are emerging as a unique class of materials in the field of photonics due to their intriguing optoelectronic properties. The combination of 1T-TaS2 with HPs is proposed as a viable solution to overcome the drawbacks of each category thanks to charge transfer phenomena.

In this work, we studied the phase transitions of 1T-TaS2 as a function of the cooling rate. In the case of nanothick crystals, CDW phase transitions were observed upon gradual cooling but they were totally absent afrer a vigorous cooling. On the contrary, for bulk crystals the CDW phase transitions were totally independent of the cooling rate. Furthermore, we developed 1T-TaS2/HPs heterostructures and we investigated charge transfer phenomena by XPS and UPS spectroscopy, both revealing electron transfer from 1T-TaS2 towards perovskite. Charge transfer could also enable the development of high-performance hybrid optoelectronic devices based on these materials.

DS 4.10 Tue 12:30 H3

The effect of a perpendicular electric field on charge-spin interconversion coefficients in proximitized graphene on 1T-TaS_2 monolayer — •Juraj Mnich[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

The proximity-induced spin-orbit coupling and exchange interactions in the graphene-based heterostructures provides an effective way to manipulate with charge-spin interconversion coefficients. In the talk we focused on charge-spin interconversion in bilayer and trilayer heterostructures of 1T-TaS_2 and graphene. By modulating the temperature, we can access the charge density wave phase and switch between the magnetic and non-magnetic phases of 1T-TaS_2 affecting consequently the graphene electrons. Using linear response theory we showed the dependence of charge-spin interconversion coefficients on a perpendicular applied electric field. For the specific configurations of the 1T-TaS_2 and graphene we observed a change in both the sign and the magnitude of the non-equilibrium spin density as a response to the perpendicular electric field. This result indicates a possibility of using electric fields as a tool to control the direction of spin density.

This work was supported by the APVV-SK-CZ-RD-21-0114 and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008.

DS 4.11 Tue 12:45 H3

Self spin-orbit torque in proximitized graphene on 1T-TaS_2 monolayer — •Martin Gmitra[1,4], Maedeh Rassekh[1], Juraj Mnich[1], and Marko Milivojević[2,3] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

We show that self spin-orbit torque induced in graphene-based van der Waals heterostructures represents a platform to extract the Rashba phase – a proximity-induced spin-orbit coupling parameter. Performing first-principles calculations, tight-binding modeling, and non-equilibrium Greens function transport calculations for graphene on 1T-TaS_2 monolayer we found that charge current in graphene generates non-equilibrium spin accumulation and self-torque in graphene due to the proximity-induced spin-orbit coupling and exchange interaction. The Rashba spin-orbit torque is a dominant contribution and weakly depends on the direction of magnetization in 1T-TaS_2. We propose that the magneto-optical Kerr effect can directly extract the Rashba spin-orbit coupling phase.

This work was supported by the APVV-SK-CZ-RD-21-0114, EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008, and IMPULZ IM-2021-42.

DS 5: Thin Oxides and Oxide Layers

Time: Tuesday 14:00–15:15 Location: H3

DS 5.1 Tue 14:00 H3

How to functionalize 2D states at oxide interfaces by controlled redox reaction — •Pia Maria Düring, Andreas Fuhrberg, Timo Krieg, Verena Reva, and Martina Müller — FB Physik, Universität Konstanz, 78457 Konstanz

Oxide electronics provide the key concepts and materials for enhancing silicon-based semiconductor technologies with novel functionalities. In a recent paper, we provide evidence for individually emerging hole- and electron-type 2D band dispersions at Fe-$SrTiO_3$ heterostructures [1]. The emergence of p- or n-type bands is closely linked to the Fe oxidation state which enables the possibility to tune the interface properties to set or even switch between negatively (n) charged electrons or positively (p) charged holes. One of the main processes that controls the interface properties is the oxygen exchange between the film and the substrate. Using our UHV-MBE system, we grow high-quality ultra-thin TM (e.g. Fe, Co and Hf) oxide films on $SrTiO_3$ substrates by systematically varying the growth parameters, e.g. (i) growth temperature, (ii) substrate annealing, and (iii) metal film thickness. The present work discusses the effect of different growth parameters on the interfacial properties like oxygen vacancies, the oxidation state of the TM oxide as well as the concentration of defects in $SrTiO_3$, which strongly influences the valence band alignment between electron and hole band bending. In this way, we can effectively control the properties of the 2D interface to ultimately add ferroic functionalities to these confined electronic states.

[1] P. M. Düring et al., Advanced Materials, 2024, 2390217.

DS 5.2 Tue 14:15 H3

Adsorption-controlled growth of α-(Al,Ga)2O3 and β-(Al,Ga)2O3 on Al2O3 by suboxide molecular-beam epitaxy (S-MBE) — •Sushma Raghuvansy[1], Marco Schowalter[1], Alexander Karg[1], Manuel Alonso-Orts[1,2], Martin Williams[1], Stephan Figge[1], Andreas Rosenauer[1,2], Martin Eickhoff[1,2], and Patrick Vogt[1,3] — [1]Institute of Solid-State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359, Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany — [3]Max Planck Institute for solid state research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Gallium oxide (Ga2O3) is a promising ultra-wide band gap semiconductor with extremely high (predicted) breakdown field for high performance power electronics.

α-Ga2O3 is isostructural to α-Al2O3, and allows alloying over the entire composition range from Ga2O3 (x=0) and Al2O3 (x=1) in α-(AlxGa1-x)2O3 [1]. For β-(AlxGa1-x)2O3, range with which Al can be alloyed is $0 < x < 0.61$, which leads

to a bandgap range of 4.6-5.9 eV [2].

In this contribution, we demonstrate the growth of high quality α-(Al,Ga)2O3 on Al2O3 (10-10) and Al2O3 (11-20) and β-(Al,Ga)2O3 on Al2O3 (0001) by suboxide molecular beam epitaxy (S-MBE). We investigated the influence of Al flux and growth parameter space of (Al,Ga)2O3 alloys on differently oriented Al2O3 substrates.

[1] R. Jinno et al., Science Advances 7 (2021) [2] T. Oshima et al., Jpn. J. Appl. Phys. 48, 070202 (2009)

DS 5.3 Tue 14:30 H3

Tuning the interlayer coupling in $La_{0.7}Sr_{0.3}MnO_3$ / $LaNiO_3$ multilayers with strong perpendicular-magnetic-anisotropy — •Jörg Schöpf[1], Valentina Piva[1], Paul H. M. van Loosdrecht[1], Padraic Shafer[2], Divine P. Kumah[3,4], Xuanyi Zhang[3,4], Lide Yao[5], Sebastiaan van Dijken[6], and Ionela Lindfors-Vrejoiu[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, USA — [3]Department of Physics, Duke University, Durham, USA — [4]Department of Physics, North Carolina State University, Raleigh, USA — [5]OtaNano-Nanomicroscopy Center, Aalto University, Aalto, Finland — [6]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

We report on the magnetic interlayer coupling between Ru-substituted $La_{0.7}Sr_{0.3}MnO_3$ thin films separated by few unit cell thin $LaNiO_3$ spacers, grown by pulsed-laser-deposition and investigated by SQUID-mangetometry, magnetotransport and the magneto-optive-Kerr effect. The magnetic anisotropy in Ru-substituted $La_{0.7}Sr_{0.3}MnO_3$ thin films, in combination with light compressive strain of a LSAT substrate, allows to tune the magnetic anisotropy from easy-plain to strong perpendicular-magnetic-anisotropy. $LaNiO_3$, allows for strong FM- or AFM-coupling between the manganite layers depending on spacer thickness. We propose a layer-by-layer type magnetization reversal in the case of strong PMA, introduced by substituting 10% of Mn by Ru, while films with lower substitution of 5% and weaker PMA instead show signs of collective, spin-flop-type transitions.

DS 5.4 Tue 14:45 H3

Multinary compositionally graded, spatially addressable materials libraries by pulsed laser deposition — •Jorrit Marius Bredow, Marius Grundmann, and Holger von Wenckstern — Felix Bloch Institute for Solid State Physics, Leipzig University

The discovery of novel, functional materials is increasingly based on the investigation of multinary materials with large composition spaces. Therefore, combinatorial synthesis and high-throughput characterization methods are preferable for the discovery of functional multi-component materials. Here, pulsed laser deposition (PLD) from segmented targets allows the synthesis of spatially addressable materials libraries (SA-ML) with continuous compositional gradients[1].

We demonstrate that PLD is a viable method for synthesizing multi-component SA-ML using n-fold azimuthally segmented targets. We present a roadmap for the fabrication of fivefold segmented targets using MgO, CoO, NiO, CuO, and ZnO, which can be readily applied to different material combinations. Moreover, we compare two approaches to target and deposition process design for PLD of SA-ML. The composition of the SA-ML is determined by high-throughput energy dispersive X-ray spectroscopy confirming the successful synthesis of a fivefold compositionally graded SA-ML by combinatorial PLD. Aditionally, the height distributions and elemental compositions are simulated with the thickness distribution parameters of the binary oxides and the simulation results are compared to the experimental data.

[1] H. von Wenckstern, Z. Zhang, F. Schmidt, J. Lenzner, H. Hochmuth, and M. Grundmann, CrystEngComm, 15, 10020, 2013.

DS 5.5 Tue 15:00 H3

Tri-functionality in a Single Oxide Interface-Based Nanostructure with Reconfigurable Logic-in-Memory Applications — •Soumen Pradhan[1], Kirill Miller[1], Fabian Hartmann[1], Merit Spring[2], Silke Kuhn[1], Victor Lopez-Richard[3], Michael Sing[2], Ralph Claessen[2], and Sven Höfling[1] — [1]Julius-Maximilians-Universität Würzburg, Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Deutschland — [2]Julius-Maximilians-Universität Würzburg, Würzburg-Dresden Cluster of Excellence ct.qmat, Experimentelle Physik 4, Deutschland — [3]Department of Physics, Federal University of São Carlos, Brazil

We demonstrate transistor (T), memristive (M), and memcapacitive (MC) functionalities in nanowires, based on quasi-two-dimensional electron system in $LaAlO_3/SrTiO_3$ heterostructures depending on the biasing condition at lateral gates. Combining one T and one M, the device can be utilized for short term and long term synaptic plasticity. However, arranging two T in parallel and series with one M, the structures show logic OR and AND gates, respectively. In addition, the devices can memorize the logic output even after grounding the inputs taking advantage of its long term memory. Interestingly, the single structure can be reconfigured between OR and AND logic. Our findings on oxide nanostructures together with logic-in-memory and reconfigurability in logic as well as in functionality open a path towards oxide-based monolithic integrated circuits for brain inspired neuromorphic computing.

DS 6: Thin Film Application

Time: Wednesday 9:30–11:45 Location: H3

DS 6.1 Wed 9:30 H3

Fluorescent SiON-Doped Si Thin Films in Miniature Temperature Sensor Fabrication Using Machine and Deep Learning with Low Root Mean Square Error — Ali Karatutlu[1], Timuçin Emre Tabaru[2], •Zehra Gizem Mutlay[1], Esra Kendir Tekgül[1], Nurhan Güneş[2], and Bülend Ortaç[1] — [1]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University, Ankara, Türkiye — [2]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, Sivas, Turkey

SiON-doped Si, discovered by our project team last year (DOI: Advanced Optical Materials, 2023, DOI: 10.1002/adom.20230009), has a special molecular matrix with a refractive index that can be controlled depending on the amount of SiON. The counterpart structures, such as SixNy, SiOxNy, or Si-rich Si3N4, are conventional structures with general properties such as mechanical durability, thermal stability, chemical resistance, electrical insulation, and optical transparency. We report that SiON-doped Si can have a relatively even higher refractive index from 2.07 to 2.56 near the telecom wavelength of 1310 nm, depending on the SiON content. In terms of application, SiON-doped Si thin films were tested at room temperature to 200°C using different packaging materials such as borosilicate glass and aluminum, and their use as miniature temperature sensors will be demonstrated. The preliminary temperature-fluorescence spectrum correlation was investigated using machine learning and deep learning methods that yield the root mean square error of this system to be as low as 2°C.

DS 6.2 Wed 9:45 H3

Electron-transparent free-standing ultrathin membranes for studying gas-solid and liquid-solid interfaces at high pressures — •Max Gertig[1], Carlos Morales[1], Andreas Schubert[2], Carlos Alvarado[2], Christian Wenger[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]IHP Leibniz-Insitut für innovative Mikroelektronik, Frankfurt (Oder), Germany

The chemical reactions of heterogenously catalyzed processes take place at the gas-solid and liquid-solid interfaces. Thus, significant efforts have been dedicated to developing new methods to study them under realistic conditions. In recent years, electron-transparent graphene windows have been used in ambient pressure X-ray photoelectron spectroscopy (AP-XPS) to separate liquids and gases at ambient pressure from a high vacuum. Following this design, we present free-standing ultrathin (up to 10 nm) Al_2O_3 membranes fabricated by atomic layer deposition (ALD) which are electron-transparent to tender and hard X-rays. Three different commercial supports are used: TEM SiN perforated membranes (1 μm), single-hole stainless steal apertures (20 μm), and TEM Cu-grids (80 μm). Their conformity has been examined by scanning electron microscopy (SEM) and atomic force microscopy (AFM), whereas their chemical composition and homogeneity by energy dispersive X-ray (EDX) mapping. Additionally, confocal μ-Raman microscopy complements the chemical and structural characterization. Conventional free-standing graphene membranes have also been fabricated for comparison purposes.

DS 6.3 Wed 10:00 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. Preliminary work in the literature suggests that the phase transition temperature of the anatase to rutile structural phase transition of TiO_2 is lowered for by alloying Cu. However, that the band gap of $Cu_xTi_{1-x}O_2$ decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates by conventional rf-sputtering employing a TiO_2 ceramic target and Cu wires as Cu source. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D

phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

DS 6.4 Wed 10:15 H3

VO_2 Smart Windows for Applications: A Study of $Cu_xTi_{1-x}O_2$ Buffer Layers in Multilayer Thin Film Systems — •Hao Lu[1,2], Martin Becker[1,2], Jan Luka Dornseifer[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Giessen, Germany — [2]Center of Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Giessen, Germany

Alloying the TiO_2 with CuO_2 yielding $Cu_xTi_{1-x}O_2$ may provide a suitable buffer layer for optical smart windows based on VO_2. Preliminary work in the literature suggests that the phase transition temperature of the anatase to rutile structural phase transition of TiO_2 is lowered for by alloying Cu. However, that the band gap of $Cu_xTi_{1-x}O_2$ decreases with increasing x compared with the wide band gap of TiO_2. We successfully grew polycrystalline $Cu_xTi_{1-x}O_2$ alloys with x up to 31% on quartz substrates. We determined the crystal phase of the deposited thin films by XRD and Raman spectroscopy and established a 2D phase map versus substrate temperature during growth and Cu content x. It shows that increasing Cu content considerably lowers the growth temperature where rutile $Cu_xTi_{1-x}O_2$ thin films can be obtained. Furthermore, we find that the morphology of the $Cu_xTi_{1-x}O_2$ thin films changes with increasing x. Currently, we are assessing the trade-off between band gap, morphology, and growth temperature required for obtaining the most suitable rutile $Cu_xTi_{1-x}O_2$ buffer layer from the viewpoints of the best materials properties as well as a suitability for future commercialization in smart windows.

session break

DS 6.5 Wed 10:45 H3

Achieving superconductivity in infinite-layer nickelate thin films by aluminum sputtering deposition — •dongxin zhang[1], A. Raji[2], L. M. Vicente-Arche[1], A. Gloter[2], M. Bibes[1], and L. Iglesias[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, 91405, France — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, 91405, France

After decades of research, the recent discovery of superconductivity in hole doped infinite-layer nickelates (ABO2) has offered new perspectives to deepen the understanding of high-temperature superconductivity. infinite-layer (IL) nickelates are synthesized by topotactic reduction that selectively removes all apical oxygens of the precursor perovskite ABO3 phase. This is typically achieved by an ex-situ complex annealing using CaH2 as a reducing agent. However, the progress in this field is hampered by significant challenges in materials synthesis and the limited number of research groups capable of producing high-quality superconducting (SC) samples.Here, we present a new method to synthesize SC IL nickelates Pr0.8Sr0.2NiO2 thin films using an aluminum overlayer deposited by sputtering as a reducing agent. We optimized the aluminum deposition conditions and achieved SC samples reduced either in-situ or ex-situ. In-situ Al reduction enhances the quality of the SC Pr0.8Sr0.2NiO2 films, with a maximum transition temperature Tconset of 17 K. This simplified synthesis approach, more accessible than existing ones, enables more research groups to produce high-quality SC nickelate samples, Possibly advancing experimental understanding of superconductivity in IL nickelate.

DS 6.6 Wed 11:00 H3

Deposition and characterisation of NbTiN thin films for application in SRF cavities — •Bharath Reddy Lakki Reddy Venkata, Aleksandr Zubtsovskii, and Xin Jiang — Chair of Surface and Materials Technology, University of Siegen, Germany

Superconducting radio frequency (SRF) cavities are key components for modern particle accelerators. While bulk niobium (Nb), with the highest lower critical magnetic field, Hc1 (0.18 T), and transition temperature, Tc (9.23 K), among elemental superconductors, has dominated SRF applications, the performance of bulk Nb cavities has reached theoretical limits. Recent research focuses on the use of superconducting thin films of Nb or other alternative higher Tc materials, such as NbN, NbTiN, Nb3Sn, MgB2, etc, to enhance SRF cavity performance and cost efficiency. However, their lower Hc1 limits high accelerating gradients and quality factors. Gurevich's SIS multilayer theory offers a breakthrough to shield an underlying superconductor from the applied magnetic fields, thus increasing the maximum accelerating gradient beyond the bulk Nb limits. This study investigates NbTiN thin films deposited on Si substrates using reactive DC- and HiPIMS techniques. Deposition parameters were optimised to achieve improved microstructure and superconducting properties, enabling their integration into SIS structures. To understand the microstructural characteristics of NbTiN films, positron annihilation spectroscopy (PAS) was employed alongside SEM, XRD, AFM, and EDX, offering deeper insights into how deposition techniques and parameters affect material performance.

DS 6.7 Wed 11:15 H3

T-dependent switching of molecular spin-crossover (SCO) monolayers — •Fabian Streller[1], Kirill Gubanov[1], Stephen Goodner[2], Marat Khusniyarov[2], and Rainer Fink[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich Alexander Universität Erlangen Nürnberg — [2]Lehrstuhl für Anorganische und Allgemeine Chemie, Friedrich Alexander Universität Erlangen Nürnberg

Spin-crossover (SCO) complexes are regarded as promising materials in spintronics, molecular electronics and ultra-high-density memory systems applications. Switching between diamagnetic low-spin (LS) and paramagnetic high-spin (HS) species is triggered by external stimuli, e.g., change of temperature, pressure, or illumination with light.[1] One major challenge is the transfer from solution or bulk towards thin films or even monolayers on well-defined surfaces without quenching of the switching behaviour. Six-coordinate iron(II) complexes have been used as SCO materials. This material is attached to the surface via a bidental phenanthroline ligand containing moieties suitable for bonding to the substrate. We report on a step-by-step formation of SCO-active single-layer films on Au(111) surfaces. Thus created specimens were characterized by atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and temperature dependent near edge x-ray absorption fine structure (NEXAFS) to follow the molecular switching. Research is funded by the BMBF (contract 05K22WE2) [1] B. Rösner, M. Milek, A. Witt, B. Gobaut, P. Torelli, R. H. Fink, M. M. Khusniyarov Angewandte Chemie. 2015, 127, 13168-13172.

DS 6.8 Wed 11:30 H3

High Accuracy Reflection Prediction Model for Multi-Layer Anti-Reflection Coatings Using Deep Learning and Machine Learning — •Iremnur Duru, Semih Oktay, and Timuçin Emre Tabaru — Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey

In order to optimize the thickness parameters, this work employs Machine Learning (ML) and Deep Learning (DL) approaches to develop an accurate reflection prediction model that will direct the design of filters with multilayer Anti-Reflection Coating (ARC). A dataset of information derived from 3000 (1500 Ge- Al2O3, 1500 Ge- SiO2) computer simulations based on the thicknesses of multilayer structural materials has been used to create this model. Al2O3 and SiO2 served as the second layers in both coatings, with Ge serving as the substrate. Reflectance values for wavelengths ranging between the 3-5 *m and 8-12 *m bands characteristic of the mid-wave infrared (MWIR) and long-wave infrared (LWIR) bands are included in the data set. The average reflectance in the given 2-layer data set was at least 0.36 at thicknesses of 515 nm Ge and 910 nm SiO2. In terms of predicting reflectance values, the results demonstrate that machine learning (ML) models*specifically, decision tree, random forest and bagging methods perform better than the DL model and offer a useful guide for conceptualizing and manufacturing optical thin-film filters.

DS 7: Spins in Molecular Systems: Strategies and Effects of Hyperpolarization

Time: Wednesday 9:30–11:45 Location: H14

Invited Talk DS 7.1 Wed 9:30 H14

Enhancing Organic Spin Valves Through Spinterface Engineering — •Shuaishuai Ding and Wenping Hu — Institute of Molecular Aggregation Science, School of Science, Tianjin University, Tianjin, China

Organic spin valves hold immense promise for efficient spintronic devices, driving advancements in information processing and storage technologies. The spinterface, the interface between an organic semiconductor and a ferromagnetic electrode, plays a crucial role in the performance of these devices. However, the inherent instability of the spinterface poses challenges that must be addressed to fully realize this potential. To tackle these issues, we have developed a comprehensive approach that combines innovative fabrication techniques and material engineering. Electrode transfer technology enhances interfacial properties by enabling the precise deposition of high-quality ferromagnetic electrodes onto organic semiconductors, while doping with F4-TCNQ effectively improves spin injection efficiency through modulation of electronic and magnetic characteristics. Moreover, the engineering of controllable bottom spinterfaces allows for precise regulation of spin injection, resulting in highly tunable device performance. By leveraging the spinterface, we have achieved in-situ control of device

tunability, significantly expanding the multilevel resistance modulation of organic spin valves. These advancements not only address key challenges of unstable spinterface but also establish novel methods for device modulation, marking an important leap forward in organic spintronics.

DS 7.2 Wed 10:00 H14

Hyperpolarised electron spins as a sensitive probe for investigating structure–function relationship in organic energy materials — •Till Biskup — Universität Rostock, Rostock, Germany

Energy conversion and storage is of paramount importance, and organic functional materials are increasingly being used for this purpose. Hyperpolarised electron spins as created, e.g., by light excitation act as sensitive probe of their environment. This allows to investigate the structure–function relationship of these materials by using time-resolved electron paramagnetic resonance (TREPR) spectroscopy. Insights range from morphology and details of the aggregation behaviour in both, film and solution to triplet routes to the electronic structure of these materials far beyond exciton delocalisation. Here, we focus particularly on the effects of conjugation break and systematic backbone variation on exciton delocalisation as well as solvent and cooling rate on aggregate formation. TREPR spectroscopy provides insight into these effects with molecular resolution that is not available by and complementary to other methods.

DS 7.3 Wed 10:15 H14

The CISS magnetoresistance effect for polyalanine and polyproline molecules studied by ambient STM — •Thi Ngoc Ha Nguyen[1], Lech Tomasz Baczewski[2], Tobias Theiss[3], Tanja Gulder[3], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Ger- many — [2]Reichenhainerstr., 70 — [3]Institute of Organic Chemistry, Faculty of Chemistry and Mineralogy, Leipzig University, Leipzig, Germany

The chirality induced spin selectivity (CISS) effect has been up to now measured in a wide variety of systems but its exact mechanism is still under debate. Whether the spin polarization occurs at an interface layer or builds up in the helical molecule is yet not clear. We investigated the current transmission through helical polyalanine molecules, revealing a strong and length dependent dipole moment, as a part of a tunnel junction realized with a scanning tunneling microscope. Depending on whether the molecules were chemisorbed directly on the magnetic Au/Co/Au substrate or at the STM Au-tip, the magnetizations of the Co layer had been oriented in the opposite direction in order to preserve the symmetry of the IV-curves. These results show that besides the helicity also the electric dipole play a crucial role. Latest experiments with polyproline with a small electric dipole moment showed that the CISS effect is almost vanishing. Our results can be explained by a spin-polarized or spin-selective interface effect, induced and defined by the helicity and electric dipole orientation of the molecule at the interface.

session break

DS 7.4 Wed 10:45 H14

Analysis of polaron pair lifetime dynamics and secondary processes in exciplex driven TADF OLEDs using organic magnetic field effects (MFE) — •Annika Morgenstern[1], Dominik Weber[2], Lukas Hertling[1,3], Konstantin Gabel[1], Ulrich T. Schwarz[1], Daniel Schondelmaier[2], Dietrich R.T. Zahn[1,3], and Georgeta Salvan[1,3] — [1]Institute of Physics, TU Chemnitz — [2]Physical Engineering and Computer Science, WH Zwickau — [3]MAIN, TU Chemnitz, Chemnitz

MFE in TADF materials have been shown to influence the reverse intersystem crossing and to impact on electroluminescence and conductivity. Here, we present a novel model combining Cole-Cole and Lorentzian functions to describe low and high MFE originating from hyperfine coupling, the Δg mechanism, and triplet processes. We applied this approach to organic light-emitting devices of third generation based on TCTA and TPBi, exhibiting blue emission, to unravel their loss mechanisms. The quality of the regression function was evaluated using k-fold cross-validation. The scoring was compared to various alternative fitting functions, which were previously proposed in literature. Density functional theory calculations, photoluminescence, and electroluminescence studies validated the formation of a TADF exciplex system. Furthermore, we propose successful encapsulation using a semi-permeable polymer, showing promising results for magnetic field sensing applications. This study provides insights into the origin of MFE in exciplex-TADF materials, with potential applications in optoelectronic devices and sensing technologies.

DS 7.5 Wed 11:00 H14

Employing CISS for Modification of Skyrmion Diffusion and Size — •Fabian Kammerbauer[1], Yael Kapon[2], Theo Balland[1], Shira Yochelis[2], Yossi Paltiel[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

Chirality-induced spin selectivity (CISS) is a phenomenon that has garnered significant attention due to its ability to generate large spin polarizations in organic molecules and its associated effects, such as the magnetic switching of ferromagnets induced by chiral molecules [1]. In hybrid systems, these chiral molecules have been found to influence magnetic properties, including changes in the magnetization [2]. This study explores the interaction between chiral molecules, specifically alpha-helix polyalanine, and chiral spin structures such as magnetic skyrmions. The skyrmions are stabilized in ferromagnetic/heavy metal multilayers via the Dzyaloshinskii-Moriya interaction [3]. Through magneto-optic Kerr effect imaging, we demonstrate that chiral polypeptides can alter the stability of skyrmions by shifting the temperature and magnetic field ranges where they remain stable. Furthermore, we reveal the impact of chiral molecules on skyrmion size and thermal skyrmion diffusion.

[1] R. Naaman et al. Nat. Rev. Chem. 3, 250 (2019)
[2] Y. Kapon et al. J. Chem. Phys. 159, 064701 (2023)
[3] K. Everschor-Sitte et al. J. Appl. Phys. 124, 240901 (2018)

DS 7.6 Wed 11:15 H14

Microscopic and Macroscopic CISS Effect Characterization: Moving from MBE to Sputter-Deposited Au/Co/Au Substrates — •Lokesh Rasabathina[1], Thi Ngoc Ha Nguyen[1], Julia Krone[1], Annika Morgenstern[1], Franziska Schölzel[1,2], Markus Gössler[1], Karin Leistner[1], Aleksandr Kazimir[4], Jannik Knoche[4], Christina Lamers[4], Irene Coin[4], Lech Thomasz Baczewski[5], Christoph Tegenkamp[1], Georgeta Salvan[1,2], and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology,Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Leipzig University, Leipzig, Germany — [5]Polish Academy of Sciences, Warszawa, Poland.

Adsorption of alpha-helical polyalanine molecules on metallic substrates enables interfacial selective electron transport with a defined spin direction, a phenomenon known as Chirality Induced Spin Selectivity (CISS). We combine microscopic STM/STS of hybrid spin-valve structures with macroscopic MOKE magnetometry for CISS effect characterization on Au/Co/Au substrates. Microscopically we observe magneto resistance changes across the hybrid spin-valve structure and macroscopically we find a coercivity enhancement of the Co layer after exposure to molecules. To use more complex systems, we moved from MBE to sputterd substrates and discuss the challenges related to this transition.

DS 7.7 Wed 11:30 H14

Towards a quantum sensing approach to single-cell chemical and mechanical analysis using nanoscale NMR — •Baha Sakar[1], Sirswa Kuldeep Shree Ram[1], Maximilian Püllmann[1], Frank Sauer[2], Rustem Valiullin[1], Josef A. Käs[2], and Nabeel Aslam[1] — [1]Felix-Bloch-Institut für Festkörperphysik - Universität Leipzig, Leipzig, Deutschland — [2]Peter-Debye-Institut für Physik der weichen Materie - Universität Leipzig, Leipzig, Deutschland

Understanding single-cell mechanical and chemical properties is key to exploring cellular behavior and dysfunction, influencing processes like development, immune response, and disease progression, including cancer metastasis. While fluorescence microscopy enables structural insights and tracking, it lacks the chemical specificity of conventional NMR. The latter is however limited to ensemble measurements and cannot resolve single-cells. In this study, we utilize a quantum sensing platform based on NV centers in diamond, which are atomic-scale spin defects capable of detecting nuclear spins with sensitivities up to fifteen orders of magnitude higher than conventional NMR, enabling single-cell resolution. By applying resonant microwave pulse sequences and specially designed magnetic fields, we probe the NMR signal of the cells' nuclear spins. In this talk, we will discuss the steps towards studying the micromechanical and chemical properties of single cells, distinguishing between intracellular and extracellular molecular diffusion processes. Furthermore, we will present initial results of correlating fluorescence microscopy and NMR spectroscopy with the goal to investigate the link between cell mechanics and tumor aggressiveness.

DS 8: Optical Analysis of Thin Films I

Time: Wednesday 12:00–13:00 Location: H3

DS 8.1 Wed 12:00 H3

Initial stages of Palladium growth on vicinal Si(001)-(2*1) surfaces — •Sandhya Chandola[1], Norbert H. Nickel[1], Julian Plaickner[2], Jörg Rappich[1], Karsten Hinrichs[1], and Norbert Esser[2] — [1]Nanoscale Solid-Liquid Interfaces, Helmholtz-Zentrum Berlin für Materialien und Energie,Schwarzschildstr. 8, 12489 Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Although palladium-based silicides are of great interest in many microelectronic applications, their formation mechanisms are still not fully understood, especially for thin films where the silicidation reaction may be controlled from the initial Pd-Si interactions at the interface.

The early stages of palladium silicide formation have been investigated in ultra-high vacuum (UHV), using Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy on vicinal Si(001) surfaces with different degrees of ordering. Raman spectroscopy has identified silicide-like reacted phases at the Si-Pd interface upon annealing, with the appearance of several phonon modes which are in very good agreement with vibrational modes obtained from ab initio calculations for Pd incorporation into Si surface layers.

The growth morphology of the Pd-Si structures was shown to be dependent on the initial surface reconstruction with in-situ RAS and ex-situ AFM (atomic force microscopy) clearly distinguishing between two types of structures depending on the substrate template.

DS 8.2 Wed 12:15 H3

Ultrafast Charge Carrier Dynamics in Niobium Probed in the Visible Spectral Range — •Noah Stiehm[1], Shirly Espinoza[2], Mateusz Rebarz[2], Saul Vazquez Miranda[2], Erik Müller[3], Hannes Töpfer[3], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Technische Universität Ilmenau, Fachgebiet Technische Physik I, Weimarer Straße 32, 98693 Ilmenau, Germany — [2]ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 25241 Dolní Břežany, Czech-Republic — [3]Technische Universität Ilmenau, Fachgebiet Theoretische Elektrotechnik, Helmholtzplatz 2, 98693 Ilmenau, Germany

With the recently developed experimental method of femtosecond time-resolved spectroscopic ellipsometry (trSE) [1], it is possible to obtain the transient dielectric function of a sample after excitation in a pump-probe scheme. We present results of applying the technique to study the ultrafast charge carrier dynamics in the transition metal Niobium. We show that it is possible to observe bleaching in the dielectric function for several 100 picoseconds and up to 1 nanosecond, depending on the pump wavelength, resulting from exciting charge carriers into higher conduction bands, where they relax into band minima and remain stable for some time until recombination.

The initial results from this study at room temperature provide valuable insight into the ultrafast charge carrier dynamics and good motivation to conduct further investigations under cryogenic conditions in the superconducting phase.

[1] S. Richter *et al.*, Rev. Sci. Instrum. 92, 033104 (2021).

DS 8.3 Wed 12:30 H3

Investigation of metal surfaces using Surface Resonant Raman Scattering — •Sarang Bhasme, Mariella Denk, Simon Kalteis, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

We have recently demonstrated the possibility to investigate surface phonons on metals by surface resonant Raman spectroscopy (SRRS), in which the Raman cross section is significantly enhanced by resonant excitation of optical transitions involving surface electronic states [1]. Here we report new investigations regarding the phonon and electron scattering mechanism on clean and adsorbate-modified Cu(110) surfaces using SRRS and reflectance difference spectroscopy (RDS) under ultra-high vacuum (UHV) conditions and variable temperatures. We have modified the Cu(110) surface electronic states via ion bombardment and by adsorption of small molecules such as oxygen or CO to explore its effect on the Raman signals. We find that both the phonon and the electron related scattering strongly depend on the details of the surface cleanliness and structural properties, underscoring the influence of the surface electronic structure and adsorbate interactions on the Raman signatures.

[1] M. Denk et al., Phys. Rev. Lett. 128, 216101 (2022).

DS 8.4 Wed 12:45 H3

Watching hydrogen diffusion into Lutetium and Yttrium thin films with Pd cap layers — •Zahra Hojjati, Philipp Flad, and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

Hydrogenated Lutetium is one of the materials that may have a potential to be used as high-temperature superconductor under high pressure. Recently, reports have indicated that the Lu-H-N system undergoes a phase transition to blue when hydrogenated, with unconfirmed reports suggesting superconductivity. Therefore, we investigate hydrogen-lutetium interactions and the dynamics of hydrogen diffusion within lutetium, which is influenced by the ambient temperature, crystal structure and the hydrogen concentration. Hydrogen diffusion in metals involves interstitial diffusion through the lattice and surface absorption. We find that lutetium is a good hydrogen storage material due to its diffusion properties.

We analyzed the progression of the blue hydrogenation front in Lutetium and subsequently measured the drift velocity for each sample. We calculated the activation energy required for protons to overcome the potential barrier using the Arrhenius equation. Following this, we determined the diffusion constant based on the diffusion equation. We also carry out the same experiments with Yttrium.

DS 9: Optical Analysis of Thin Films II

Time: Thursday 9:30–12:45 Location: H3

Invited Talk DS 9.1 Thu 9:30 H3

Inverse Problems and Uncertainty Quantification for the analysis of thin films and nanostructured surfaces — •Sebastian Heidenreich[1], Nando Hegemann[1], Victor Soltwisch[2], and Markus Bär[1] — [1]Mathematical Modelling and Data Analysis, PTB, Abbestr. 2-12, 10587 Berlin — [2]Radiometry with Synchrotron Radiation, PTB, Abbestr. 2-12, 10587 Berlin

For the analysis of thin films and nanostructured surfaces, indirect optical measurement techniques are often used to determine the optical and geometrical properties by solving an inverse problem. Due to measurement errors and model errors, the results are subjected to uncertainties. In the talk we give an overview about statistical inverse problems with applications in the metrology of thin films and nanostructured surfaces. We start with a discussion of the advantages and disadvantages of frequently used Least-Squares, then consider the Maximum-Likelihood method and introduce the Bayesian approach as a statistical method [1]. We apply the Bayesian approach to thin film examples as well as to line grating structures and show how to deal with measurement uncertainties and model errors. Furthermore, we discuss some drawbacks of the Bayesian method and present recent developments like polynomial chaos, transport maps or neural networks to tackle these drawbacks [2]. –[1] Soltwisch, Fernandez Herrero, Pflüger, Haase, Probst, Laubis, Krumrey, Scholze, J. Appl. Cryst. 50, 2017; Heidenreich, Gross, Bär, Metrologia 55(6), 2018. [2] Hegemann, Heidenreich, J. Open Software 8 (89), 2023; Hagemann, Hertrich, Casfor, Heidenreich, Steidl, Mach. Learn:Sci. Technol. 5, 2024.

Invited Talk DS 9.2 Thu 10:00 H3

Metrological spectroscopic and imaging Mueller matrix ellipsometry for the analysis of thin films and nanostructured surfaces — •Bernd Bodermann[1], Matthias Wurm[1], Manuela Schiek[2], Jana Grundmann[1], and Tim Käseberg[1] — [1]Optical Nanometrology, PTB, Bundesallee 100, 38116 Braunschweig — [2]Center for Surface and Nano-Analytics (ZONA) Johannes Kepler University Linz, Austria

Spectroscopic Mueller ellipsometry is a widely used method for analysing thin films and nanostructured surfaces. The extension to imaging ellipsometry enables measurements on small measurement objects << 1 mm2 and investigations of local parameter variations. However, as an integral and indirect measurement method, the determination of the corresponding measurement uncertainties is challenging and requires complex analysis methods. Imaging ellipsometry, involves an even higher level of complexity both in terms of data analysis and the necessary metrological system characterisation. We give an overview of various experimental sources of uncertainty including structure-induced contributions and how these can be characterised. Both deterministic and stochastic contributions of the measurement system as well as the samples under test will be discussed. Additionally, we present investigations of sensitivity-enhanced ellipsometry, by e.g. exploiting local plasmonic or dielectric resonances in the sample structure, and advanced methods that use additional structures to amplify and/or guide resonances for the detection and characterisation of periodic and non-periodic structures.

session break

DS 9.3 Thu 10:45 H3

Structured Light Microscopy for Optical and Topological Characterization — •Denis Ukolov, Polina Gromova, and Peter Lemmens — IPKM, TU-BS, Braunschweig, Germany

Structured light beams with orbital angular momentum (OAM) are applied to study topological properties of thin films and metasurfaces. Using a laser confocal microscope with integrated interferometry, we investigate phase distributions and topological features of chiral structures.

Experimental data are compared with simulations to understand the interaction of OAM with surface geometry and its topological effects. This method offers a novel approach to characterizing surface properties in complex systems.

Work supported by DFG EXC-2123 QuantumFrontiers - Light and Matter 390837967.

DS 9.4 Thu 11:00 H3

Synchrotron-based VUV ellipsometry on passivated Si samples for optical thin film metrology — •Julian Plaickner[1], Alexander Gottwald[2], Mattia Mulazzi[2], Jörg Rappich[3], Karsten Hinrichs[3], Christoph Cobet[4], Johanna Reck[5], and Norbert Esser[1] — [1]Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — [2]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [3]Nanoscale Solid-Liquid Interfaces, Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Albert Einstein Str. 15, 12489 Berlin — [4]Center for Surface and Nanoanalytics, Johannes Kepler Universität, Altenbergerstr. 69, 4040 Linz — [5]SENTECH Instruments GmbH, Schwarzschildstr. 2, 12489 Berlin

The vacuum ultraviolet (VUV) spectral range spectral range is characterized by a lack of reliable data on optical properties due to the extreme surface sensitivity and the requirements of a high brightness light source. A method for determining traceble optical data with well-defined uncertainty budget is tested on novel reference materials. For this purpose, chemically passivated vicinal silicon surfaces were measured between 2 and 30 eV with the synchrotron-based VUV ellipsometer[1] at the Metrology Light Source (MLS) of the PTB. X-ray photoelectron spectroscopy (XPS) and IR ellipsometry measurements serve as quality cross checks for the prepared surfaces. In the spectral range between 2 and 6 eV, results are compared to reference measurements made with commercial SENTECH ellipsometers.

DS 9.5 Thu 11:15 H3

Tailoring Properties of Epitaxially Grown Bismuth Telluride Thin Films through Stoichiometric Control — •Felix Hoff, Christoph Ringkamp, Alexander Kiehn, Thomas Schmidt, Dasol Kim, Jonathan Frank, Timo Veslin, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

The Earth's crust contains a significant number of minerals formed by elements such as Bi and Te, which is surprising given their scarcity. This rich mineral diversity can be attributed to strong interlayer interactions within layered chalcogenides, leading to complex phase diagrams. Bismuth tellurides, in particular, exhibit various stacking sequences that influence their properties as thermoelectrics and topological insulators. While their structural and thermoelectric properties are well-studied in bulk forms, high-quality thin films and their optical and vibrational properties remain underexplored. We address this gap by examining the vibrational and dielectric properties of epitaxially grown thin films of nine distinct BiTe compositions grown on Si (111). Using Raman and fs pump-probe spectroscopy, we characterized the lattice dynamics while optical spectroscopy was employed to determine the dielectric properties. The variation in phonon frequencies with respect to the Bi share can be attributed to the differing strengths of the interlayer bonds. The height of the dielectric absorption peak increases with increasing Bi share, accompanied by a shift in the absorption maximum to lower photon energies. Our results demonstrate the potential of the BiTe system as a versatile and tunable platform for thin film applications.

DS 9.6 Thu 11:30 H3

VUV ellipsometry for the determination of thin film optical constants — •Mattia Mulazzi[1], Julian Plaickner[2], Jörg Rappich[3], Alexander Gottwald[1], and Norbert Esser[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587, Berlin, Germany — [2]Technische Universität Berlin, Hardenbergstr. 36, 10623, Berlin, Germany — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Motivated by the purpose of determining the optical constants of thin films materials, we present our investigation method based on spectroscopic ellipsometry in the vacuum-ultraviolet spectral range using monochromatised synchrotron radiation. The measurements are characterised by low noise and high accuracy, both quantified according to state-of-the-art metrological procedures, and are well-suited to be fit by numerical methods to obtain the refractive index and the absorption coefficient in a non-parametric way, i.e., independent of the underlying physics of the material under investigation. We show exemplary measurements on surfaces of hydrogen-passivated Si, native SiO2 on Si, graphene on Si and the evaluation steps necessary to determine the optical constants from the measured data.

session break

DS 9.7 Thu 12:00 H3

Optical absorption by two-dimensional excitons (with and without screening) — •Stefan Zollner and Carlos Armenta — New Mexico State University, Las Cruces, NM

Two-dimensional excitons form not only in 2D layered materials (such as transition metal dichalcogenides) or in quantum wells. They also dominate the visible absorption by 2D van Hove singularities in 3D semiconductors. As an example, we measured and calculated the optical absorption of germanium near the E_1 and $E_1 + \Delta_1$ transitions. The 2D character of these transitions stems from the large optical mass along the (111) direction, where the highest valence bands and the lowest conduction band are nearly parallel. Elliot's formalism for the Sommerfeld enhancement of optical absorption (as modified by Tanguy for 2D excitons) provides an excellent description of these absorption peaks, if the momentum matrix element from $\vec{k} \cdot \vec{p}$-theory is used as the optical dipole matrix element. We also discuss how band filling with Fermi-Dirac statistics after intense laser excitation reduces the absorption. We are not aware of a (Banyai-Koch) theory that can be applied to the screening of 2D excitons. This work was supported by the US Air Force (FA-9550-24-1-0061).

DS 9.8 Thu 12:15 H3

All-optical quality-control of indenene intercalation into graphene/SiC — •Cedric Schmitt[1,2], Simone Sotgiu[3], Stefan Enzner[2,4], Jonas Erhardt[1,2], Elena Stellino[3], Domenico Di Sante[5], Giorgio Sangiovanni[2,3], Ralph Claessen[1,2], Simon Moser[1,2], and Leonetta Baldassarre[3] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Department of Physics, Sapienza University of Rome — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [5]Department of Physics and Astronomy, University of Bologna

Intercalating two-dimensional quantum materials beneath a sheet of graphene provides effective environmental protection and facilitates ex situ device fabrication. However, developing a functional device requires rapid, large-scale screening methods to evaluate the quality of the intercalant, which to date can be monitored only by slow, UHV-based surface science techniques. In this study, we utilize ex situ Raman micro-spectroscopy to optically and non-destructively identify the quantum spin Hall insulator indenene, a monolayer of indium sandwiched between a SiC(0001) substrate and a single sheet of graphene. Color modulation combined with indenene's distinctive low-frequency Raman fingerprint enables rapid assessment of its homogeneity and crystalline quality. Density functional perturbation theory indicates that this Raman signature originates mainly from indenene's shear and breathing modes, while additional higher-order modes are tentatively attributed to defect-assisted and two-phonon Raman processes.

DS 9.9 Thu 12:30 H3

Moiré lattice of twisted bilayer graphene as template for non-covalent functionalization — •Tobias Dierke[1], Stefan Wolff[1], Roland Gillen[1], Tamara Nagel[2], Jasmin Eisenkolb[2], Sabine Maier[1], Milan Kivala[3], Frank Hauke[2], Andreas Hirsch[2], and Janina Maultzsch[1] — [1]Chair of Experimental Physics, FAU Erlangen-Nürnberg, Erlangen — [2]Department of Chemistry and Pharmacy, FAU Erlangen-Nürnberg — [3]Organisch-Chemisches Institut, Centre for Advanced Materials, Universität Heidelberg

We present an innovative approach to achieve spatial variations in the degree of non-covalent functionalization of twisted bilayer graphene (tBLG). The tBLG with local twist angle variations between * 5° and 7° was non-covalently functionalized with 1,4,5,8,9,11- hexaazatriphenylenehexacarbonitrile (HATCN) molecules. We observe a correlation between the twist angle of tBLG and the degree of functionalization, determined through Raman spectroscopy. We propose that the adsorption of HATCN molecules follows the moiré pattern of twisted bilayer graphene, preferentially avoiding AA-stacked regions and primarily attaching to regions with local AB-stacking order, resulting in an overall ABA-stacking arrangement. This hypothesis, is further supported by density functional theory (DFT) calculations [1]. [1] Dierke et al., Angew. Chemie Int. Ed., accepted (2024), DOI: 10.1002/anie.202414593

DS 10: Transport Properties

Time: Thursday 11:30–12:30 Location: H14

DS 10.1 Thu 11:30 H14

A tunable room temperature nonlinear Hall effect in elemental bismuth thin films — •Pavlo Makushko[1], Sergey Kovalev[1], Yevhen Zabila[1], Igor Ilyakov[1], Alexey Ponomaryov[1], Atiqa Arshad[1], Gulloo Lal Prajapati[1], Thales V. A. G. de Oliveira[1], Jan-Christoph Deinert[1], Paul Chekhonin[1], Igor Veremchuk[1], Tobias Kosub[1], Yurii Skourski[1], Fabian Ganss[1], Denys Makarov[1], and Carmine Ortix[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V. — [2]Università di Salerno, Fisciano (SA), Italy

The nonlinear Hall effect with time-reversal symmetry is a second-order electronic transport phenomenon that induces frequency doubling and occurs in non-centrosymmetric crystals with Berry curvature dipole. This effect was typically reported in complex compounds characterized by Dirac or Weyl electrons at low temperatures. Here, we report a room temperature nonlinear Hall effect in polycrystalline thin films of the centrosymmetric elemental bismuth. The nonlinear transversal currents are induced by electrons at the (111) free surface, which possesses a Berry curvature triple. The nonlinear transverse voltage can be boosted by the geometric nonlinear Hall effect in arc-shaped bismuth stripes. The geometric curvature induced frequency doubling is extended to the second-harmonic generation in the terahertz spectral range. We also demonstrate efficient high-harmonic generation in polycrystalline bismuth films and bismuth-based heterostructures across a broad range of terahertz frequencies.

[1] P. Makushko et al., Nature Electronics 7, 207 (2024).

DS 10.2 Thu 11:45 H14

Electrochemical characterization of CeO_2/YSZ multilayer systems with well-defined interfaces — •Julius K. Dinter[1], Anja Henss[1,2], and Matthias T. Elm[1,2] — [1]ZfM, JLU Gießen — [2]Institute of Experimental Physics, JLU Gießen

Mixed ionic and electronic conductors (MIECs) are key components for a variety of electrochemical devices. Their functionality depends on their ability to store or transport both electrons and ions. However, most materials with high ionic conductivity exhibit poor electronic conductivity and vice versa. A common approach to overcome this challenge is the preparation of artificial mixed conductors by mechanically mixing a good electronic conductor with an ionic conductor. Consequently, these artificial MIECs are characterized by a high number of interfaces, which can significantly affect charge storage and charge transport in the composites. A detailed understanding of the impact of these interfaces on the electrochemical properties is essential for the design and improvement of electrochemical devices with enhanced functionality. We present the preparation and characterization of multilayer heterostructures of ceria (CeO_2) and yttria-stabilized zirconia (YSZ). The multilayers with constant thickness but varying number of interfaces were prepared by pulsed laser deposition to obtain thin film structures with well-defined interfaces. Structural characterization was performed using Raman microscopy and time-of-flight secondary ion mass spectrometry. The electrochemical properties were characterized by electrochemical impedance spectroscopy at different temperatures and under varying atmospheric conditions.

DS 10.3 Thu 12:00 H14

Magneto transport in bilayer graphene cavities — •Florian Schöppl[1], Michael Barth[1], Ming-Hao Liu[2], Klaus Richter[1], and Angelika Knothe[1] — [1]Institut für Theoretische Physik, 93053 Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan City 701, Taiwan

The remarkable sample quality of bilayer graphene in combination with the unprecedented electronic control of the band-structure makes bilayer-graphene an excellent platform for electron optics. While the purity of the system allows for ballistic transport on the micrometer scales [1,2], the trigonal warping of the band structure close to each K points induces a valley dependent selection of momenta leading to unique transport and scattering properties [3,4]. Interested in the interplay of symmetry breaking induced by a variety of all-electronic gate confinements and the trigonal warping, we implement various quantum mechanical tight binding models as well as semiclassical simulations and deploy them to investigate magneto transport through bilayer graphene cavities.

[1]L. Seemann et al., Gate-tunable regular and chaotic electron dynamics in ballistic bilayer graphene cavities, Phys.Rev. B (2023) [2]L. Banszerus et al., Ballistic Transport Exceeding 28*m in CVD Grown Graphene, Nano Lett. 2016 [3]C. Gold et al., Coherent Jetting behind a gate-defined channel in bilayer graphene, Phys.Rev. Lett. (2021) [4]J.K. Schrepfer e t al. Dirac fermion optics and directed emession from single- and bilayer graphene cavities, Phys. Rev. B (2021)

DS 10.4 Thu 12:15 H14

Electrical transport across thin catalyst/defect-engineered titania corrosion protection layer interfaces for photoelectrochemical applications — •Julius Kühne[1,2], Tim Rieth[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technichal University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Producing value-added products via light-driven photoreduction represents a promising approach to sustainably address increasing CO2 emissions and meet the growing global energy demand. However, such solar fuels systems require passivating layers to chemically protect semiconductor light absorbers from harsh reaction environments. Despite great progress in the development of atomic layer deposited (ALD) protection layers, the factors governing efficient charge injection into the catalytic component remain not well understood. The nanoscale thickness of these ultrathin layers presents unique challenges, particularly for in-plane electrical measurements, complicating the reliable characterization of their transport properties compared to bulk materials. Here, the charge transport characteristics between various defect-engineered TiO2 protection layers grown with ALD and metal catalyst layers are investigated. By analyzing contact resistivity, carrier transport, and interface kinetics, this work seeks to deepen understanding of the interface between catalyst and protection layer.

DS 11: Thermoelectric and Phase Change Materials

Time: Thursday 15:00–16:00 Location: H3

DS 11.1 Thu 15:00 H3

Bond strength and force constants in RESbS — •Franziska Zahn[1], Christopher Benndorf[2], Hans H. Falk[1], Konrad Ritter[1], Sergiu Levcenko[1], Edmund Welter[3], Oliver Oeckler[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektron Synchrotron DESY, Hamburg, Germany

Our recent study on bond strength in different materials has shown that elemental Sb exhibits characterics of regular covalent and multicenter bonding based on the behavior of force constants with increasing interatomic distance. *RE*SbS are Sb-containing rare-earth (*RE*) pnictide chalcigenides that show special electronic and magnetic properties. They consist of different layeres, including Sb monolayers that alternate with *RE*-S double layers. To study the structural and vibrational properties of *RE*SbS with *RE* = La, Ce, Pr, and Nd in more detail, extended X-ray absorption fine structure spectroscopy (EXAFS) was performed at the Sb K-edge at ten different temperatures ranging from 20 to 295 K. The temperature dependence of the bond length variation σ^2 (mean square relative displacement) was evaluated using a correlated Einstein model, providing static disorder and force constants. The behavior of the force constants with incrasing interatomic distance is compared to other materials and to elemental Sb in particular. This contributes to the fundamental understanding of physical properties of *RE*SbS and their potential origin.

DS 11.2 Thu 15:15 H3

Enhancing mechanical flexibility and thermoelectric efficiency of amorphous TiNiSn — •Denis Music — Department of Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden

Thermoelectrics can convert heat to electricity without greenhouse gas emissions and hold significant potential as energy sources for wearable devices. Current research focuses on designing compounds that combine high conversion efficiency with mechanical flexibility. Half-Heusler phases, such as TiNiSn, demonstrate promising chemical stability and thermoelectric efficiency, but their inherent brittleness limits their application in flexible devices. To address this shortcoming, amorphous TiNiSn thin films were synthesized by sputtering on various substrates, such as Kapton, silk, and paper, to evaluate their bending response. These thin films show good adhesion to the substrates, as predicted by density functional theory, and do not delaminate under mechanical loading. Bending tests up to 154 degrees reveal minimal crack formation, indicating a high degree of flexibility. Consequently, amorphous TiNiSn is a promising candidate for flexible thermoelectric devices. To further enhance the thermoelectric efficiency of these devices, density functional theory and Boltzmann transport theory were employed to tune the electronic structure and identify suitable doping elements among 3d and 4d transition metals. Experiments were carried out to validate these predictions, yielding an order of magnitude increase in performance at room temperature.

DS 11.3 Thu 15:30 H3

Atomic arrangement in MBE grown chalcogenide thin films: structural investigation based on LEED-IV — •Maximilian Buchta[1], Christoph Ringkamp[1], Lucas Bothe[1], and Matthias Wuttig[2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

If chalcogenides such as GeTe or Sb2Te3 are confined to reduced dimensions, for instance by reducing the film thickness, distortions in the atomic arrangement of the crystal emerge, which have been investigated by techniques such as X-ray diffraction (XRD). However, for the chalcogenides SnTe and SnSe, density functional theory (DFT) predicts pronounced distortions not only for thin films but also at the vicinity of the surface, which cannot be resolved by XRD. Further, as the distortions occur in both out-of-plane and in-plane directions, advanced structural characterization techniques are necessary to determine the atomic arrangement. In this work, Low Energy Electron Diffraction (LEED) Intensity vs. Electron Energy (LEED-IV) curves will be utilized to determine the surface atomic arrangement of tin-based chalcogenide thin films (SnTe and SnSe), grown by Molecular Beam Epitaxy (MBE), providing direct experimental evidence for structural predictions based on DFT.

DS 11.4 Thu 15:45 H3

Characterization of Nucleation and Growth Processes in the Phase Change Material GeTe upon Laser-Induced Switching — •Ramon Pfeiffer, Pascal Schröder, Elias Hildebrand, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

We have investigated how germanium telluride (GeTe) phase change material behaves during laser-induced switching at a wavelength of 658 nm. Starting with an amorphous GeTe matrix, which we have crystallized using laser pulses, GeTe has been reverted back to an amorphous state before recrystallizing it again. To analyze concomitant changes, we have examined individual crystal grains using electron backscatter diffraction (EBSD) and topographic changes by atomic force microscopy (AFM). Additionally, we have explored larger spot sizes during the second crystallization phase to assess the influence of a crystalline matrix on nucleation and growth dynamics within the material. These experiments revealed distinct nucleation and growth mechanisms that depend on the parameters used for crystallization.

DS 12: Gaede-Jubiläumssitzung

The Gaede Prize was founded 40 years ago by Dr Manfred Dunkel and is awarded annually for outstanding scientific work in basic research and application, for which the use of vacuum is relevant. To mark this anniversary, Selina Olthof (2019 prizewinner), Philip Willke (2022), Philip Hofmann (2011), and Andreas Waag (1998) from the illustrious list of prizewinners will give presentations in this session, covering a broad spectrum from the prize-relevant fields of thin films, surface science, semiconductor physics, and nanotechnology.

Time: Thursday 16:15–18:30 Location: H3

Invited Talk DS 12.1 Thu 16:15 H3

Probing the Electronic Structure of Halide Perovskites — •Selina Olthof — Department of Chemistry, University of Cologne — Chair of Material and Surface Analysis, University of Wuppertal

Halide perovskites are a novel class of thin film semiconductors that have revolutionized the field of photovoltaics, nowadays even surpassing in record efficiency the conventional silicon-based cells. Their remarkable defect tolerance, solution-based processability and tunable band gap make them highly promising for next-generation optoelectronic technologies.

This talk will provide a brief introduction to halide perovskites, highlighting the origins of their exceptional material properties. Next, I will introduce UV photoelectron spectroscopy (UPS) as well as reflection electron energy loss spectroscopy (REELS) as powerful tools to gain deeper insight into device relevant material properties. Specifically, I will discuss our investigations into the valence and conduction band density of states in tin and lead-based 3D perovskites. By combining photoelectron spectroscopy results with density functional theory, we identified the roles of atomic positions, bond hybridization, and lattice distortions in shaping the electronic properties.

Additionally, I will introduce our recent work on reduced-dimensionality perovskites (2D layers), which are gaining attention for their potential to optimize interfaces and enhance solar cell efficiencies. Here, I will present a systematic study using alkyl-based organic cations with varying chain length, which we used to track effects of interlayer spacing on the electronic and optical properties.

Invited Talk DS 12.2 Thu 16:45 H3

Quantum Science with Single Atoms and Molecules on Surfaces — •Philip Willke — Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

The quantum nature of a physical system often emerges from its fundamental building blocks and demands a deep understanding to leverage its benefits for future quantum devices. In this talk, I introduce the combination of electron spin resonance (ESR) and scanning tunneling microscopy (STM) as a new platform for coherent control of spins on surfaces (1). This technique enables for instance the addressing of individual atoms on surfaces with exceptional energy resolution. It allowed for high-resolution magnetic sensing, for instance by resolving their hyperfine interaction between the electron and nuclear spins. Recently, we have extended this technique to achieve spin resonance on individual molecules (2), which is particularly exciting as it extends ESR-STM into the realm of molecular quantum technologies: Promising new avenues involve organizing spins through molecular self-assembly into larger structures, alongside the application of on-surface chemistry techniques. As an example, we demonstrate how constructing new complexes through tip-assisted on-surface assembly can lead to spin systems with improved dynamic spin properties (3), that can be coherently controlled. (1) Chen, Y. et al., Advanced Materials, 35 (27), 2107534 2023. (2) Zhang, X. et al. Nat. Chem., 14, 59-65 2022. (3) Huang, W. et al. arXiv.2410.18563 2024.

session break

Invited Talk DS 12.3 Thu 17:30 H3

Gallium Nitride Technology - the second pillar of microelectronics — •Andreas Waag — Nitride Technology Center NTC, TU Braunschweig

The highly efficient radiative recombination makes GaN ideally suited for microLEDs with dimensions as small as 1 μm and even below. Besides display applications, their capability to produce optical patterns with high resolution, which can be modulated at extremely high frequencies, makes them suitable for numerous other applications.

Besides chip-based microscopy and highly efficient sensing, we explore these exciting properties for a new highly significant application: utilizing microLEDs in optical processing units for artificial intelligence workloads.

The talk will focus on technological challenges of chip processing and hybrid integration with silicon CMOS microelectronics. For all these applications, nitride technology and the exciting properties of GaN semiconductor devices are a key.

Invited Talk DS 12.4 Thu 18:00 H3

Ultrafast X-ray photoelectron spectroscopy and photoelectron diffraction — •Philip Hofmann — Department of Physics and Astronomy, Aarhus University, Denmark

X-ray photoelectron spectroscopy (XPS) is an experimental tool capable of accurately determining the core level binding energies of atoms. This energy is not only element-specific but also provides detailed information on the atoms' oxidation state and chemical environment, making XPS an essential tool for studying catalytic processes. XPS line shapes have also attracted considerable interest, leading to the development of many-body theories to study the solid's electronic and vibrational properties. Finally, the core level photoemission intensity can be interpreted as a diffraction pattern that gives access to the emitting atom's local geometrical environment in an experimental approach called X-ray photoelectron diffraction (XPD).

The increasing availability of ultrafast X-ray sources at free electron lasers now opens the opportunity to take XPS and XPD into the ultrafast time domain and this talks will give two recent examples. For graphene, it is shown that a study of the time-dependent XPS line shape can reveal detailed insight into the excitation of the system, directly giving access to parameters such as the electronic temperature. A demonstration of XPD is given in which the motion of surface atoms of the topological insulator Bi_2Se_3 is tracked after the excitation of a coherent optical phonon.

DS 13: Poster

Time: Thursday 18:00–20:00 Location: P1

DS 13.1 Thu 18:00 P1

Establishing Circular Dichroism Spectroscopy as predictor for CISS in molecular thin films — •Franziska Schölzel[1,3], Dominik Hornig[2,3], Lokesh Rasabathina[1], Olav Hellwig[1,3], Michael Mehring[2,3], and Georgeta Salvan[1,3] — [1]TU Chemnitz, Institute of Physics, 09126 Chemnitz, Germany — [2]TU Chemnitz, Institute for Chemistry, 09111 Chemnitz, Germany — [3]TU Chemnitz, Research Center for Materials, Architectures and Integration of Nanomembranes, 09126 Chemnitz, Germany

Circular Dichroism Spectroscopy which utilizes the differential absorption of left and right circularly polarized light to distinguish between the enantiomers of a chiral molecule. Previously it has been shown that the method is able to predict the strength of the chirality induced spin selectivity (CISS) effect [1]. Although many studies show that CISS relies on the interface between a chiral molecule and a magnetic substrate, CD spectroscopy is mainly used for the analysis of molecules in solution [1]. Therefore, it is crucial to develop a method for the interpretation of CD exhibited by molecular thin films.

In this study we present a homebuilt setup to implement the analysis of thin films systems into the Jasco J-1500 CD spectrophotometer. Furthermore, we propose a way to overcome artefacts that may be caused by optical anisotropy of the film and the substrate [2].

[1] Chem. Rev. 124, 4, 1950-1991 (2024) [2] J. Am. Chem. Soc. 143, 21519-21531 (2021)

DS 13.2 Thu 18:00 P1

Wannier description using CP2K — •Nisarg Trivedi, Maximilian F. X. Dorfner, and Frank Ortmann — School of Natural Sciences, Technische Universität München

Wannier functions provide an ideal basis for simulating quantum transport using Model Hamiltonians (i.e., tight binding models). Most Wannier generation tools use a plane-wave basis to expand the Wannier functions. However, using a gaussian basis to expand such functions can make simulations more efficient by using the sparsity of the matrices. Here, we present a procedure to obtain moderately localized Wannier functions on an atom-centered gaussian basis. Interfaced with the CP2K software, the method uses the Kohn-Sham Hamiltonian and Overlap matrices obtained from DFT simulation in the same atom-centered gaussian basis to obtain the Bloch states and then transform them into Wannier functions. We present the results of the application of this method on different polymers, which show excellent reproduction of band structure using a simple tight binding model based on the respective Wannier functions for all studied polymers.

DS 13.3 Thu 18:00 P1

Geometry and electronics of helical nanostructures — •Faezeh Shabani[1], Sibylle Gemming[1], Florian Günther[2], Jeffrey Kelling[1], Hadis Ghodrati Saeini[1], Christoph Tegenkamp[1], Thi Ngoc Ha Nguyen[1], and Georg Kuenze[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil — [3]Universität Leipzig, Leipzig, Germany

Helical nanostructures are intriguing systems where geometry and chirality drive unique electronic phenomena, including the chiral-induced spin selectivity (CISS) effect. This interplay enables efficient spin polarization in electron transport, offering exciting prospects for spintronic applications. In this study, the electronic band structure of helical nanostructures is explored, highlighting how their geometry influences transport as well as spin-dependent properties. These insights will inspire further investigations into biological helices, such as peptides and proteins, which share similar structural motifs and could broaden our understanding of spin polarization in natural systems. This work is part of TRR 386 HYPMOL, funded by DFG. (www.hypmol.net)

DS 13.4 Thu 18:00 P1

local charge transport properties of n-type organic semiconductor films based on T2-(NDI-T2)2 — •Zihao Liu[1], Hajar Komekoz[1], Nisarg Trivedi[2], Dietrich R. T. Zahn[1], Michael Sommer[1], Frank Ortmann[2], and Georgeta Salvan[1] — [1]Fakultät für Naturwissenschaften, Semiconductor Physics group, Technische Universität Chemnitz — [2]TUM School of Natural Sciences,Technische Universität München

Due to the advantages of organic semiconductor thin films, such as weak spin-orbit coupling and low spin scattering, organic materials have emerged as a strong alternative to traditional metallic spacer layers in the field of spin valve devices with vast potential for future spintronic applications. This study investigates conjugated organic semiconductor materials, specifically T2-(NDI-T2)2, and its related compounds with different side chain lengths focusing on their electrical properties on the micrometer and nanometer scales. High-quality organic semiconductor thin films were fabricated on gold substrates by spin coating. The dielectric function ϵ and the film thicknesses were determined by spectroscopic ellipsometry. Kelvin Probe Force Microscopy (KPFM) and conductive atomic force microscopy (c-AFM) were employed to analyze the local charge transport properties of the films systematically. The findings provide crucial insights into the influence of molecular orientation on conductivity and charge carrier mobility providing a solid foundation for further understanding and application of organic semiconductor materials

DS 13.5 Thu 18:00 P1

A graph-theoretical approach to spin-polarised quantum walks in chiral environment — •Saba Arshad[1], Sibylle Gemming[1], and Shahid Iqbal[2] — [1]TU Chemnitz, Chemnitz, Germany — [2]NUST, Islamabad, Pakistan

Exploring the model where a particle or system of particles moves between neighboring nodes couple with autonomous spins on the edges, leading to the propagation of entanglement. The work highlights how entanglement, along with spin oscillations and relaxation dynamics, offers significant advantages while transmitting directed quantum information through the quantum walks, providing faster quantum computations. This approach establishes a connection between spin dynamics and quantum computation, with potential applications in cryptography, quantum key distribution, super-dense coding, teleportation, and quantum computing, leveraging entangled states for secure and efficient information processing.

DS 13.6 Thu 18:00 P1

Self-Assembly Kinetics of Polyalanine α-helix Monolayers: Insights from Coarse-Grained Molecular Dynamics Simulations — •Hadis Ghodrati Saeini[1], Thi Ngoc Ha Nguyen[1], Faezeh Shabani[1], Olav Hellwig[1,2], Christoph Tegenkamp[1], Sibylle Gemming[1], Florian Günther[3], and Jeffrey Kelling[1,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute for Ion Beam Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo (USP), São Carlos, Brazil — [4]Institute for Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany

Helical molecules, such as polyalanine α-helices, are promising candidates for spintronic applications due to their strong spin-filtering ability via the Chiral-Induced Spin Selectivity (CISS) effect. Understanding their intermolecular interactions and collective behavior is essential for harnessing their properties in practical applications. This study employs molecular dynamics simulations with coarse-grained molecular potentials to explore the kinetics of monolayer self-assembly by deposition from solution onto a smooth van der Waals substrate.

Simulations conducted at room temperature reveal key aspects of molecular relaxation, structural organization, and dynamical time-scales. These insights enhance our understanding of the self-assembly mechanisms and stability of polyalanine monolayers, supporting their development for advanced spintronic technologies.

DS 13.7 Thu 18:00 P1

Simulation of self-assembled polyalanine α-helices films: Development and application of an empirical potential — Kevin Preis[1], Hadis Ghodrati Saeini[1], Christoph Tegenkamp[1], Sibylle Gemming[1], Jeffrey Kelling[2], and •Florian Günther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]São Paulo State University, Rio Claro, Brazil

Polypeptide molecules have been discussed as potential candidates for electronic spin-filters because of the so-called chiral-induced spin selectivity. For this reason, tremendous effort is invested to characterize the structural and electrical properties of self-assembled monolayers (SAMs) of peptide helices, e.g. polyalanine (PA) α-helices. In our work, we aim at characterizing the intermolecular interactions that govern the formation of PA-SAM films. For this, we elaborated an empirical potential that models the interaction of two isolated helices using the density functional based tight-binding method. With these potentials, energetically most favored arrangements in SAM films were simulated via a Monte-Carlo approach using the simulated annealing and the Metropolis algorithm. Statistically analyzing the relative positioning of adjacent molecules, we are able to classify the degree of frustration in SAM films. For enantiopure systems, we found that a frustration-free arrangement is possible yielding a perfect hexagonal lattice. For mixtures of different chiralities, parallel aligned domains of differently handed helices were obtained. Both of these observations are in great agreement to experimental works.

DS 13.8 Thu 18:00 P1

Thin films of atomically precise chiral bismuth oxido nanoclusters — •Dominik Hornig[1], Rico Thomas[1], Annika Morgenstern[2], Franziska Schölzel[2], Thi Ngoc Ha Nguyen[2], Christoph Tegenkamp[2], Georgeta Salvan[2], and Michael Mehring[1] — [1]TU Chemnitz, Institute of Chemistry, Germany — [2]TU Chemnitz, Institute of Physics, Germany

The adsorption of chiral molecules on metallic surfaces induces electron spin polarization at the interface, enabling novel applications in chiral opto-spintronics. This effect, known as chiral-induced spin selectivity (CISS), strongly depends on the binding and ordering of the species on surfaces.[1] In our studies, we investigate the adsorption behavior of chiral bismuth oxido nanoclusters (BiO-NCs) on gold (Au) surfaces. The chiral BiO-NCs represent monodisperse nanoclusters which can be modulated by an exchangeable ligand shell. This has been demonstrated for the stable $[Bi_{38}O_{45}]$ cluster architecture and enables targeted modification of the BiO-NC with regard to optical properties.[2,3] By functionalizing BiO-NCs with amino acids such as Boc-L-methionine and Boc-L-phenylalanine, the chiral nanoclusters $[Bi_{38}O_{45}(Boc\text{-}L\text{-}Met\text{-}O)_{24}]$ or $[Bi_{38}O_{45}(Boc\text{-}L\text{-}Phe\text{-}O)_{24}]$ were synthesized. Furthermore, tuning of physical properties is possible by doping these atomically precise nanoclusters with other metals. Here we present the preparation of thin films of atomically precise chiral BiO-NCs and results of ellipsometry, UV-Vis, STM and STS measurements. [1] Nat. Rev. Chem. 2019, 3, 250-260. [2] Langmuir 2024, 40, 16320-16329.[3] Nanomaterials 2022, 12, 1815.

DS 13.9 Thu 18:00 P1

Twist angle dependent proximity induced spin-orbit-coupling in graphene/NbSe2 heterostructures — •Thomas Naimer[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Pavol Jozef Safarik University in Kosice, 04001 Kosice, Slovakia

We investigate the effect of the twist angle on the proximity spin-orbit coupling (SOC) in graphene/niobium diselenide (Gr/NbSe2) heterostructures from first principles. The low energy Dirac cones of several different commensurate twisted supercells are fitted to a model Hamiltonian, allowing us to analyze the twist-angle dependency of the SOC in detail. This reveals the possibility to triple the Rashba SOC, when going from 0° to 30° twist angle. Furthermore, at a critical twist angle of 23° the in-plane spin structure acquires a significant radial component, enabling collinear charge-to-spin conversion. Analyzing the Dirac cone with respect to allowed Umklapp processes and orbital decomposition shines light on the observed twist angle dependencies. In addition we evaluate the potential for (collinear and perpendicular) charge-to-spin conversion in such heterostructures within linear response theory. All authors acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH. T. N. and J. F. were also supported by the European Union Horizon 2020 Research and Innovation Program 881603 (Graphene Flagship). M.G. acknowledges additional financial support provided by the Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114 and Slovak Academy of Sciences project IMPULZ IM-2021-42.

DS 13.10 Thu 18:00 P1

Wet-Chemical Transfer and Post Characterization of Hexagonal Boron Nitride Grown on Ge(001)/Si Substrates — •Monika Choudhary[1], Max Franck[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP-Leibniz-Institut für Innovative Mikroelektronik, Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

This study presents a poly (methyl methacrylate) (PMMA) assisted transfer process for hexagonal boron nitride (hBN) epitaxially grown on Ge(001)/Si substrates via chemical vapor deposition using borazine at 900-980°C. The transfer involves sequential etching of Si at 95°C in KOH solution [1] and of Ge in NH4OH, H2O2, and H2O solution (1/1/5) at 75°C [2]. The PMMA/hBN is then transferred onto SiO2/Si and TiN/Si substrates, confirmed by optical microscopy, Raman and X-ray photoelectron spectroscopy analyses. Furthermore, metal-insulator-metal devices are fabricated by gold deposition on hBN/TiN, yielding a resistivity of 5.1e-10 ohm*cm and a dielectric constant of 2.4, as determined by current-voltage and capacitance-voltage measurements. Additionally, hBN/graphene/hBN heterostructures are fabricated and characterized using optical microscopy and Raman analyses. Hall bar devices are then created by defining structures on the hBN/graphene/hBN stack using photolithography and reactive ion etching.

[1] P. Pal, et al. Micro and Nano Systems Letters 9 (2021):4. [2] S. Sioncke, et al. Solid State Phenomena 145-146 (2009):203-206.

DS 13.11 Thu 18:00 P1

Tuning the electronic structure of MoSe2 through molecular adsorbates — •Carolin Sabrina Schüle, Joschua Büble, and Heiko Peisert — Institut für Physikalische und Theoretische Chemie Universität Tübingen, Deutschland

Layered transition metal dichalcogenides have emerged as a promising alternative to conventional semiconductor materials. The electronic properties of TMDCs can be tuned by the adsorption of molecules, including weakly interacting, physisorbed carbon molecules. As example, a quenching of the low-temperature defect photoluminescence of MoS2 was observed after adsorption of metal-phthalocyanines, depending strongly on the central metal atom of the phthalocyanine.1 We studied interface properties of phthalocyanines (CoPc and CoPcF16) on MoSe2 and p-doped MoSe2 as example for comparably weakly interacting molecules, and compare them to HATCN - a strong electron acceptor. For the cobalt phthalocyanines, the exchange of the metal centre has only a small effect on the position of the highest occupied molecular orbital (HOMO), whereas fluorination of the molecular backbone lowers the HOMO considerably. The formation of dipols, interface states, as well as a band bending in the MoSe2 bulk substrates was observed, depending on the molecule under consideration. (1) DOI: 10.1021/jacs.1c07795.

DS 13.12 Thu 18:00 P1

Synthesis of MoS_2 films for electronic and optoelectronic device applications — •Axel Printschler, Md Tarik Hossain, Julian Picker, Christof Neumann, and Andrey Turchanin — Friedrich-Schiller-Universität Jena, Institute of Physical Chemistry, Jena, Deutschland

Transition metal dichalcogenides (TMDs) are a class of 2D materials that have exceptional promise for a wide range of electronic and optoelectronic applications. In particular, TMD-based field-effect transistors (FETs) are continually in the focus of research because of their potential to overcome the limitations of traditional silicon-based devices. To efficiently fabricate FETs based on TMD monolayers, it is crucial to synthesize continues mono- or few layers of these materials on wafer scale and/or enable their growth at a predefined position on the wafer. In this study, we compare different methods for bottom-up synthesis of MoS_2 monolayers and thin films and characterize their properties for device applications. To this end, we employ CVD growth from solid and liquid state precursors as well as MOCVD growth using gaseous precursors. The synthesized films are characterized using complementary spectroscopy and microscopy techniques including optical and atomic force microscopy (AFM), X-ray photoelectron, Raman and photoluminescence (PL) spectroscopy, which is further complemented by electrical and optoelectrical measurements of the microfabricated FET devices.

DS 13.13 Thu 18:00 P1

Conventional and nanoscale NMR investigation of NbSe2 for various temperatures, magnetic field strengths and orientations — •Mokessh Kannah Ciwan[1], Marcel Martin[1], Jakob Nachtigal[1], Yejin Lee[4], Nicola Poccia[2,3], Uri Vool[4], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]Department of Physics, University of Naples Federico II, Naples, Italy — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Niobium diselenide (NbSe2) is a transition metal dichalcogenide (TMD) that has attracted particular interest for decades due to the coexistence/competition of charge density waves (CDW) and the superconducting state in the bulk crystal. To this end, nuclear magnetic resonance (NMR) can be used to measure relaxation times and shifts in the resonance frequency, which reveal how the charge carriers in these phases interact with the nuclei of the host material.

Using conventional NMR, we investigate the electronic behaviour of bulk NbSe2 over a wide range of magnetic field amplitudes and orientations as well as temperatures down to the CDW phase. Additionally, we are working towards nanoscale NMR using nitrogen vacancy (NV) centers in diamond as quantum sensors. This method allows NMR measurements on um-scale exfoliated flake down to the monolayer. In this direction we have already achieved first promising results. Findings from both bulk and flake measurements will be presented.

DS 13.14 Thu 18:00 P1

A Hybrid Organic-hBN Platform for Quantum Sensing — •Xuan-Kai Zhou, Yan-Tung Kong, Ruo-Ming Peng, and Jörg Wrachtrup — Universität Stuttgart, 3. Physikalisches Institut, Allmandring 13, Stuttgart, Deutschland

Optically activated molecular spin qubits are promising candidates for quantum sensing applications due to their customizable molecular design, enabling biocompatibility and close proximity to target environments. However, organic molecules under ambient conditions often suffer from weak emission signals, instability, and degradation caused by solvent evaporation, air exposure, and low resistance to photobleaching during measurements. In this work, we address these challenges by encapsulating organic molecules within two-dimensional hexagonal boron nitride (2D-hBN) rather than diluting them in conventional host organic polymers such as p-terphenyl. This hybrid organic-2D material heterostructure stabilizes the fluorescence of organic molecules, potentially enhancing the performance of optically detected magnetic resonance (ODMR) measurements. Furthermore, this innovative encapsulation method integrates physical chemistry into 2D materials approaching the monolayer limit, significantly advancing sensing capabilities, including surface-sensitive techniques and biocompatible detection strategies.

DS 13.15 Thu 18:00 P1

Towards infrared photodetection with an ultra-low carrier density moiré superconductor — Giorgio Di Battista[1], •Leon G. Schubert[1], Kin Chung Fong[2,3], Andrés Díez-Carlón[1], Kenji Watanabe[4], Takashi Taniguchi[5], and Dmitri K. Efetov[1,6] — [1]Fakultät für Physik, LMU — [2]Department of Physics, Harvard University — [3]Quantum Engineering and Computing Group,

Raytheon BBN Technologies — [4]Research Center for Functional Materials, NIMS, Tsukuba — [5]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba — [6]Munich Center for Quantum Science and Technology (MCQST)

Single-photon detectors (SPDs) offer remarkable capabilities for highly-sensitive detection of electromagnetic radiation. To achieve high performance, state-of-the-art SPDs rely on the photon-induced breaking of Cooper pairs in superconductors (SCs). However, extending SPD capabilities to lower photon energies requires novel SC materials with significantly lower charge carrier densities which offer a larger relative perturbation of the SC state. The moiré superconductor magic-angle twisted bilayer graphene (MATBG) holds great promise with its unprecedentedly low carrier density of $\sim 10^{11}\mathrm{cm}^{-2}$ which is ~ 5 orders of magnitude lower than conventional SCs. We demonstrate a proof-of-principle experiment to detect single near-infrared photons by voltage biasing a MATBG device near its SC phase transition. Our work offers insights on the MATBG-photon interaction and opens new opportunities for developing novel quantum sensors with the potential for single photon detection in the terahertz spectrum.

DS 13.16 Thu 18:00 P1

Qauntum anomalous Hall effect in Cr-doped BST — •Edoardo Tosi[1,2], Gertjan Lippertz[1], Anjana Uday[1], Bibek Bhujel[1], Alexey Taskin[1], Marco Moretti[2], and Yoichi Ando[1] — [1]University of Cologne — [2]Polytechnic University of Milan

The quantum anomalous Hall (QAH) effect in a magnetic topological insulator (TI) represents a new state of matter originating from the interplay between topology and magnetism. The defining characteristics of the QAH ground state are the quantized Hall resistivity and vanishing longitudinal resistivity in the absence of an external magnetic field. Manipulating the QAH state is of great importance in both the understanding of topological quantum physics and the implementation of dissipationless electronics.

To observe the QAH effect, fabrications of thin-film devices are required which allows for tuning the Fermi level across the Dirac point. It is necessary to improve growth conditions for the ternary compound (Bi1-xSbx)2Te3 such that the composition between n-type Bi2Te3 and p-type Sb2Te3 can be almost perfectly compensated. Decreasing the thickness of the MBE grown films, reduces the bulk-to-surface ratio and leads to TI samples where the surface transport is dominating. Doping ultrathin films with Cr allows to obtain the ferromagnetic state, which opens a gap in the surface states, leading to the QAH effect at low temperatures.

In this contribution we report our efforts to realize the QAH effect in the magnetic topological insulator Cr-doped (Bi,Sb)2Te3 (CBST) grown by molecular beam epitaxy (MBE) on an InP substrate.

DS 13.17 Thu 18:00 P1

VO2 oscillator with advanced neuron-like feature originating from blinking filament — •Zhong Wang, Kajal Tiwari, Yishen Xie, Jae-Chun Jeon, Ke Xiao, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle(Saale), Germany

The insulator-metal-transition of VO2 gives rise to the electric oscillation that has extensive applications in neuromorphic computing[1]. Although the oscillation feature is typically stable and deterministic, advanced neuromorphic applications require more complex and adaptive device properties[2]. Here we discover the neuron-like bursting with the non-deterministic separation time in the VO2 thin film-based device, which is only detectable in a narrow temperature range below transition. This feature of VO2 indicates the dynamical process beyond ordinary insulator-metal-transition and capacitive charging. By scanning near-field optical microscopy and modelling, we identify the flipping filament formation in multiple positions as the physical origin of the complex feature observed. Our work unveils the mechanism underlying VO2 oscillator that could assist future device design for neuromorphic computing.

[1] P. Schofield et al., Advanced Materials 35, 2205294 (2023).
[2] S. Kumar et al., Nature Reviews Materials 7, 575 (2022).

DS 13.18 Thu 18:00 P1

Advanced modeling of X-ray reflectivity for metallic multilayer systems with GenX 3 — •Rico Ehrler[1,2] and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Research Center MAIN, D-09126 Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany

X-ray reflectivity (XRR) is a versatile, nondestructive technique for probing thin film systems at grazing incidence, offering insights into layer thickness, roughness, and density. However, due to the inherent phase problem in X-ray techniques, extracting these parameters from the XRR data requires careful sample modeling. Especially for metallic multilayers with a complex microstructure, creating a well parametrized model may be challenging. We explore different modeling approaches using the open-source software "GenX 3"[1] on the example of sputter deposited, magnetic Co/Pt multilayer systems. A simplified model without the complex multilayer structure is found to fit the data surprisingly well, when limiting the XRR to a reasonable range. We then add the actual multilayer, modeled with a damped, periodic function following a graded-interface approach to account for the complex microstructure.[2] Finally, real space transmission electron microscopy (TEM) images are used to motivate and validate the models.

[1] A. Glavic and M. Björck, J. Appl. Cryst., **55**, 1063-1071 (2022)
[2] V. Munteanu et al., J. Appl. Cryst., **57**, 456-469 (2024)

DS 13.19 Thu 18:00 P1

In-Situ XAS study of ZnO and Mn-ZnO thin films — •Sulaiman Al Salem[1,2], Sreeju Sreekantan Nair Lalithambika1[2], Shagun Thakur[3], Simone Techert[1,2,3], and Christian Jooss[3] — [1]Institute of X-ray Physics, University of Göttingen, 37077 Germany — [2]Structural Dynamics in Chemical Systems, Deutsches Elektronen-Synchrotron, DESY, Notkestrasse 85, D-22607, Hamburg, Germany — [3]Institute of Materials Physics, University of Göttingen, 37077 Germany

High-performance catalysts with low overpotential for oxygen evolution reaction (OER) are critical for green energy transition. Transition metal-doped ZnO thin films make it a promising catalyst for efficient OER. Understanding the electronic properties of such materials in a catalytically relevant environment is crucial for tailoring and tuning these materials for OER applications. X-ray Absorption Spectroscopy (XAS) is a powerful spectroscopic technique that is element-selective and environment-sensitive. We present an investigation into the electronic structure of Zinc Oxide (ZnO) and Mn-doped thin films using XAS at the Oxygen K-edge as well as the Zn and Mn L-edges. The XAS spectra, which serve as the basis for further investigation upon Mn-doping, show the characteristic peaks of the elements present in the films. Besides, soft x-ray XAS spectra at in-situ ZnO and Mn-doped ZnO - water interface conditions were measured further to study the electronic structure at catalytically relevant conditions.

DS 13.20 Thu 18:00 P1

Martensitic Transformation in Ultrathin Layered Stacks of $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$ — •Nancy Töws, Pascal Strathkötter, Roland Schubert, Inga Ennen, Judith Bünte, Laila Bondzio, Dario Stierl, and Andreas Hütten — Universität Bielefeld, Dünne Schichten und Physik der Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld, Germany

Magnetic shape memory alloys, such as various Heusler alloys, have been extensively studied over the past decade for their potential in magnetocaloric applications. In the realm of thin-film technology, stacking different Heusler alloys in layered systems offers a microstructural design framework initiated through the interaction of strain fields during the martensitic transformation of the stack*s individual components*.

Here, we present results on the stacking of two well-known FeNi alloys, $Fe_{85}Ni_{15}$ and $Fe_{71}Ni_{29}$, and the resulting physical properties. We report on investigations conducted using structural, magnetic, and thermal methods, alongside findings on the progression of martensitic and austenitic transformations within these distinct layered systems.

*Reference: Ramermann et al., *Nano Scaled Checkerboards: A Long-Range Ordering in NiCoMnAl Magnetic Shape Memory Alloy Thin Films with Martensitic Intercalations,* Appl. Sci. 2022, 12(3), 1748; https://doi.org/10.3390/app12031748.

DS 13.21 Thu 18:00 P1

Structural and electronical investigation of the Electrode/MoS2 interface by electron microscopy and photoemission — •Eric Juriatti, Christoph Späth, Heiko Peisert, and Marcus Scheele — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Tübingen, Germany

In search for new semiconducting devices the group of transition-metal dichalcogenides (TMDCs) like molybdenum disulfide (MoS2) is of increasing scientific interest. The exceptionally unique electronic properties, including the tunability of the band gap by exfoliation, of these layered semiconductors allow further miniaturization of devices like photodetectors, which are promising candidates to fulfill Moore*s law in future applications.

The successful manufacturing of astonishingly fast and responsive TMDC photodetectors contacted by gold electrodes was recently demonstrated. However, the influence of the electrodes on the TMDC/metal interface properties, which would supposedly also affect charge carrier transport in devices, has not been studied in detail so far.

In this study, different metals which are typical electrode materials were deposited as thin films on clean MoS2 bulk crystals to mimic the resulting TMDC/Metal interface. The resulting heterostructure was investigated by X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS). In addition, scanning electron microscopy (SEM) was performed to study the growth of the metals on the TMDC surface.

DS 13.22 Thu 18:00 P1

Transition metal oxide doped ZnO films for electro-synthesis — •Shagun Thakur, Pia Henning, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Germany

Understanding the crystal structure and morphology is crucial for investigating the electrocatalytic activity of inorganic materials. Zinc oxide doped with transition metal oxides are interesting candidates for electro-conversions owing to their unique reactivity. The ZnO crystal exhibits different polarity and surface stability in different crystallographic directions [1][2]. With this aim of producing well-defined ZnO films, we utilized the advancements of thin film technology.

Sputtering is used for growing epitaxial undoped and Mn-doped ZnO thin films with temperature and oxygen control. We will also use pulsed laser deposition which is modified by attaching molecular beam sources to prepare such surfaces with precise fine-doped elements and stoichiometry control. These films will be later compared.

This work presents our ongoing studies on transition metal-doped ZnO thin films, focusing on magnetic dopants and their impact on catalytic activity via sputtering and hybrid PLD systems.

[1] C.-H.P. Sung-Ho Na, First-Principles Study of the Surface of Wurtzite ZnO and ZnS - Implications for Nanostructure Formation, The Journal of the Korean Physical Society, 54 (2009) 5

[2] S. Akhter, K. Lui, H.H. Kung, Comparison of the chemical properties of the zinc-polar, the oxygen-polar, and the nonpolar surfaces of zinc oxide, The Journal of Physical Chemistry, 89 (1985) 1958-1964

DS 13.23 Thu 18:00 P1

Tuning high-T_C ferromagnetism and perpendicular magnetic anisotropy in van der Waals magnet $Cr_{1+\delta}Te_2$ — •Laura Pflügl, Pia Henning, Anna Tschesche, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In recent years, chromium tellurides ($Cr_{1+\delta}Te_2$) have gained significant interest due to their promising characteristics, such as ferromagnetic ground states with tunable transition temperatures and perpendicular magnetic anisotropy (PMA) which open up various possible applications in spintronics [1]. However, the fabrication of high-quality stochiometric and epitaxial $Cr_{1+\delta}Te_2$ thin films is difficult and calls for advanced synthesis techniques. Using a hybrid setup combining pulsed laser deposition for Cr and a molecular beam source for Te, we deposited $Cr_{1+\delta}Te_2$ thin films with precise stoichiometry control [2]. Changes of the magnetism were previously reported in $Cr_{1+\delta}Te_2$ due to extreme air-sensitivity and nonself-limited oxidation [3]. Since our films are epitaxially stabilized on a substrate, they are free from defect introduction and offer air stability by forming a passive surface oxide layer. We will address the ongoing challenges during the growth of this material and put forward effective tuning by varying deposition control parameters.

[1] Y. Fujisawa et al., Phys. Rev. Mater., 4 (2020) 114001.

[2] A. Tschesche, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

[3] A. Coughlin et al., ACS Materials Letters, 5 (2023) 1945-1953.

DS 13.24 Thu 18:00 P1

Investigating interfacial mechanisms and switching behavior in GST-124/Sb_2Te_3 superlattices using Atom Probe Tomography — •Athanasia Piperidou[1], Jan Köttgen[1], Lucas Bothe[2], Lukas Conrads[1], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Chalcogenide-based phase-change materials like $GeSb_2Te_4$ (GST) are crucial for non-volatile storage technologies due to their rapid and reliable switching. Reducing the energy required for transitions between amorphous and crystalline states can improve device performance significantly, as demonstrated in phase-change memories using superlattices (SLs). Here we investigate the switching behavior of MBE-grown 60nm GST-124/Sb_2Te_3 SLs. Using a pulsed laser, we induce amorphization and recrystallization processes. Atom Probe Tomography (APT) is used to compare the structural and chemical characteristics of interfaces in recrystallized and as-deposited regions. APT's three-dimensional, near-atomic resolution reveals changes in morphology and element distribution, shedding light on the mechanisms driving switching. Our results show that the SL structure enhances switching efficiency through unique interfacial mechanisms, offering insights for the design of next-generation memory devices.

DS 13.25 Thu 18:00 P1

Deposition of Medium-Entropy Telluride Thin Films via Hybrid Pulsed Laser Deposition — •Niklas Kohlrautz, Pia Henning, and Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

High- and medium-entropy materials (HEMs and MEMs) are known for their great multifunctional properties, such as ordered magnetism and promising catalytic behavior [1]. Moreover, tellurides are recognized for their novel magnetic properties, including room-temperature ferromagnetism and large magnetic anisotropy, as well as catalytic potential [2][3]. Designing novel high-entropy tellurides opens new possibilities for discovering multifunctional materials. Toward the goal of synthesis of novel HEMs, we fabricated MEM tellurides (FeCrNiTe) via hybrid pulsed laser deposition (PLD). In this presentation, we will address the challenges in growing $(FeCrNi)_xTe$ and the detailed structural and physical characterization. FeCrNiTe films were synthesized on $SrTiO_3(001)$ substrates providing FeCrNi via the standard PLD process and Te through a molecular beam source, allowing easy Te stoichiometry control. Systematic studies of growth parameters yielded high-quality epitaxial thin films with elemental surface homogeneity. We are investigating the magnetic, electric and electrocatalytic properties of the films, comparing the results with the crystal structure.

[1] Z. Zhang et al., Chemical Engineering Journal 2024, 498, 155736.

[2] A. Tschesche et al., R.S., doi.org/10.21203/rs.3.rs-4861088/v1.

[3] N. Oueldna, Materials Horizons 2024, 11(10), 2323-2354.

DS 13.26 Thu 18:00 P1

Thin Film Effects in Ultra-thin, MBE-grown In_2Te_3-Films — •Lucas Bothe[1], Maximilian Buchta[1], Felix Hoff[2], Timo Veslin[2], Christoph Ringkamp[2], Ka Lai Mak[1], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

InSbTe (IST) as an unconventional Phase Change Material is of significant interest in recent years. However, the related binary compound In_2Te_3 is less studied. With its small direct band gap and high absorption coefficient, it is an interesting candidate for e.g. photodetectors.

Here, a thin film series of In_2Te_3 was fabricated employing Molecular Beam Epitaxy (MBE) to achieve highly textured thin films. These films are characterized via XRD, RHEED and Raman spectroscopy. Next to the structural bulk values measured for the thickest In_2Te_3 sample, a decrease in the out-of-plane lattice constant by up to 0.4 A with decreasing film thickness is reported. The in-plane lattice constants however increase for thinner films. This trend with reduced film thickness contrasts known thin-film effects in metavalently bonded materials like Sb_2Te_3 or Bi, as In_2Te_3 is not expected to exhibit metavalency. Furthermore, the structural changes in the thin films are unlikely to arise from strain, given the Te-terminated Si surface promotes van der Waals growth, preventing alignment of the Si and In_2Te_3 in-plane lattice constants.

In addition, thickness-dependent vibrational properties were determined by Raman spectroscopy.

DS 13.27 Thu 18:00 P1

The interface wz-GaN/rs-ScN studied by depth profiling photoelectron spectroscopy — Fabian Ullmann[1,2] and •Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

Theoretical predictions show extreme high polarization gradients and polarization-induced surface charge densities at interfaces of rock salt ScN and wurtzite GaN.

Experimental investigation were made by depth profiling X-ray photoelectron spectroscopy (XPS) along the interface of rs-ScN and wz-GaN grown by molecular beam epitaxy (MBE).

DS 13.28 Thu 18:00 P1

Deposition of Cr self-intercalated $Cr_{1+\delta}Te_2$ thin films by Hybrid Pulsed Laser Deposition — •Pia Henning, Laura Pflügl, Anna Tschesche, Tobias Meyer, and Jasnamol Palakkal — Institute of Material Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

$Cr_{1+\delta}Te_2$ thin films exhibited an increased interest over the last few years, due to their tunable magnetic anisotropy and ferromagnetism with T_C ranging from 150 K to 350 K [1]. This tunability of magnetic properties is sensitively linked to the stoichiometry, governed by the self-intercalation of Cr species between $CrTe_2$ layers [1]. Therefore, the sensitive control of δ in addition with the insurance of high crystalline quality, with epitaxial and low defect growth, is crucial for a profound discussion and comparison of thin film properties. In this work, we used a hybrid pulsed laser deposition (PLD) unit attached with Te molecular beam source for growing high quality $Cr_{1+\delta}Te_2$ thin films [1]. We studied the influences of different growth parameter settings on the thin film quality and properties. We were able to carefully modify the δ and thickness of the films and investigated their correlation with the magnetic and electronic properties. This material system is a promising candidate for spintronics application due to room temperature ferromagnetism, anisotropic magnetoresistance and huge perpendicular magnetic anisotropy. Our findings manifest the advantages of this technique for depositing further novel transition metal chalcogenides. [1] A. Tschesche, P. Henning, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

DS 13.29 Thu 18:00 P1

Investigating Lateral Molecular Heterogeneity with Phase-Resolved Vibrational SFG Microscopy — •Ben John, Alexander P. Fellows, Tuhin Khan, Martin Wolf, and Martin Thämer — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Understanding molecular heterogeneity at interfaces is crucial for applications in fields such as biophysics and materials science. Systems like lipid rafts in biological membranes or functionalized surfaces in microfluidics require techniques capable of resolving molecular structures, orientations, and compositions with high sensitivity and spatial resolution. Phase-resolved vibrational sum-frequency generation (vSFG) microscopy has emerged as a powerful tool to meet these needs, offering vibrational specificity, orientational sensitivity via second-order selection rules, and sub-micron spatial resolution through frequency up-conversion. Despite its potential, traditional vSFG microscopy has faced significant technical challenges in detecting weak signals from monolayers and spatially mapping them. We address these limitations with an advanced phase-resolved vSFG microscope, which achieves improved signal-to-noise ratios and spatial resolution. Using this system, we successfully image phase-separated monolayers of mixed chiral lipids, revealing spatial heterogeneity in molecular orientations and packing structures. This breakthrough positions phase-resolved vSFG microscopy as a transformative approach for characterizing interfacial molecular systems, enabling deeper insights into the complex behaviors of molecular assemblies in both natural and engineered environments.

DS 13.30 Thu 18:00 P1

Structural and optical properties of β-Ga_2O_3 thin films obtained by spray pyrolysis — •Polina Shamrovska[1,2], Oleksandr Selyshchev[1], Narmina Balayeva[1], Volodymyr Kudin[2], and Dietrich Zahn[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

β-Ga_2O_3 thin films have gained significant research interest due to their wide bandgap, high thermal stability and breakdown voltage, making them suitable *e.g.* for UV photodetectors. Here, β-Ga_2O_3 thin films were deposited on c-plane sapphire substrates via spray pyrolysis, a cost-effective technique suitable for large-scale production. For deposition, we used $Ga(NO_3)_3$ dissolved in a 1 : 1 water-ethanol mixture or water with 1% polyethyleneimine, followed by annealing at 800 °C or 1000 °C. The films were characterized by SEM, AFM, Raman, XRD, spectroscopic ellipsometry, UV-vis spectroscopy, and electrical resistance measurements by the four-point probe.

The stoichiometric β-phase Ga_2O_3 films revealed a preferred $(\bar{2}01)$ orientation in agreement with previous results [1]. The samples showed transparency of up to 99% in the visible range and a sharp absorption edge in the UV range with bandgaps of 4.9 to 5.3 eV. The resistivity of the films was in the GΩ range. The results obtained reveal that spray pyrolysis allows the fabrication of highly crystalline, transparent, and high-resistive β-Ga_2O_3 films suitable for further studies as UV photodetectors.

[1] Akazawa, Housei, Vacuum, 2016, 123: 8-16.

DS 13.31 Thu 18:00 P1

"Green" Aqueous Synthesis and Characterization of Cu_2NiSnS_4 and Cu_2ZnSnS_4 Nanocrystal Thin Films — •Oleksandra Ivakhno-Tsehelnyk[1], Oleksandr Selyshchev[1], Serhiy Kondratenko[2], Volodymyr Dzhagan[3], Lukas Hertling[1], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes, Chemnitz University of Technology, 09107 Chemnitz, Germany. — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine. — [3]Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 03038 Kyiv, Ukraine.

We investigated thin films of Cu_2NiSnS_4 (CNTS) and Cu_2ZnSnS_4 (CZTS) nanocrystals (NCs) obtained by "green" colloidal synthesis [1,2]. This synthesis approach provides a way to non-toxic and scalable production for sustainable and low-cost light-absorbing nanomaterials. To assess the potential of thin films of these NCs for photovoltaic and other possible applications, electrical studies are necessary. Colloidal NCs were deposited on glass substrates by spin coating and annealed at temperatures starting from 180 °C to obtain conductive thin films. Analytical techniques such as Raman spectroscopy, AFM, XRD, spectroscopic ellipsometry, and 4-point probe measurements were used to characterize their structural, optical, and electrical properties. We discuss the optical and electrical differences related to Zn-to-Ni substitution in the NC structure and establish the correlation between electrical properties of the films and elemental composition in both colloidal NCs and annealed films.

DS 13.32 Thu 18:00 P1

An in-situ μGISAXS growth study of CoFeB thin film on ion beam sculptured Si template — •Vishnu Narayan Manoj Kumar[1], Praveen Kumar Dubey[2], Prasanta Karmakar[3], Kristian A Reck[4], Benedikt Sochor[1], Yusuf Bulut[1], Thomas Strunskus[4,5], Franz Faupel[4,5], Stephan V Roth[1,6], Peter Müller Buschbaum[7], Ajay Gupta[2], and Sarathlal Koyiloth Vayalil[1,2] — [1]DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]UPES, Bidholi, Dehradun, India-248007 — [3]VECC, 1/AF, Bidhannagar, Kolkata -700064, India — [4]Chair for Multicomponent Materials, Department of Materials Science, Kiel University Kaiserstr. 2, 24143 Kiel, Germany — [5]Kiel Nano, Surface, and Interface Science, KiNSIS, Kiel University, Christian-Albrechts Platz 4, 24118 Kiel, Germany — [6]Division of Coating Technology, KTH Royal Institute of Technology, Teknikringen 48, 100 44 Stockholm, Sweden — [7]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, Garching 85748, Germany

In this work, the growth and structural evolution of CoFeB thin films deposited on nanopatterned Si templates prepared by N_2^+ ion beam irradiation has been done using in-situ micro GISAXS. Different growth regimes have been identified using appropriate growth models. Thin film is found to replicate the sawtooth ripple geometry of the templates up to a large extent of film thickness near 15nm. Strong uniaxial magnetic anisotropy has been observed in this system. Direction of magnetic easy axis is found to be changing with annealing.

DS 13.33 Thu 18:00 P1

Structure evolution of multi-component Ti-Nb-Zr-based thin films with Ag addition during heat treatment — •Anna Benediktová, Lucie Nedvědová, Zdeněk Jansa, Palaniappan Subramanian, Michal Procházka, and Ján Minár — University of West Bohemia, Pilsen, Czech Republic

Multicomponent and high-entropy alloys represent an intensively studied group of materials. Due to their potential to be chemically and structurally very stable, wear resistant and hard, they have also become the subject of study as biomaterials. Conventional metallic biomaterials usually have many disadvantages, including inadequate antibacterial properties leading to infections and possible implant loss. To improve the surface properties, thin films with different amounts of silver as an antibacterial agent were prepared by magnetron sputtering. Their structure in the as-deposited state and the evolution of the structure during heat treatment were analyzed in detail by diffraction techniques (XRD, SAED) and by scanning and transmission electron microscopy (SEM, TEM). The chemical states of the surface were investigated by X-ray photoelectron spectroscopy (XPS). The chemical stability of the films in phosphate buffered solution (pH ~ 7.4) was evaluated by electrochemical methods such as potentiodynamic polarization and electrochemical impedance spectroscopy.

DS 13.34 Thu 18:00 P1

Microscale Domain Structures in AlScN Thin Films — •Ella Dieball[1], Nicolas Hayen[1], Otto Lippmann[1,3], Philipp Jordt[1], Niklas Wolff[2], Lorenz Kienle[2], Fabian Westermeier[4], Michael Sprung[4], and Bridget Murphy[1,4,5] — [1]Institute of Experimental and Applied Physics, Kiel University, Germany — [2]Institute of Material Sciences, Kiel University, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [5]Ruprecht Haensel Laboratory, Hamburg, Germany

Thin films of Aluminium-Scandium Nitride (AlScN) are used as central components in magnetoelectric surface-acoustic wave sensors utilized extensively within the Collaborative Research Center 1261 "Biomagnetic Sensing".

High resolution XRD experiments were conducted at microfocus beamline P10 at PETRA III. Bragg diffraction on AlScN thin films grown on GaN was investigated at the [0 0 0 2], [0 0 0 4] and [0 1 -1 5] reflections. The material exhibits an unexpected domain structure on the μm scale, which is associated with Scandium-rich and Scandium-depleted regions.

Additional synchrotron experiments are in planning to further investigate AlScN, e.g. grazing incidence diffraction or absorption measurements around the Scandium K-edge.

DS 13.35 Thu 18:00 P1

In Operando Grazing Incidence Diffraction in AlScN Surface Acoustic Wave Sensors — •Otto Carlos Lippmann[1,2], Nicolas Hayen[1], Philipp Jordt[1], Jana Meyer[5], Fabian Lofink[5], Henrik Wolframm[4], Didier Wermeille[7], Laurence Bouchenoire[7], Florian Bertram[3], and Bridget Murphy[1,3,6] — [1]Institute of Experimental and Applied Physics, Kiel, Germany — [2]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [3]Deutches Elektronen Synchrotron, DESY, Hamburg, Germany — [4]Faculty of Engineering, Kiel, Germay — [5]Fraunhofer Institute for Silicon Technology ISIT, Itzehoe, Germany — [6]Ruprecht-Haensel Laboratory, Hamburg, Germany — [7]European Synchrotron Radiation Facility, Grenoble, France

Magnetic field sensors based on thin-film surface acoustic wave (SAW) technology are widely utilized in Collaborative Research Center 1261 "Biomagnetic Sensing". The use of Aluminium-Scandium-Nitride (AlScN) as the piezoelectric material allows for significant improvements in device sensitivity.

To investigate the microstructure of AlScN during the excitation of acoustic modes, an *in operando* setup was developed for high-resolution X-ray diffraction (XRD). This setup induces standing waves and allows the observation of diffraction patterns. A comparison of grazing-incidence diffraction (GID) of the [0 1 3] Bragg reflection between the stationary and operating state shows a shift in the signal peak position. Additional experiments are planned, along with the development of a new setup for time-resolved experiments. These efforts aim to enhance the understanding of SAW propagation in these materials.

DS 13.36 Thu 18:00 P1

Deterministic single ion-implantation of Er into thin film lithium niobate — •Maranatha Andalis, Reiner Schneider, and Klaus D. Jöns — Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP) and Department of Physics, Paderborn University, 33098 Paderborn, Germany

Incorporating rare earth ions (REIs) into lithium niobate-on insulators (LNOI) is of great interest in scalable photonic integrated circuits (PIC), enhancing the potential of LNOI with added functionalities enabled by the REIs. Erbium ions can be incorporated into LNOI using ion implantation and implemented at telecom wavelengths. Together with Ionoptika Ltd., we have customized a single ion implantation system called Q-One with up to 40 kV acceleration voltage. For most quantum applications, the site-selective implantation of a single REI is required. Our results show single Er ion implantation into LNOI with 85% efficiency using secondary electron emission detection. The Q-One single ion implanter, with its high-resolution mass-filtered focused ion beam, nanometer-precision stage, and choice of ion source, holds significant potential in deterministic ion implantation, crucial for scalable quantum technologies with REIs.

DS 13.37 Thu 18:00 P1

Impact of ITO electrodes on the electrical and optical properties of a smart window — •Rebecca Cizek[1], Florian Sutter[1], Stephan Heise[1], Kai Gehrke[2], Eckhard Lüpfert[1], and Robert Pitz-Paal[1] — [1]German Aerospace Center, Institute of Solar Research, Oldenburg, Almería, Köln, Germany — [2]German Aerospace Center, Institute of Networked Energy Systems, Oldenburg, Germany

This study investigates the impact of indium tin oxide (ITO) electrodes on the performance of smart windows utilizing reversible metal electrodeposition (RME). RME is a promising technique for fabricating electrochromic devices, offering dynamic control over light transmission. ITO electrodes, known for their high conductivity and transparency, play a critical role in facilitating the electrochemical processes that govern the reversible metal deposition and dissolution on the window surface. The effects of ITO electrode characteristics, such as conductivity, surface morphology, and transparency, are explored in relation to the electric and optical performance of the smart window. Long-term measurements are conducted with voltage applied over several hours to assess the durability and performance of the electrodes under operation.

DS 13.38 Thu 18:00 P1

Antibacterial activity of ZnO and Al doped ZnO nanocoatings — •Maria Stefanova[1], Dimitrina Petrova[1,2], Vladimira Videva[1], Dimitre Dimitrov[1,3], Nadia Todorova[4], and Vera Marinova[1] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]South-West University Neofit Rilski, Blagoevgrad, Bulgaria — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research Demokritos, Athens, Greece

Here we report on thin coatings of metal oxides (ZnO and ZnO doped with Al (AZO)) deposited by ALD technology. Their structural, surface-morphological and optical properties were investigated by AFM analysis, UV-Vis and fluorescence spectroscopy, as well as surface contact angle measurements. The antibacterial activity against Escherichia coli bacteria was evaluated in the dark and under ultraviolet light illumination. AZO nanocoatings were found to demonstrate more effective antibacterial action, mostly due to the improved sensitivity at UV spectral range as well as hydrophilicity in comparison with ZnO. The studied nanocoatings can serve as effective antimicrobial agents in a variety of applications.

Acknowledgements: This work is supported by the Bulgarian National Science Fund under the grant number KP-06-N-58/12 and the Research equipment of distributed research infrastructure INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science.

DS 13.39 Thu 18:00 P1

Chiral Induced Spin Selectivity Cooling — •Ohad Golan[1], Yossi Paltiel[1], and Ron Naaman[2] — [1]Hebrew University of Jerusalem, Jerusalem, Israel — [2]Weizmann Institute of Science, Rehovot, Israel

Chiral Induced Spin Selectivity (CISS) is a quantum phenomenon in which electron spins become selectively polarized as they pass through chiral materials. This effect enhances spin-dependent interactions without the need for external magnetic fields, playing a crucial role in various spintronic and chemical processes. Building on this principle, the Chiral Induced Spin Selectivity Cooling (CISSCO) effect exploits CISS to generate a temperature gradient across chiral materials. When current flows through a chiral system from a source to a drain, spin alignment at the source increases local entropy, leading to heating, while spin randomization at the drain reduces entropy, resulting in cooling. Unlike conventional thermoelectric and magnetocaloric effects, CISSCO requires no magnetic materials, enabling efficient and highly localized cooling. This groundbreaking mechanism has the potential to transform nanoscale heat management, offering an innovative solution for cooling micro- and submicron electronic devices.

DS 13.40 Thu 18:00 P1

NaCl-assisted TAC synthesis of MoSe2 films for optical humidity sensor applications — •Blagovest Napoleonov[1], Katerina Lazarova[1], Dimitrina Petrova[1,2], Vladimira Videva[1,3], Dimitre Dimitrov[1,4], and Vera Marinova[1] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]South-West University Neofit Rilski, Blagoevgrad, Bulgaria — [3]Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria — [4]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

We present the synthesis of MoSe2 through the Thermal Assisted Conversion (TAC) method with Mo liquid precursor solution composed of MoO3 dissolved in a 1:1 mixture of H2O and H2O2, with NaCl as an additive. The precursor solution enables controlled delivery of Mo during the TAC growth. The presence of NaCl influences the growth kinetics and crystallization during the annealing step. Raman spectroscopy, TEM, AFM and XPS measurements were employed for comprehensive material characterization, revealing the effectiveness of this precursor combination in synthesizing high-quality MoSe2 films. Based on optical reflectance measurements, the MoSe2 films demonstrate sensitivity to relative humidity changes by reflectance variation. These results led to the development of an optical humidity sensor, showcasing the material's potential in sensor applications. Acknowledgements: This work is supported by the Bulgarian Science Fund under the grant number KP-06-COST/15 under the COST Action CA20116 OPERA European Network for Innovative and Advanced Epitaxy.

DS 13.41 Thu 18:00 P1

Functionalization of Al-doped ZnO nanolayers for display applications — •Stefani Bogoeva[1], Vladimira Videva[1], Dimitrina Petrova[1,2], Vera Marinova[1], and Dimitre Dimitrov[1,3] — [1]Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]Faculty of Engineering, South-West University, 2700 Blagoevgrad, BG — [3]Institute of Solid State Physics, BAS, 1784 Sofia, BG

The integration of highly transparent and conductive thin films into functional structures and devices plays an important role in the advancement of next-generation technologies. Here we report about Aluminum doped ZnO (AZO) thin films synthesized on different substrates using the atomic layer deposition (ALD) technique, which allows excellent conformality. The effect of post-deposition treatments on the optical and electrical properties of the films was studied using variety of characterization techniques.

Based on the above characteristics, integration of AZO layers in liquid crystal (LC) devices and Polymer Dispersed Liquid crystals (PDLC) structures are demonstrated, with measured electro-optical characteristics and response time. Implementation of AZO layers opens prospective applications for future ITO-free optoelectronics.

Acknowledgments The research was supported by the Scientific Research Fund project No. KP-06-*-58/12, as well as the distributed scientific infrastructure INFRAMAT, part of the National Roadmap of Bulgaria for scientific infrastructure, financially supported by the Ministry of Education and Science.

DS 13.42 Thu 18:00 P1

A high-field, high power instrument for (nonlinear) Terahertz Emission Spectroscopy — •Jonas Woeste[1,2], Nikola Stojanovic[2], Sergey Pavlov[2], Sergey Kovalev[3], and Michael Gensch[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany — [2]DLR - Institute of Optical Sensor Systems, Berlin, Germany — [3]Fakultät Physik, Technische Universität Dortmund, Dortmund, Germany

The quest to understand nonlinear terahertz phenomena has driven the development of advanced instruments towards the capability to detect faint terahertz transients with sub-cycle time resolution. The instrument presented here is optimized for a mJ-level laser amplifier operating at kHz repetition rates. It generates high-field THz pulses with peak fields of a few 100 kV/cm spanning frequencies from 0.3-1 THz. Using ultrashort NIR pulses for tilted-pulse-front pumping of a lithium-niobate crystal, pulse energies of up to 5 μJ are achieved. Demonstration experiments include studies on various doped semiconductors, graphene, and chip-integrated Dirac materials giving insights into different nonlinear and non-perturbative quantum phenomena.

DS 13.43 Thu 18:00 P1

Techno-Enviro-Economic Evaluation for Thin-film Solar Cells Integrated with Hybrid Renewable Energy System — •Tawfik Hussein — Mechanical Engineering Dep., National Research Centre (NRC), El Buhouth st.,Dokki, Cairo, Egypt

Thin-film solar cells (TFSC) have surfaced as a potentially viable substitute in recent years. TFSC have emerged as a transformative technology in the renewable energy sector, offering unique advantages such as lightweight construction, flexibility, and cost-effectiveness compared to conventional crystalline silicon photovoltaics.

The main objective of this study is to design an optimal hybrid renewable energy system (HRES) integrating TFSC in order to achieve efficient use of the available renewable energy sources (RES). Therefore, a HRES consisting of different RES integrated with TFSC is proposed to cover reliable electricity to a scientific farm in Egypt with technical, environmental, and economic evaluation. The research highlights the performance of TFSC under varying environmental conditions, emphasizing their superior efficiency in low-light and high-temperature scenarios. All the parameters, such as system performance, net present cost, and carbon emissions, are considered.

The results showed that the proposed TFSC delivers highly efficient energy generation at significantly lower costs compared to traditional configurations. From an environmental perspective, it achieves a significant reduction in carbon emissions and demonstrates improved sustainability.

DS 13.44 Thu 18:00 P1

Molecular packing and alignment of prototypical acenes in organic 2D-material heterostructures — •Jan Vincent Schreiber and Gregor Witte — Philipps-Universität Marburg, Molekulare Festkörperphysik, 35032 Marburg, Germany

Heterostructures comprised of thin films of organic molecules and two-dimensional materials, notably monolayers of transition metal dichalcogenides, are emerging as a promising class of systems for applications in organic electronics. Unlike metallic surfaces, two-dimensional materials interact with adsorbates primarily through van der Waals forces, resulting in substrate-adsorbate interactions comparable in strength to intermolecular forces. This delicate balance means that even minor variations in surface characteristics or growth conditions can significantly affect the relative molecular alignment. A systematic investigation of the molecular model systems pentacene and 5,7,12,14-pentacenetetrone allows comparison of the influence of electrostatic forces on the film alignment. Techniques ranging from scanning tunnelling microscopy to optical polarisation microscopy highlight the necessity of understanding these interactions across multiple length scales. We demonstrate that for most substrates, specific molecular orientations optimize the system's structural energy, a phenomenon known as van der Waals epitaxy. Our findings emphasize the need for rigorous structural studies to unravel the interplay between molecular structure and substrate properties.

DS 13.45 Thu 18:00 P1

Spectroscopy of organic dye/TMDC heterostructures — •Christoph von der Oelsnitz[1,2], Julian Schröer[1,2], Tim Völzer[1,2], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]Institut für Physik, Universität Rostock, Albert-Einstein-Straße 23, 18059 Rostock, Deutschland — [2]Department LL&M, Albert-Einstein-Straße 25, 18059 Rostock, Deutschland

Heterostructures composed of organic molecules adsorbed onto transition metal dichalcogenide (TMDC) monolayers can exhibit charge separation after optical excitation, making these systems promising candidates for optoelectronic applications. In this study, we investigate heterostructures consisting of the organic dyes copper phthalocyanine (CuPc) and 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) deposited onto TMDC monolayers and hexagonal boron nitride (hBN), with the latter serving as a non-interacting reference system. First, the preparation of the dye layers via thermal vapor deposition was calibrated and performed. Subsequently, we investigated the dye/TMDC and dye/hBN heterostructures using various spectroscopic methods. In the event of charge separation in the dye/TMDC system, photoluminescence quenching of the dye is expected.

DS 13.46 Thu 18:00 P1

Substrate-driven Molecular Orientation of BQQDI-based Organic Thin Films — •Jeya Vishva Jeyaraj Pandian and Gregor Witte — Philipps-Universität Marburg, FB Physik

Thin films of PhC_2-BQQDI, a high-performance n-type organic semiconductor, exhibit preferential molecular orientations depending on the substrate. On weakly-interacting amorphous SiO_2 substrates, the molecules adopt an upright orientation. Furthermore, a co-existence of thin-film phase was observed depending on the growth parameters, which is characterised by the increased molecular tilt angle with respect to the surface of the substrate. Notably, a domination of thin-film phase was observed at elevated temperatures. This phenomenon contradicts a commonly observed growth behaviour in organic thin films, whereby bulk phase prevails under such growth conditions. However, post-deposition annealing results in a transition from thin-film phase into bulk phase with significant dewetting. In contrast to SiO_2, on surfaces of alkali halides such as KCl, the molecules exhibit a recumbent orientation. Furthermore, an epitaxial growth was observed, driven by the templating effect of the underlying substrate. These findings pave the way for a phase-selective preparation of thin films of PhC_2-BQQDI which can be used to deepen the understanding of electronic transport in devices based on PhC_2-BQQDI.

DS 13.47 Thu 18:00 P1

The influence of stoichiometry on molybdenum oxide-based memristors — •Katerina Maskanaki[1], Gion Kalemai[2,3], Evangelos K. Evangelou[1], and Anastasia Soultati[2] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Institute of Nanoscience and Nanotechnology (INN), National Center for Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece — [3]Department of Physics, University of Patras, 26504 Patra, Rio, Greece

Transition metal oxides (TMOs) are a promising class of materials for neuromorphic computing and processing systems demonstrating a variety of resistive switching (RS) mechanisms. However, little is known about the correlation between its stoichiometry and RS. This study is focused on the development and characterization of molybdenum oxide memristors with different stoichiometry. Both, fully-stoichiometric (MoO_3) and sub-stoichiometric (MoO_{3-x}) molybdenum oxide devices showed good resistive switching behavior. However, the stoichiometric memristor exhibited better RS properties with endurance of 250 cycles, ON/OFF ratio > 10^2 and high retention of 2×10^4 s, compared to the poor RS behavior of the device based on the MoO_{3-x} film. This impressive memristive behavior could be attributed to the excess of oxygen vacancies in the case of fully-stoichiometric memristor in respect to the sub-stoichiometric MoO_{3-x} which play crucial role in the conductive behavior of the device. The high reproducibility observed in MoO_3-based memristor highlights their potential for practical applications and scalability.

DS 13.48 Thu 18:00 P1

In and ex situ detection of oxygen vacancies in HfO2 - advanced by PLD growth control and (HAX)PES spectroscopy — •Berk Yildirim[1], Seema Seema[1], Oliver Rehm[1], Pia Düring[1], Andreas Fuhrberg[1], Andrei Gloskovskii[2], Christoph Schlueter[2], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]DESY, Hamburg, Germany

Hafnium dioxide (HfO2) has emerged as a promising ferroelectric material, particularly suitable for non-volatile memory devices. Ferroelectricity in HfO2 is closely linked to oxygen vacancies (OV), but their direct experimental observation is challenging. This study uses tailored growth conditions to systematically control the OV concentration in HfO2 thin films as an essential prerequisite for their in and ex situ detection. In our pulsed laser deposition (PLD) system, parameters such as temperature, laser fluence, and oxygen partial pressure were varied to prepare HfO2 thin films with defined OV concentrations. In situ X-ray photoelectron spectroscopy (XPS) and ex situ hard X-ray photoelectron spectroscopy (HAXPES) provided detailed insight into OV distribution with different depths sensitivity, while structural properties were examined by in situ RHEED and ex situ X-ray diffraction (XRD) as well as atomic force microscopy (AFM). In and ex situ (HAX)PES analysis indicates a direct relationship between oxygen supply and the OV content via analysis of the Hf3+/Hf4+ spectral weight. In addition, the structural analysis points towards a systematic dependence between the onset of epitaxy and oxygen supply.

DS 13.49 Thu 18:00 P1

Oxygen vacancy mediated epitaxial superstructure thin film in tungsten sub-oxides — •Kyeong Jun Lee[1], Hyowon Seo[2], Yeong Gwang Kim[2], Yong-Jun Kwon[3], Bongju Kim[1], Minu Kim[1], Chan Ho Yang[3], Hyun Hwi Lee[4], Sangyoun Park[4], Gyungtae Kim[5], Jung-ho Kim[6], Young Jun Chang[2], and Seo Hyoung Chang[1] — [1]Department of Physics, Chung-Ang University, Seoul 06974, South Korea — [2]Department of Physics, University of Seoul, Seoul 02504, South Korea — [3]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, South Korea — [4]Pohang Accelerator Laboratory, POSTECH, Pohang 37673, South Korea — [5]National NanoFab Center, Daejeon 34141, South Korea — [6]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA

In metal oxides, oxygen vacancies are key to enhancing energy conversion and unconventional properties. Crystallographic shear (CS) planes in these structures are vital for electrochemical electrodes. While powders and polycrystals are well studied, research on single crystals or epitaxial films is essential to link oxygen vacancies with electronic and crystal structures. We fabricated epitaxial {103} CS superstructures in tungsten sub-oxides (Magnéli phases) on NdGaO3 (110)o substrates. X-ray scattering, AFM, and TEM confirmed epitaxial growth. W L3 RIXS revealed W6+ 5d0 and W6+ 5d1 states, showing oxygen vacancies' role in mediating superstructures and electronic properties.

DS 13.50 Thu 18:00 P1

Electronic structure of the TiO2/AlInP heterointerface studied by photoemission spectroscopy — •Mohammad Amin Zare Pour[1,2], Sahar Shekarabi[1], Jonathan Diederich[3], Negin Mogharehabed[2], Christian Höhn[3], Wolfram Jaegermann[4], Dennis Friedrich[3], Roel van de Krol[3], Agnieszka Paszuk[2], and Thomas Hannappel[1] — [1]Grundlagen von Energiematerialien, Technische Universität Ilmenau — [2]Paszuk group, Technische Universität Ilmenau — [3]Institut für solare Brennstoffe, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [4]Fachgebiet Oberflächenforschung, Technische Universität Darmstadt

Many world-record photoelectrochemical cells use AlInP as a window layer for selective electron transport passivated with TiO2, which is stable in electrolytes. The electronic and atomic properties of the TiO2/AlInP heterointerface in dependence to AlInP surface terminations to were examined. TiO2 was deposited by atomic layer deposition on various AlInP surface reconstructions and the TiO2/AlInP interface band diagram was experimentally examined. XPS/UPS studies reveal that TiO2 deposition reduces AlInP band bending, while remaining surface states pin the fermi level and still induce band bending towards the interface. Based on AlInP surface reconstruction, the valence band offset ranges from 1.7 to 1.9 eV. The presence of an oxide layer hinders the growth of TiO2 relative to clean surfaces. AlInP window layers are prevalent in III-V heterostructures, therefore mapping the TiO2/AlInP interface's electrical properties can optimize photoelectrochemical interfaces and more.

DS 13.51 Thu 18:00 P1

Resonance Raman and DFT analysis of structural and point defects in transparent conductive oxide SnO2:X (X=Ta, F) — •Lukas Prager[1], Carlos Romero Muñiz[2], Frans Munnik[1], Justus Haag[1], Ramon Escobar Galindo[3], and Matthias Krause[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Departamento de Física de la Materia Condensada, Universidad de Sevilla, Avda. Reina Mercedes s/n, 41012-Sevilla, Spain — [3]Departamento de Física Aplicada I, Escuela Politécnica Superior, Universidad de Sevilla, Virgen de África 7, 41011-Sevilla, Spain

Structural and point defects have a crucial influence on the electronic and optical properties of transparent conductive oxides. In this contribution we characterize different types of defects in SnO2:X (X = Ta, F) by the combination of laser-wavelength dependent Raman spectroscopy and state-of-the-art density functional theory (DFT) calculations using hybrid functionals.

Sn-vacancy- and O-interstitial-type point defects are found in transparent conductive SnO2:Ta thin films grown at 575 °C. These defects are responsible for strong, fingerprint-like Raman lines out of the phonon range of SnO2 [1], which are resonance-enhanced in the visible spectral range. The defects induce strong distortions of the electronic structure in the upper range of the valence band of Ta-doped SnO2. Moreover, the DFT calculation reveal a localized, molecular nature of the O interstitial and a delocalized nature of the Sn vacancy defect.

[1] M. Krause, et al., J. Mat. Chem. A 11, 17686-17698, (2023).

DS 13.52 Thu 18:00 P1

Ion Beam Sputter Deposition of Aluminium oxide Thin Films for electronic applications — •Prakrthi Alankaru Narayana[1,2], Aurelio García-Valenzuela[1], Jens Zscharschuch[1], Charlotte Kielar[1], Holger Lange[1], Claudia Neisser[1], Thomas Seyller[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Germany

Aluminium oxide (Al2O3) has drawn considerable interest from the research community due to its versatility in microelectronics particularly as a high-k dielectric in Complementary Metal Oxide Semiconductor (CMOS) devices. Ion Beam Sputter Deposition (IBSD), a physical vapor deposition method, facilitates the formation of Al2O3 thin films with fewer defects, improved composition, and better adhesion than compared to other physical deposition methods.

This work focuses on optimizing ion beam parameters to improve film properties such as stoichiometry, surface roughness, crystallinity, optical transmittance, and dielectric constant. Furthermore, the influences of oxygen flux and annealing on film properties have been investigated. To demonstrate the applicability of the deposited Al2O3 films, they have been utilized as a high-k dielectric material in metal-insulator-metal capacitors.

[1] P. T. Ahmadi, et al. Journal of Vacuum Science & Technology A 42, 063402 (2024).

[2] D. Niu et al. Surface and Coatings Technology 291, 318 (2016).

DS 13.53 Thu 18:00 P1

Band gap engineering of $SrNbO_3$ using anions — •Abhishek Sharma, Jasnamol Palakkal, and Christian Jooss — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Green energy is the demand of this generation for a better, eco-friendly future. Solar energy, being a renewable source can fulfill our demand through solar energy harvesting, which converts available sunlight to electrical energy. Transparent conducting oxide $SrNbO_3$ is a promising material for use in silicon tandem solar cells due to its wide bandgap (1.99 eV) and flexibility of the transparency window to be varied across different wavelengths using defects concentration [1]. Cationic and anionic defect engineering also varies this material's electrical conductivity from a metallic conductor to a ferroelectric insulator [2]. Upon introducing Sr vacancies, we changed the plasma frequency of $SrNbO_3$ from the visible light region (1.99 eV) to the near-infrared region (1.37 eV) [1]. In our ongoing work, we further vary the electrical and optical properties using anion modification in the form of oxygen defects and nitrogen anion introduction. A hybrid pulsed laser deposition unit with plasma sources for gases is being used carefully to control the anions in this materials system.

1. Palakkal et al., arXiv:2410.01253.
2. Chen. et.al., ACS Nano, 2017, 11, 12519-12525.

DS 13.54 Thu 18:00 P1

Thickness dependence of transport in thin crystalline FeTe films — •Paul Zhuromskyy, Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Iron chalcogenides present an intriguing material class for solid state physics; they have been shown to display antiferromagnetism, tunable superconductivity, inverted phase change behaviour, and unique interface effects when brought into contact with topological insulators. The layered compound FeTe has been predicted to be a topological semimetal. Although it has been the subject of numerous investigations, so far little attention has been given to the effects of nanoscale confinement below a thickness of 100 nm. Besides electrical transport, we have also analyzed optical and vibrational properties with regards to topological effects and phase transitions of FeTe for decreasing film thicknesses, from 80nm down to a few monolayers, and identified inflection points at which the phase transitions and conduction behaviour change due to confinement effects. Due to the importance of interfaces for topologically nontrivial materials, this presents a step towards the understanding of electronic phenomena in iron chalcogenides, as well as finding practical applications for FeTe in nanoelectronics. Our findings reveal that the complexity of solid-state systems makes them challenging to model but offers tunable parameters like quantum confinement to create novel phenomena and materials. Characterizing these dependencies helps uncover new connections and property design opportunities.

DS 13.55 Thu 18:00 P1

Charge Density Waves and resulting properties of polycrystalline CuTe Films — Johannes Holters, •Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Charge density waves (CDWs) are periodic modulations of charge density in materials, often coupled with structural distortions and electronic property changes. The layered transition metal monochalcogenide CuTe exhibits a CDW phase below 335 K in single crystals, accompanied by a Peierls distortion along its Te-chains, which confines electron transport to a quasi-1D channel. While this phenomenon has been extensively studied in bulk single crystals, its manifestation in polycrystalline thin films is less well characterized. Here, we investigate the CDW phase and topological properties of sputter-deposited CuTe thin films with varying thickness. We observe that the CDW transition persists in these films, and its characteristics are influenced by thickness and microstructure. By modeling the resistivity curves, we extract key physical parameters, like the CDW transition temperature and its broadening due to the grain size distribution. Further, we explore the topological semimetal (TSM) characteristics in the non-CDW state (T>335K), examining features such as magnetoresistance and the planar Hall effect. Our results highlight the robustness of the CDW in polycrystalline CuTe and its sensitivity to film structure, extending the understanding of CDW behavior beyond bulk crystals. These findings reveal the interplay between CDWs, TSMs and microstructure, offering potential for novel device applications.

DS 13.56 Thu 18:00 P1

Mechanical stress of Ge films upon ion irradiation — •Karla Paz Corrales[1], Aaron Reupert[2], Berit Marx-Glowna[3], Martin Hafermann[1], Elke Wendler[1], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 3, 07743 Jena, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Lessingstraße 12-14, D-07743 Jena, Germany — [3]Helmholtz Institute Jena, Fröbelstieg 3, D-07743 Jena, Germany

Mechanical stress in thin films significantly affects the performance, reliability, and durability of optoelectronic components. Polycrystalline films are considered to be in a "stressed state" due the mismatch of the thermal expansion coefficients between the film and substrate. Amorphous Ge films (~600nm) were deposited on fused silica substrates by magnetron sputtering. Subsequent annealing was performed at 600°C for 1h and 7h in vacuum to achieve crystallization. GIXRD patterns show peaks related to the polycrystalline Ge with preferred orientation along the [111] direction. Laser curvature measurements showed compressive stress for amorphous Ge-films, while the polycrystalline Ge samples became tensile stressed after annealing. In situ curvature measurements during ion-irradiation, using Au ions with 1.8 MeV on the polycrystalline Ge, show a decrease in stress with increasing irradiation fluence. Furthermore, optical measurements were performed after irradiation, and a reduction in the reflectance region of 450 to 650 nm and a shift of the absorption region up to ~1000 nm were observed due to ion beam-induced defect formation.

DS 13.57 Thu 18:00 P1

Single-Phase Crystallization and Optimization for Optical and Electrical Properties of Sputtered In_3SbTe_2-SnTe Thin Films — •Zhengchao Zhu, Thomas Schmidt, Christian Stenz, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide phase-change materials (PCMs) are known for their distinct differences in dielectric property i.e. $\epsilon(\omega)$ and electrical conductivity between their amorphous and crystalline states. This ability to rapidly switch between phases under light or electrical pulses makes them promising for applications in data storage and solar energy systems. One of the next-generation PCMs, In_3SbTe_2 (IST), exhibits a transition from dielectric to metallic behaviour when crystallized, a characteristic that spans the entire infrared spectrum and offers gigantic potential for advancing nanophotonic technologies. However, IST faces a limitation at high temperatures, where it decomposes into InSb and InTe, leading to reduced phase contrast and diminished performance. SnTe, with its similar lattice structure to IST, shows excellent miscibility with IST and can prevent phase separation. Never the leer, mixtures containing 30%-60% IST still exhibit tendencies of phase separation. This study aims to synthesize single-phase alloys using magnetron sputtering, evaluating phase separation across different stoichiometries. Subsequent investigations will focus on determining crystallization temperatures, electrical conductivity, and optical constants of the samples.

DS 13.58 Thu 18:00 P1

Bond Confinement Induced Tayloring of Optical Properties — •Thomas Schmidt, Peter Kerres, Felix Hoff, Julian Mertens, Yiming Zhou, Maria Häser, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide materials, such as GeTe and Sb_2Te_3, exhibit a broad range of properties that enable applications in thermoelectrics and phase change material (PCM) memory storage, where rapid and reversible switching between amorphous and crystalline states alters optical and electrical characteristics. Recent studies on textured chalcogenide thin films have focused on understanding structure-property relationships, particularly how properties evolve with film thickness. It is also explored how confinement influences atomic arrangement and bonding. Changes in bonding, particularly the transition from metavalent to covalent-like bonding, are linked to significant variations in material properties with decreasing thickness. In this work, we investigate the optical contrast of chalcogenide films by analyzing the thickness-dependent changes in the dielectric function. These findings are compared with the dielectric function of a mono-elemental system molecular beam epitaxy (MBE)-grown Bi films with thicknesses ranging from 2 to 30 nm to establish a link between bonding and optical properties.

DS 13.59 Thu 18:00 P1

Coherent Control of Optical Phonon Modes in Bi Thin Films Using Polarization and Double-Pulse Excitation — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], Felix Nöhl[1], Abdur Rehman Jalil[3], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

A new approach in the coherent control of optical phonon modes has been explored, enabling advances in material manipulation. By integrating polarization control with temporal modulation of double-pulse excitation, we show the selective and independent modulation of A1g and Eg phonon modes in a 12.5 nm bismuth thin film using a femtosecond pump-probe setup. This method takes advantage of the unique polarization dependencies of each phonon mode and quantum interference effects resulting from varying time delays between two pump pulses. The proposed approach is widely applicable to various materials and offers an unique level of active control over optical phonon excitation. This advancement could be relevant for emerging phononic technologies, such as nanoscale heat management, phononic data processing, and telecommunications. These applications are particularly vital for addressing the "THz gap" in the 1-10 THz spectral range, marking a crucial progress for the next generation of high-speed information transfer.

DS 13.60 Thu 18:00 P1

Ultra-fast exciton and charge carrier dynamics in monolayer MoS_2 seen in the transient spatial dielectric function — •Jakob Seyfarth[1], Andy Engel[2], Noah Stiehm[1], Younes Slimi[1], Lucas Krätschmer[1], Markus Olbrich[2], Theo Pflug[2], Alexander Horn[2], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Fachgebiet Technische Physik I, Technische Universität Ilmenau, Weimarer Straße 32, 98693 Ilmenau, Germany — [2]Laserinstitut Hochschule Mittweida, Schillerstraße 10, 09648 Mittweida, Germany

We present the charge carrier dynamics of monolayer MoS_2 on c-cut sapphire measured using pump-probe imaging reflectometry and interferometry with a spatial resolution of 0.65 micrometers and temporal resolution of 40 femtoseconds [1]. The time-resolved spatial dielectric function shows a diffusion which can be related to the dynamics of charge carriers. The dynamics can be attributed to specific events in the band structure of MoS_2 by comparing the results of a specific probe photon energy with previous time-resolved spectroscopic ellipsometry results [2]. References: [1] O. Herrfurth, T. Pflug, M. Olbrich, M. Grundmann, A. Horn, and R. Schmidt-Grund; Femtosecond-time-resolved imaging of the dielectric function of ZnO in the visible to near-IR spectral range; Appl. Phys. Lett. 115, 212103 (2019) [2] L. Krätschmer, Y. Slimi, L. Trefflich, S. Espinoza, M. Rebarz, J. Seyfarth, T. Pflug, M. Olbrich, N. Stiehm, B. Hähnlein, C. Sturm, A. Horn, J. Andreasson, M. Grundmann, S. Krischok, and R. Schmidt-Grund; Ultrafast Exciton and Charge Carrier Dynamics in Monolayer MoS2 Measured with Timeresolved Spectroscopic Ellipsometry; tbp

DS 13.61 Thu 18:00 P1

Anomalous Nernst effect in Fe-Ge-N thin films for power generation applications — •Robin Kidangan Paul[1], Imants Dirba[1], Oliver Gutfleisch[1], Jakub Vít[2], Petr Levinský[2], Kyo-Hoon Ahn[2], Karel Knížek[2], Markéta Jarošová[2], Jaroslav Kohout[2], Stanislav Mráz[3], Marcus Hans[3], and Jochen Schneider4[3] — [1]Functional Materials, Technical University of Darmstadt, Germany — [2]Institute of Physics of the CAS, Praha, Czech Republic — [3]Materials Chemistry, RWTH Aachen University, Aachen, Germany

With the growing demand for sustainable energy solutions, thermoelectric devices that convert heat directly into electricity have gained significant interest. While conventional thermoelectric devices based on the Seebeck effect are well-established, their complex designs and geometric limitations have hindered large-scale adoption. Anomalous Nernst Effect (ANE)-based devices have recently emerged as a promising alternative, offering simpler geometries and device flexibility. However, their adoption is constrained by lower efficiencies and output voltages compared to Seebeck-based counterparts. This study focuses on addressing these challenges by exploring materials with high ANE coefficients. Among the candidates, Fe4N has attracted attention due to its cost-effectiveness, nontoxicity, and tunability through elemental doping. DFT calculations of the Berry curvature indicate that doping Fe4N with Ge can enhance its ANE coefficient. In this work, thin films of doped Fe4-xGexN were fabricated onto MgO substrates using magnetron sputtering. Crystal structure, microstructure and transport properties are systematically characterized.

DS 13.62 Thu 18:00 P1

Resolving crystalline domains in an amorphous matrix via APT — •Elias Hildebrand[1], Jan Köttgen[1], Ramon Pfeiffer[1], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Controlling crystallization from the amorphous state is critical for the development of new energy-efficient, non-volatile data storage technologies. The direct observation of crystalline nuclei is a challenging task because they are undetectable using classical X-ray diffraction.

In recent years, atom probe tomography (APT) has been established as an analytical technique for studying the microscopic structure of materials. Furthermore, it has been shown that for some chalcogenide materials (i.e., metavalently bonding materials), the difference between their amorphous and crystalline phases can be observed directly in APT data by utilizing the Probability of Multiple Events (PME).

In this project, APT is used to characterize amorphous and crystalline domains on a microscopic scale. The samples are produced using an in-house switching setup (the Phase Change Optical Tester) to reliably create crystalline regions within an amorphous matrix.

With this combination of techniques, we aim to achieve a better understanding of the crystallization mechanisms in chalcogenide glasses. This novel approach may help bridge the gap left by XRD measurements for small nuclei and thus improve control over crystallization and understanding of nucleation and growth on a nanometer scale.

DS 13.63 Thu 18:00 P1

Electrical switching dynamics of Ge-Sb-Te alloys for phase-change memories — •Alexander Kiehn[1], Ramon Pfeiffer[2], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Phase-change materials composed of Ge-rich Ge-Sb-Te alloys are promising candidates for next-generation phase-change memory (PCM) due to their non-volatile nature, temperature stability, and fast switching speeds. These properties make them ideal for in-memory computing or applications in sensor systems, where fast, energy-efficient and reliable memory is crucial. However, in order to integrate PCMs into the usual semiconductor devices, it is necessary to reduce the switching voltage and current. This is influenced by the stoichiometry of the sputtered Ge-Sb-Te layer, which was varied in this study. Using industry-standard CMOS fabrication processes, chips were manufactured based on a confined cell PCM design. Based on the electrical switching results, trends in thermal stability and the resulting voltage requirements are clearly shown for increasing Ge content. These trends are supported by further investigating the crystallization behavior in optically-switched thin films.

DS 13.64 Thu 18:00 P1

Tailoring Metavalent Materials: Exploring the Structural and Functional Properties of $(GeTe)_x(SnTe)_{1-x}$ Alloys — •Jari Klinkmann[1], Lucas Bothe[1], Felix Hoff[2], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Metavalent materials have attracted significant interest due to their unique property portfolio, including medium electrical conductivities, high optical dielectric constants, large Born effective charges, and high Grüneisen parameters. GeTe and SnTe in particular are highly relevant for applications in thermoelectrics and phase-change memories. Here, we provide a comprehensive study of $(GeTe)_x(SnTe)_{1-x}$ alloys fabricated using molecular beam epitaxy (MBE). Structural characterization using x-ray diffraction alongside polarization-resolved Raman spectroscopy reveal the stoichiometry dependence of the rhombohedral-to-cubic phase transition, characterized by the loss of Raman-active modes in the cubic phase. Furthermore, coherent phonon investigations captured via femtosecond pump-probe spectroscopy detail the phase transition temperature evolution. Electrical and optical characterizations demonstrate the impact of stoichiometry on material properties, highlighting opportunities for tailoring these alloys for advanced technological applications.

DS 14: Members' Assembly

Time: Thursday 18:30–20:00 Location: H3

All members of the Thin Films Division are invited to participate.

DS 15: Organic Thin Films, Organic-Inorganic Interfaces

Time: Friday 9:30–11:45 Location: H3

Invited Talk DS 15.1 Fri 9:30 H3

Structure formation and growth at the metal-organic interface — •Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University Linz, Austria

The evolution of the structural, electronic and optical properties of organic thin films strongly depend on the ordering, aggregation and orientation of the molecules within the very first or a few deposited monolayers. The chosen substrate and its intentional modification (e.g. by pre-adsorption of inorganic or organic species) may thus have a strong influence on the structural, electronic and optical properties of the growing organic thin film. Using complementary experimental methods, namely, surface optical spectroscopy (RDS, DRS), diffraction (LEED) and microscopy (STM, PEEM), supported by empirical models and ab-initio calculations we aim to identify (and eventually quantify) the underlying driving forces. We will present examples on the 2D condensation of organic molecules on metal surfaces, the structural and orientational ordering in 2D (and quasi 1D) monolayer phases and its influence on the further growth of the organic thin film. Finally, we will illustrate the effects of modification / templating of the substrate on the structure and properties of the organic layers.

DS 15.2 Fri 10:00 H3

Thin film heterostructures based on Co/Ni synthetic antiferromagnets on polymer tapes: towards a sustainable flexible spintronics — •Mariam Hassan[1], Sara Laureti[2], Christian Rinaldi[3], Federico Fagiani[3], Gianni Barucca[4], Manfred Albrecht[5], and Gaspare Varvaro[2] — [1]Institute of Physics, TU Chemnitz, Germany — [2]CNR-ISM, nM2-Lab, Italy — [3]Department of Physics, Politecnico di Milano, Italy — [4]Università Politecnica delle Marche, Dipartimento SIMAU, Italy — [5]Institute of Physics, University of Augsburg, Germany

The PGMs-free Co/Ni-system offers several advantages for spin-based devices such as low damping and high spin polarization, and they contribute to a more sustainable future. Moreover, these films could be good substrates for the investigation of the chiral-induced spin selectivity "CISS" effect. In this work, flexible synthetic-antiferromagnets with perpendicular-magnetic-anisotropy (PMA-SAFs) and GMR-spin-valves (SVs) containing a SAF-reference electrode and a Co/Ni-free layer were deposited on flexible polyethylene naphthalate tapes with different combinations of buffer and capping layers (Pt, Pd, Cu/Ta). High-quality SAFs with a fully compensated antiferromagnetic region and SVs with a sizeable GMR ratio were obtained. The best performances are achieved with PGMs used as buffer layer and Cu as capping layer[1]. The results indicate that complex Co/Ni-based heterostructures with reduced content of PGMs deposited on flexible tapes allow for the development of novel shapeable and sustainable spintronic devices.

[1]ACS Appl. Mater. Interfaces. 14 (2022) 51496-51509.

DS 15.3 Fri 10:15 H3

highly crystalline, cleavable, and transferable semi-conducting 2D imine COF film — •diksha srivastava[1], vipin mishra[2], showkat h. mir[3], jyotirban dey[1], jayant k. singh[1], manabendra chandra[1], and thiruvancheril g. gopakumar[1] — [1]Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]KU Leuven, Celestijnenlaan 200F, Leuven B-3001, Belgium — [3]University of Kashmir, Hazratbal, Srinagar 190006, Jammu and Kashmir, India

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are emerging crystalline organic polymers with potential applications in thin-film electronics, sensing, and catalysis, driven by their stability, tunable electronic properties, and versatile functionality. We present a scalable method for synthesizing 2D imine-COF films on dielectric glass substrates via a Schiff base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA) over 15 hours. This yields highly crystalline 2D networks with film thicknesses ranging from 100 nm to a few monolayers and lateral dimensions up to 2 cm. Sonication exfoliation is employed for producing free-standing films. Structural characterization via SEM, TEM, and AFM confirms highly crystalline 2D structures. XPS analysis validates the chemical composition, while optical measurements indicate a semi-conducting band gap. DFT calculations show a semiconductor-like band structure with strong band dispersion near the conduction and valence band edges, signifying efficient charge transport and potential for future electronic applications.

session break

DS 15.4 Fri 10:45 H3

Excited state dynamics in thin films of planar and twisted azaperopyrene derivatives — •Jakob Steidel[1], Robert Eichelmann[2], Jakob Sawatzki[1], Lutz Gade[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, Germany

Azaperopyrene derivatives are a class of organic semiconductors with a high potential for applications in optoelectronic devices. The molecular π-system of planar octaazaperopyrenedioxide (OAPPDO-H) is substituted with chlorine yielding OAPPDO-Cl, a molecule with a twisted structure.

In this contribution we utilised transient absorption spectroscopy to elucidate excited state dynamics of OAPPDO derivatives with planar and twisted molecular π-systems in thin films. On a short time scale of several hundred femtoseconds we observed fast population of excited states and fluorescence in both materials. The lifetimes of these processes show a similar dependency on the intensity of the excitation pulse. On a long time scale of several nanoseconds striking differences were observed. While the lifetimes of the excited state in OAPPDO-Cl increased and saturated with increasing excitation intensity, the lifetimes in OAPPDO-H showed a maximum at a medium excitation intensity of 400 nJ per pulse. We assign this behaviour to the opening of an additional decay pathway due to triplet-triplet-annihilation that requires cofacial arrangement of two molecules. Only planar OAPPDO-H can arrange in such a way, while the increased steric hindrance in OAPPDO-Cl suppresses this intermolecular interaction.

DS 15.5 Fri 11:00 H3

Thermally Tuning the Optical Properties of Discrete NDI-T2 Oligomer Thin Films — •Alexander Ehm[1], Fabian Eller[2], Meike Kuhn[2], Rukiya Matsidik[1], Michael Sommer[1], Eva M. Herzig[2], and Dietrich R. T. Zahn[1] — [1]Faculty of Natural Sciences, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, D-95447 Bayreuth, Germany

In the pursuit of developing and optimizing n-type organic semiconductors for the use in organic electronics, materials derived from naphthalene diimide (NDI) and bithiophene (T2), such as P(NDI2OD-T2), are highly interesting [1]. Changing the average molecular orientation via thermal annealing, and thereby their opto-electronic properties, allows finetuning for specific applications [2].

Recently, we showed that the optical anisotropy of the discrete oligomers NDI-(T2-NDI)2 and T2-(NDI-T2)2 can be influenced by thermal annealing [3]. Here, we extend this study and reveal that the photoluminescence and optical anisotropy, as found by variable-angle spectroscopic ellipsometry of T2-(NDI-T2)2 can be continuously tuned by the choice of the annealing temperature. The

correlation with molecular alignment is investigated using grazing-incidence wide-angle X-ray scattering.

[1] Chen et al. J. Am. Chem. Soc. 2009, 131, 8
[2] Vu et al. ACS Macro Lett. 2023, 12, 140
[3] Ehm et al. Phys. Status Solidi B Basic Res. 2024, 2400202

DS 15.6 Fri 11:15 H3

Highly-Robust Double Neuromorphic Device Based on Perovskite/Molybdenum Oxide-Sulfide Compound Heterojunction — •Gion Kalemai[1,2], Michael-Alexandros Kourtis[3], Anastasia Soultati[1], Apostolos Verykios[1], Dimitris Davazoglou[1], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology (INN) National Center for Scientific Research Demokritos, Agia Paraskevi, Athens, Greece — [2]Department of Physics, University of Patras, Patra Rio, Greece — [3]Institute of Informatics & Telecommunications, National Center for Scientific Research Demokritos, Agia Paraskevi, Athens, Greece

This study addresses the fundamental perovskite memristor limitations by integrating a robust molybdenum oxide-sulfide (MoO3-MoS2) mixed layer beneath a RbCsMAFA quadruple cation perovskite, precisely engineered through sulfurization of sub-stoichiometric MoO3-x. The resulting neuromorphic device exhibits impressive RS, with an ON-OFF ratio of 100, high retention & endurance, and a 0.5sec switching speed. Analysis confirm the successful control in the MoO3-MoS2 structure, which introduces trap states within the bandgap, facilitating SCLC and enabling robust memory function.

The composite, demonstrates enhanced synaptic emulation capabilities, such as PPF-PPD, and STP-LTP, replicating key synaptic functions for neuromorphic computing. Notably, this device offers excellent stability under 85°C, an enhanced ON-OFF ratio under illumination. Thus, the potential of sub-stoichiometrically engineered architectures is underlined.

DS 15.7 Fri 11:30 H3

Spatially resolved work-function manipulation of azobenzene-functionalized self-assembled monolayers by optical stimulation — Jan Böhnke[1], Beatrice Andres[1], Larissa Boie[1,2], Angela Richter[1], Cornelius Gahl[1], Martin Weinelt[1], and •Wibke Bronsch[1,3] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen, Switzerland — [3]Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14-km 163.5 in AREA Science Park, 34149 Basovizza, Trieste, Italy

Strongly differing static dipole moments of the trans and cis isomers of photochromic azobenzene allow for optical work-function switching of azobenzene-functionalized self-assembled monolayers (SAMs) [1,2]. We apply these properties in a fundamental experiment to manipulate the area size of the switched SAM [3]. In our experiments we spatially resolve the transient isomerization profile of the SAM after UV illumination by means of photoemission electron microscopy imaging. We demonstrate the capability of spatial tuning of the SAM's work function and discuss the role of the laser spot profile in generating sharp edges or gradual changes of the work function across the sample.

[1] Bronsch et al., Appl. Phys. Lett. 111, 081601 (2017).
[2] Bronsch et al., J. Phys.: Condens. Matter 29, 484002 (2017).
[3] Böhnke et al., Appl. Phys. Lett. 124, 191601 (2024).

Dynamics and Statistical Physics Division
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The Dynamics and Statistical Physics Division covers theoretical and experimental activities in all areas of statistical physics, quantum dynamics and many-body systems, nonlinear dynamics and pattern formation, data analysis and machine learning as well as active matter, fluid physics, soft matter, and complex fluids. The DY section has strong links and joint sessions with the sections of Biological Physics (BP), Chemical Physics and Polymers (CPP), Socio- and Econophysics (SOE), and Low Temperatures (TT).

Overview of Invited Talks and Sessions

(Lecture halls H37, H43, and H47; Poster P3 and P4)

Invited Talks

DY 3.6	Mon	10:45–11:15	H37	**Collective behavior of photoactive macroscopic particles** — •Iker Zuriguel
DY 4.2	Mon	9:45–10:15	H43	**Physical application of infinite ergodic theory** — •Eli Barkai
DY 4.7	Mon	11:30–12:00	H43	**Modelling the movements of organisms: Movement ecology meets active particles and anomalous diffusion** — •Rainer Klages
DY 8.1	Mon	15:00–15:30	H43	**Spatio-temporal pattern formation in time-delayed optical systems** — •Svetlana Gurevich
DY 8.6	Mon	16:45–17:15	H43	**Nonlinear dynamics and time delays in metal cutting** — •Andreas Otto
DY 9.5	Mon	16:00–16:30	H47	**Large-deviation simulations of non-equilibrium stochastic processes** — •Alexander K. Hartmann
DY 14.1	Tue	9:30–10:00	H43	**Robust signal amplification and information integration via self-tuned proximity to bifurcation points** — •Isabella Graf
DY 14.7	Tue	11:30–12:00	H43	**Beyond the connectionist view: (De-)synchronizing neural networks via cell-intrinsic dynamics** — •Susanne Schreiber
DY 15.6	Tue	10:45–11:15	H47	**Beyond spheres - active matter in new shapes** — •Juliane Simmchen
DY 15.11	Tue	12:30–13:00	H47	**Emergent correlations and boundary fluctuations in epithelial cell sheets** — •Silke Henkes
DY 17.1	Tue	14:00–14:30	H43	**Mechanistic origins of temperature scaling in the early embryonic cell cycle** — •Lendert Gelens
DY 24.1	Wed	15:00–15:30	H43	**Dynamics of odd and chiral active systems** — •Hartmut Löwen
DY 24.7	Wed	16:45–17:15	H43	**Odd dynamics and universal flows of passive objects in a chiral active fluid** — •Cory Hargus, Federico Ghimenti, Julien Tailleur, Frédéric van Wijland
DY 24.11	Wed	18:00–18:30	H43	**How to model frictional contacts in sheared and active colloids** — •Friederike Schmid, Kay Hofmann, Kay-Robert Dormann, Benno Liebchen
DY 31.6	Thu	10:45–11:15	H37	**Strong coupling and coherence in quantum thermodynamics** — •Janet Anders, Federico Cerisola, James Cresser, et al
DY 32.1	Thu	9:30–10:00	H43	**Fluctuation-Response Relations for Non-equilibrium Systems** — •Benjamin Lindner
DY 36.1	Thu	15:00–15:30	H37	**Light-Driven Manipulation of Passive and Active Microparticles** — •Svetlana Santer
DY 44.1	Fri	9:30–10:00	H47	**From Cavitation in Soft Matter to Erosion on Hard Matter** — •Claus-Dieter Ohl
DY 46.1	Fri	11:30–12:00	H43	**Equilibrium and non-equilibrium dynamics of biological systems with memory** — •Roland Netz

Invited Talks of the joint Symposium Physics of Embryonic Development Across Scales: From DNA to Organisms (SYED)

See SYED for the full program of the symposium.

SYED 1.1	Mon	9:30–10:00	H1	**Emergent crystalline order in a developing epithelium** — Kartik Chhajed, Natalie Dye, Marko Popović, •Frank Jülicher
SYED 1.2	Mon	10:00–10:30	H1	**A tissue rigidity phase transition shapes morphogen gradients** — Camilla Autorino, Diana Khoromskaia, Bernat Corominas-Murtra, Zena Hadjivasiliou, •Nicoletta Petridou
SYED 1.3	Mon	10:30–11:00	H1	**Building quantitative dynamical landscapes of developmental cell fate decisions** — •David Rand
SYED 1.4	Mon	11:15–11:45	H1	**Control of lumen geometry and topology by the interplay between pressure and cell proliferation rate** — •Anne Grapin-Botton, Byung Ho Lee, Masaki Sano, Daniel Riveline, Kana Fuji, Tetsuya Hiraiwa
SYED 1.5	Mon	11:45–12:15	H1	**Chromosomes as active communication and memory machines** — •Leonid A. Mirny

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Invited Talks of the joint Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

See SYQS for the full program of the symposium.

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — Reyhaneh Khasseh, Sascha Wald, Roderich Moessner, Christoph Weber, •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg, Greta Villa, Kilian Seibold, Vincent Dumont, Gianluca Rastelli, Mateusz Michałek, Alexander Eichler, Javier del Pino
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Sessions

DY 1.1–1.3	Sun	16:00–18:15	H2	**Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)**
DY 2.1–2.11	Mon	9:30–12:30	H31	**Nonequilibrium Quantum Systems (joint session TT/DY)**
DY 3.1–3.11	Mon	9:30–12:45	H37	**Active Matter I (joint session DY/BP/CPP)**
DY 4.1–4.11	Mon	9:30–13:00	H43	**Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications I**
DY 5.1–5.7	Mon	9:30–11:15	H47	**Statistical Physics: General**
DY 6.1–6.6	Mon	11:30–13:00	H47	**Critical Phenomena and Phase Transitions**
DY 7.1–7.7	Mon	15:00–17:00	H37	**Active Matter II (joint session BP/CPP/DY)**
DY 8.1–8.11	Mon	15:00–18:30	H43	**Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications II**
DY 9.1–9.12	Mon	15:00–18:30	H47	**Statistical Physics far from Thermal Equilibrium**
DY 10.1–10.4	Mon	16:15–17:15	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
DY 11.1–11.4	Mon	17:30–18:30	H34	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
DY 12.1–12.13	Tue	9:30–13:15	H31	**Quantum Coherence and Quantum Information Systems (joint session TT/DY)**
DY 13.1–13.13	Tue	9:30–13:00	H37	**Many-body Quantum Dynamics I (joint session DY/TT)**
DY 14.1–14.9	Tue	9:30–12:30	H43	**Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)**
DY 15.1–15.11	Tue	9:30–13:00	H47	**Active Matter III (joint session DY/BP/CPP)**
DY 16.1–16.6	Tue	14:00–15:30	H37	**Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)**
DY 17.1–17.4	Tue	14:00–15:15	H43	**Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)**
DY 18.1–18.6	Tue	14:00–15:30	H47	**Pattern Formation**
DY 19.1–19.5	Wed	9:30–12:15	H17	**Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)**
DY 20.1–20.13	Wed	9:30–13:00	H37	**Many-body Quantum Dynamics II (joint session DY/TT)**
DY 21.1–21.8	Wed	9:30–11:30	H43	**Granular Matter**
DY 22.1–22.29	Wed	10:00–12:00	P3	**Poster: Statistical Physics**
DY 23.1–23.20	Wed	10:00–12:00	P3	**Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)**
DY 24.1–24.11	Wed	15:00–18:30	H43	**Focus Session: Broken Symmetries in Statistical Physics - Dynamics of Odd Systems**
DY 25.1–25.10	Wed	15:00–18:00	H44	**Statistical Physics of Biological Systems I (joint session BP/DY)**
DY 26.1–26.9	Wed	15:00–17:30	H45	**Networks, From Topology to Dynamics (joint session SOE/BP/DY)**
DY 27.1–27.14	Wed	15:00–18:00	P4	**Poster: Nonlinear Dynamics, Pattern Formation, Granular Matter**
DY 28.1–28.7	Wed	15:00–18:00	P4	**Poster: Machine Learning, Data Science**
DY 29.1–29.9	Wed	15:00–18:00	P4	**Poster: Quantum Dynamics and Many-body Systems**
DY 30.1–30.12	Thu	9:30–12:45	H31	**Quantum-Critical Phenomena (joint session TT/DY)**
DY 31.1–31.11	Thu	9:30–12:45	H37	**Focus Session: Nonequilibrium Collective Behavior in Open Classical and Quantum Systems**
DY 32.1–32.6	Thu	9:30–11:15	H43	**Nonlinear Stochastic Systems**
DY 33.1–33.13	Thu	9:30–13:00	H47	**Machine Learning in Dynamics and Statistical Physics I**
DY 34.1–34.6	Thu	11:30–13:00	H43	**Nonlinear Dynamics, Synchronization, and Chaos**
DY 35.1–35.13	Thu	15:00–18:30	H31	**Fluctuations, Noise and Other Transport Topics (joint session TT/DY)**
DY 36.1–36.9	Thu	15:00–17:45	H37	**Microswimmers and Microfluidics (joint session DY/BP/CPP)**
DY 37.1–37.9	Thu	15:00–17:15	H43	**Brownian Motion and Anomalous Diffusion**
DY 38.1–38.11	Thu	15:00–18:00	H44	**Focus Session: Innovations in Research Software Engineering (joint session BP/DY)**
DY 39.1–39.6	Thu	15:00–16:30	H47	**Machine Learning in Dynamics and Statistical Physics II**
DY 40	Thu	18:00–19:00	H43	**Members' Assembly**
DY 41.1–41.7	Fri	9:30–11:15	H37	**Quantum Dynamics, Decoherence, and Quantum Information (joint session DY/TT)**
DY 42.1–42.7	Fri	9:30–11:15	H43	**Stochastic Thermodynamics**
DY 43.1–43.12	Fri	9:30–13:00	H44	**Active Matter IV (joint session BP/CPP/DY)**
DY 44.1–44.11	Fri	9:30–12:45	H47	**Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)**
DY 45.1–45.6	Fri	11:30–13:00	H37	**Quantum Chaos (joint session DY/TT)**
DY 46.1–46.5	Fri	11:30–13:00	H43	**Statistical Physics of Biological Systems II (joint session DY/BP)**
DY 47.1–47.1	Fri	13:15–14:00	H2	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Dynamics and Statistical Physics Division

Thursday 18:00–19:00 H43

Sessions

– Invited Talks, Tutorials, Contributed Talks, and Posters –

DY 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:

https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:

https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

See BP 1 for details of this session.

DY 2: Nonequilibrium Quantum Systems (joint session TT/DY)

Time: Monday 9:30–12:30 Location: H31

See TT 2 for details of this session.

DY 3: Active Matter I (joint session DY/BP/CPP)

Time: Monday 9:30–12:45 Location: H37

DY 3.1 Mon 9:30 H37

Odd dynamics and pattern formation in mixtures of magnetic spinners and passive colloids — •Dennis Schorn[1], Stijn van der Ham[2], Hanumantha Rao Vutukuri[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

Starfish embryos aggregate into chiral crystals exhibiting odd elasticity (Tan *et al.* Nature **607**, 287 (2022)). Similar structures have been recently observed in externally driven magnetic colloids. In this talk, I present experiments and simulations of binary mixtures of magnetic spinners and passive colloids. We develop a model to predict the phase diagram of the system, which comprises four distinct phases that can be systematically reproduced in experiments. In particular, our simulations and experiments show a phase where the passive particles form a gel-like network featuring significant holes filled with self-organized rotating chiral clusters made of spinners. This phase can be reversed by changing the system's composition and magnetic field strength, featuring a system spanning spinner phase with embedded counter-rotating chiral clusters made of passive colloids. Our system may open the route towards a new type of viscoelastic active chiral matter involving nonreciprocal interactions between both species.

DY 3.2 Mon 9:45 H37

Symmetry breaking in active non-reciprocal systems — •Kim L. Kreienkamp and Sabine H. L. Klapp — TU Berlin, Germany

Non-reciprocity significantly impacts the dynamical behavior in mixtures. One of its particularly striking consequences is the spontaneous emergence of time-dependent phases that break parity-time symmetry [1-3]. Here, we study a paradigmatic model of a non-reciprocal polar active mixture with completely symmetric repulsion [4,5]. Using a combination of field theory and particle-based simulations, we identify two qualitatively distinct regimes of non-reciprocity-induced dynamics. In the regime of weak intra-species alignment, non-reciprocity leads to asymmetric clustering in which only one of the two species forms clusters. Notably, the asymmetric density dynamics is driven alone by non-reciprocal orientational couplings [4,5]. In contrast, in the strongly coupled regime, the corresponding field theory exhibits exceptional points that have been associated with the emergence of chiral phases where the polarization direction rotates over time [2]. Our simulations confirm that spontaneous chirality arises at the particle level. In particular, we observe chimera-like states with coexisting locally synchronized and disordered regions. At the coupling strengths associated with exceptional points, the spontaneous chirality peaks.

[1] Z. You et al., PNAS 117, 19767 (2020).
[2] M. Fruchart et al., Nature 592, 363 (2021).
[3] K. L. Kreienkamp and S. H. L. Klapp, NJP 24, 123009 (2022).
[4] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRE (2024).
[5] K. L. Kreienkamp and S. H. L. Klapp, to appear in PRL (2024).

DY 3.3 Mon 10:00 H37

Emergent phases in a discrete flocking model with non-reciprocal interaction — •Swarnajit Chatterjee, Matthieu Mangeat, and Heiko Rieger — Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Non-reciprocal interactions arise in systems that seemingly violate Newton's third law "actio=reactio". They are ubiquitous in active and living systems that break detailed balance at the microscale, from social forces to antagonistic inter-species interactions in bacteria. Non-reciprocity affects non-equilibrium phase transitions and pattern formation in active matter and represents a rapidly growing research focus in the field. In this work, we have undertaken a comprehensive study of the non-reciprocal two-species active Ising model (NRTSAIM), a non-reciprocal discrete-symmetry flocking model. Our study uncovers a distinctive *run-and-chase* dynamical state that emerges under significant non-reciprocal frustration. In this state, A-particles chase B-particles to align with them, while B-particles avoid A-particles, resulting in B-particle accumulation at the opposite end of the advancing A-band. This run-and-chase state represents a non-reciprocal discrete-symmetry analog of the chiral phase seen in the non-reciprocal Vicsek model. Additionally, we find that self-propulsion destroys the oscillatory state obtained for the non-motile case, and all the NRTSAIM steady-states are metastable due to spontaneous droplet excitation and exhibit motility-induced interface pinning. A hydrodynamic theory supports our simulations and confirms the reported phase diagrams.

DY 3.4 Mon 10:15 H37

Emergent phases in a discrete flocking model with reciprocal interaction — •Matthieu Mangeat[1], Swarnajit Chatterjee[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Saarland University, Saarbrücken, Germany — [2]University of Seoul, Seoul, Korea

We have undertaken a comprehensive study of the two-species active Ising model (TSAIM), a discrete-symmetry counterpart of the continuous-symmetry two-species Vicsek model, motivated by recent interest in the impact of complex and heterogeneous interactions on active matter systems. In the TSAIM, two species

of self-propelled particles undergo biased diffusion in two dimensions, interacting via local intraspecies alignment and reciprocal interspecies anti-alignment, along with the possibility of species interconversion. We observe a liquid-gas phase transition, exhibiting macrophase-separated bands, and the emergence of a high-density parallel flocking state, a feature not seen in previous flocking models. With species interconversion (species-flip dynamics), the TSAIM corresponds to an active extension of the Ashkin-Teller model and exhibits a broader range of steady-state phases, including microphase-separated bands that further enrich the coexistence region. We also find that the system is metastable due to droplet excitation and exhibits spontaneous motility-induced interface pinning, preventing the system from reaching long-range order at sufficiently low noise. A hydrodynamic theory complements our computer simulations of the microscopic model and confirms the reported phase diagrams.

DY 3.5 Mon 10:30 H37

Emergent collective behavior from cohesion and alignment — •Jeanine Shea and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin, Germany.

Collective behavior is all around us, from flocks of birds to schools of fish. These systems are immensely complex. To explore their basic characteristics, we introduce a minimal model for cohesive and aligning self-propelled particles in which group cohesion is established through additive, non-reciprocal torques [1]. These torques cause constituents to effectively turn towards one another, while an additional alignment torque competes in the same spatial range. By changing the strength and range of these torque interactions, we uncover six states which we distinguish via their static and dynamic properties. These states range from disperse particles to closely packed worm-like formations. A number of the states generated by this model exhibit collective dynamics which are reminiscent of those seen in nature.

[1] Knežević, M., Welker, T. and Stark, H. Collective motion of active particles exhibiting non-reciprocal orientational interactions. Sci Rep 12, 19437 (2022).

Invited Talk DY 3.6 Mon 10:45 H37

Collective behavior of photoactive macroscopic particles — •Iker Zuriguel — University of Navarra, Pamplona, Spain

Active matter refers to systems of interacting, self-propelled agents that convert energy into mechanical motion, representing a nice example of out-of-equilibrium systems. In this work, a novel type of active particles is introduced. These are active granular (i.e. they interact solely through physical contacts) and photoactive, meaning that they self-propel using energy from light. Therefore, by means of a programmable LED panel, we are able to change the illumination pattern and, consequently, the particle activity in space and time, allowing a precise exploration of a variety of scenarios related to collective behavior. This possibility has been exploited in microscopic systems but is genuinely new in macroscopic ones.

First, we will present the clustering behavior of these agents under homogeneous illumination. By varying the illumination intensities and changing the population size, we observed a power-law-like distribution for both the cluster sizes and durations. We identified a transition from unstable to stable clusters, as indicated by the divergence of average cluster durations. Higher particle activities and smaller populations led to the creation of small unstable clusters, while lower particle activities and larger populations result in big, stable clusters that persist over time. This transition is explained with the help of a simple model capturing the most important processes involved in cluster dynamics. In the last part of the talk, the collective behavior under inhomogeneous illumination patterns will be introduced.

15 min. break

DY 3.7 Mon 11:30 H37

Swarming model with minority interaction exhibits temporal and spatial scale-free correlations — •Simon Syga[1], Chandraniva Guha Ray[2,3,4], Josué Manik Nava Sedeño[5], Fernando Peruani[6,7], and Andreas Deutsch[1] — [1]Technische Universität Dresden — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Center for Systems Biology Dresden — [5]Universidad Nacional Autónoma de México — [6]Université Côte d'Azur, Nice — [7]CY Cergy Paris Université

Collective motion is a widespread phenomenon in social organisms, from bird flocks and fish schools to human crowds and cell groups. Swarms of birds and fish are particularly fascinating for their coordinated behavior and rapid escape maneuvers during predator attacks. Critical motion is hypothesized as an optimal trade-off between cohesive group behavior and responsiveness to well-informed individuals. However, traditional models only show criticality at the phase transition between ordered and unordered motion. Here, we extend the Vicsek model with a minority interaction, where individuals primarily follow neighbors but can switch to follow a defector moving against a well-aligned group. This triggers cascades of defections, leading to rich dynamics, including large-scale fluctuations, scale-free velocity distributions, and a scale-free return time distribution of the order parameter. Our model underscores the biological importance of minority interactions in swarming and their role in critical behavior.

DY 3.8 Mon 11:45 H37

'Predator-prey' driven swarmalator systems — •Ginger E. Lau, Mario U. Gaimann, and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Swarmalators are an active matter system of oscillators which exhibit swarming and collective motion in physical space, as well as synchronization behavior in an additional phase variable space, originally introduced by O'Keeffe *et al.* (*Nat. Commun.* 8(1), 1504, 2017). Such systems with bidirectional couplings in space and phase can be observed in nature, such as in the chorusing behavior of Japanese tree frogs characterized by Aihara *et al.* (*Sci. Rep.* 4(1), 3891, 2014). The interplay between attraction, repulsion, and phase synchronization provides several distinct regimes of self-organizational behavior. Akin to biological swarm systems responding to predator interactions, swarmalators can respond collectively to external perturbations by a repulsive driver. In previous work, driving was realized with a mobile 'pacemaker' by Xu *et al.* (*Chaos* 34(11), 113103, 2024). The present study introduces a new 'predator-prey' driven swarmalator model showing rich adaptive behavior. This could have a wide variety of potential future applications, from biological physics to swarm robotics to nature-inspired learning algorithms and methods of inference.

DY 3.9 Mon 12:00 H37

Inertial active matter governed by Coulomb friction — •Alexander Antonov[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]University of Rome La Sapenzia, Rome, Italy

Coulomb, or dry friction, is a common phenomenon that can be encountered in various systems, such as granular matter or Brownian motors. The Coulomb friction force resists the motion and, unlike the friction in wet systems, is almost independent of the relative velocity. We show that this characteristic feature of Coulomb friction leads to emergence of dynamical states when subjected to active, or self-propelled motion [1]. At low activity levels, the dynamics resembles Brownian motion, while at greater activity, a dynamic Stop & Go regime emerges, marked by continuous switching between diffusion and accelerated motion. At even higher activity levels, a super-mobile regime arises, characterized by fully accelerated motion and an anomalous scaling of the diffusion coefficient with activity. Near the transition between the Stop & Go and super-mobile regimes, we reveal a novel activity-induced phase separation in collective behavior [2]. Our theoretical findings have been also demonstrated in experiments, where vibrobots on a horizontal surface are activated by vertical oscillations generated using an electromagnetic shaker.

[1] A.P. Antonov, L. Caprini, A. Ldov, C. Scholz, and H. Löwen, Phys. Rev. Lett. 133, 198301 (2024)

[2] A.P. Antonov et al., in preparation.

DY 3.10 Mon 12:15 H37

Active nematic turbulence with substrate friction — •Peter A. E. Hampshire[1,2] and Ricard Alert[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, Dresden, Germany

Active nematics with high activity exhibit turbulent-like flows, characterized by vortices, spatio-temporal chaos and power laws in the energy spectra [1-3]. Continuum models have been successfully used to predict the scaling of the energy spectra with the wavevector. Most theoretical work has focused on free-standing, active nematic films. However, in several experimental realisations, such as bacterial colonies and epithelial monolayers, the active nematic is in contact with a solid substrate. We generalised a 2D, incompressible active nematic model to include substrate friction, and studied its impact on the transition to turbulence and the energy spectra of the turbulent-like flows. We find a variety of dynamic states including flow in lanes, stable vortices and both isotropic and anisotropic turbulence. At high activity and moderate friction, we found a power-law scaling in the kinetic energy spectrum $E(q) \sim q^3$, where q is the wavevector, at low wavevectors. The exponent of 3 can be justified with a power-counting argument. Overall, we have developed a model for active nematic turbulence on a substrate that can be compared to biological systems. [1] L. Giomi, *Phys. Rev. X* **5**, 031003 (2015). [2] R. Alert, J.-F. Joanny, J. Casademunt, *Nat. Phys.* **16**, 682-688 (2020). [3] B. Martínez-Prat*, R. Alert*, et al., *Phys. Rev. X* **11**, 031065 (2021).

DY 3.11 Mon 12:30 H37

Self-sustained patchy turbulence in shear-thinning active fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg

Bacterial suspensions and other active fluids are known to develop highly dynamical vortex states, denoted as active or mesoscale turbulence. We reveal the pronounced effect of non-Newtonian rheology of the carrier fluid on these

turbulent states, concentrating on shear thinning. As a consequence, a self-sustained heterogeneous state of coexisting turbulent and quiescent areas develops, which results in anomalous velocity statistics. The heterogeneous state emerges in a hysteretic transition under varying activity. We provide an extensive numerical analysis and find indirect evidence for a directed percolation transition. Our results are important, for instance, when addressing active objects in biological media with complex rheological properties.

DY 4: Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications I

Deterministic chaos and stochastic processes are often seen as opposites. However, not only do they share the aspect of being mechanisms for irregular temporal fluctuations, but more importantly, the theory of stochastic processes has helped to understand and quantify many aspects of chaos. Deterministic diffusion, intermittency, long-range temporal correlations can be generated by simple deterministic systems, but are conveniently characterized by concepts of stochastic processes. In both classes of systems, the inclusion of time delays in feedbacks through memory kernels has introduced additional phenomena, and more recently non-normalizable distributions have been found as causes of ageing. While a unified approach to chaos and stochastics is fascinating and satisfying from a theoretical point of view, it also has surprisingly strong application relevance. Examples include the study of turbulence, the nonlinear dynamics of wind turbines, industrial processes for metal milling and turning, laser dynamics, cardiac dynamics, and neuronal systems.

Organized by Robert Magerle (Chemnitz) and Holger Kantz (Dresden)

Time: Monday 9:30–13:00 Location: H43

DY 4.1 Mon 9:30 H43

Welcome and Remarks — •Robert Magerle[1], Holger Kantz[2], and Theo Geisel[3] — [1]Technische Universität Chemnitz, Institut für Physik, 09126 Chemnitz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

Welcome and introductory remarks.

Invited Talk DY 4.2 Mon 9:45 H43

Physical application of infinite ergodic theory — •Eli Barkai — Phys. Dept. Bar-Ilan University, Ramat-Gan, Israel

Norm conserving dynamical mappings, for example the Pomeau Manneville scenario for intermittency, exhibit either a normalized invariant density or an infinite (non-normalized) state, depending on the non-linearity of the map. In the latter case infinite ergodic theory plays a key role in the description of time averages. We will present physical applications of infinite ergodic theory in the context of stochastic Langevin dynamics [1] where the normalizing partition function diverges, and for a gas of laser cooled atoms [2]. This allows for the construction of thermodynamical relations in a non-equilibrium setting, provided that the dynamics is recurrent.

[1.] E. Aghion, D. A. Kessler, and E. Barkai Phys. Rev. Lett. 122, 010601 (2019).

[2.] E. Barkai, G. Radons, and T. Akimoto Transitions in the ergodicity of subrecoil-laser-cooled gases Phys. Rev. Lett. 127, 140605 (2021).

DY 4.3 Mon 10:15 H43

Towards a model-free inference of hidden states and transition pathways — •Xizhu Zhao[1], Dmitrii E. Makarov[2], and Aljaž Godec[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Texas at Austin, Austin, Texas, USA

Experiments on biophysical systems typically probe lower-dimensional observables, which are projections of high-dimensional dynamics. In order to infer a consistent model capturing the relevant dynamics of the system, it is important to detect and account for the memory in the dynamics. We develop a method to infer the presence of hidden states and transition pathways based on transition probabilities between observable states conditioned on history sequences for projected (i.e. observed) dynamics of Markov chains. The histograms conditioned on histories reveal information on the transition probabilities of hidden paths locally between any specific pair of states, including the duration of memory. The method can be used to test the local Markov property of observables. The information extracted is also helpful in inferring relevant hidden transitions which are not captured by a Markov-state model.

DY 4.4 Mon 10:30 H43

Interaction statistics in persistent Lotka-Volterra communities — •Joseph Baron[1], Thomas Jun Jewell[3], Christopher Ryder[4], and Tobias Galla[2] — [1]University of Bath, UK — [2]IFISC, Palma de Mallorca, Spain — [3]University of Oxford, UK — [4]University of Manchester, UK

One criticism that was levelled at Robert May's seminal ecological work, which posited random interactions to describe the stability of many-species ecological communities, was that such interactions may not arise naturally in any reasonable model of the ecosystem dynamics. In this talk, I discuss the kinds of interactions that arise between species in communities modelled by generalised Lotka-Volterra dynamics. Far from being iid random variables, there is an intricate structure of correlations between different species' interactions. These arise due to constraints on the species abundances that are imposed by the dynamics. I show that in order to correctly predict stability, one can no longer think of species as being statistically equivalent – a hierarchy amongst the species naturally emerges, even when the initial pool of species are statistically interchangeable. In a similar vein, I also show how the initial interaction network between species is warped by the Lotka-Volterra dynamics, changing the degree distribution, and introducing correlations between a species' connectivity and its interaction statistics. In the end, we see that the interactions in coexisting communities have non-trivial statistical interdependencies, and understanding this statistical structure can help us to understand which species are able to persist in a particular community.

DY 4.5 Mon 10:45 H43

Reduced order stochastic modeling of turbulent passive scalar mixing — Abhishek Joshi, Tommy Starick, •Marten Klein, and Heiko Schmidt — BTU Cottbus-Senftenberg, Cottbus, Germany

Turbulent mixing is composed of chaotic stirring (macromixing) and molecular diffusion (micromixing). The detailed numerical modeling of turbulent mixing has remained a challenge since all relevant flow scales have to be represented in a computationally feasible manner. Map-based stochastic modeling approaches address this challenge by a radical abstraction, which is accomplished by dimensional reduction and utilization of generalized baker's maps to model turbulent fluid motions. Dimensional reduction introduces limitations, but the modeling approach offers interpretability of the emerging complexity and, hence, further physical insight into turbulent mixing. In this contribution, the Hierarchical Parcel Swapping (HiPS) [Kerstein, J. Stat. Phys. 153, 142–161 (2013)] and the One-Dimensional Turbulence (ODT) [Kerstein, J. Fluid Mech. 392, 277–334 (1999)] models are used to study turbulent mixing of passive scalars. Both models aim to represent the state space of 3-D turbulent mixing by a 1-D computational domain. HiPS is a fully event-based mixing model with prescribed sampling from a turbulent cascade, whereas ODT employs an energy-based rejection sampling only for macromixing such that a turbulent cascade is the result of a prescribed physical forcing mechanism. Capabilities of both models are demonstrated for canonical single and multiple passive scalar mixing cases using standalone model formulations across diffusivities.

DY 4.6 Mon 11:00 H43

Which methods are best suited for predicting chaotic time series? — •Ulrich Parlitz — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Since the pioneering work in the 1980s on approximating the time evolution of dynamical systems using delay embedding, many methods for predicting univariate and multivariate chaotic time series have been proposed and published. Recently, the prediction of chaotic time evolution has also been used to demonstrate the performance of novel machine learning algorithms, but in many cases only low-dimensional chaos is considered, as generated by the classical Lorenz-63 system. In this talk, different prediction methods will be contrasted and compared in terms of their prediction power and complexity when applied to low- and high-dimensional chaotic time series.

15 min. break

Invited Talk DY 4.7 Mon 11:30 H43

Modelling the movements of organisms: Movement ecology meets active particles and anomalous diffusion — •Rainer Klages — Centre for Complex Systems, School of Mathematical Sciences, Queen Mary University of London

Organisms living at very different spatio-temporal scales, from migrating in the microworld to foraging at the surface of the earth, typically all display random-looking movement patterns. Understanding these complex patterns by constructing mathematical models from data provides a fundamental challenge. In this talk I first review fundamental stochastic models for understanding movement data, like random walks, Langevin equations and active Brownian particles. On this basis experimental data for the movement paths of foraging sea turtles, migrating cells and bumblee flights is analysed. For all three examples generalised overdamped Langevin equations are constructed from data revealing active and anomalous diffusive properties. I then put forward a generalised underdamped Langevin equation for modelling organismic movements, which blends key ingredients of the three fields of movement ecology, active particles and anomalous diffusion. I illustrate the application of this equation for constructing a stochastic model of bumblebee flights from experimental data and outline its theoretical foundation.

DY 4.8 Mon 12:00 H43

Self-diffusion anomalies of an odd tracer in soft-core media — Pietro Luigi Muzzeddu[1], •Erik Kalz[2], Andrea Gambassi[3,4], Abhinav Sharma[5,6], and Ralf Metzler[2] — [1]University of Geneva — [2]University of Potsdam — [3]SISSA, Trieste — [4]INFN, Trieste — [5]University of Augsburg — [6]IPF, Dresden

Odd-diffusive systems, characterised by broken time-reversal and/or parity symmetry, have recently displayed counterintuitive features such as interaction-enhanced dynamics in the dilute limit. Here we extend the investigation to the high-density limit of an odd tracer embedded in a soft Gaussian core medium (GCM) using a field-theoretic approach based on the Dean-Kawasaki equation. Our theory reveals that interactions can enhance the dynamics of an odd tracer even in dense systems. We demonstrate that oddness results in a complete reversal of the well-known self-diffusion (Ds) anomaly of the GCM. Ordinarily, Ds exhibits a non-monotonic trend with increasing density, approaching but remaining below the interaction-free diffusion, D0, (Ds < D0) so that Ds approaches D0 at high densities from below. In contrast, for an odd tracer, self-diffusion is enhanced (Ds > D0) and the GCM anomaly is inverted, such that Ds approaches D0 at high densities from above. The transition between the standard and reversed GCM anomaly is governed by the tracer's oddness, with a critical oddness value at which the tracer diffuses as a free particle (Ds = D0) across all densities. — arXiv:2411.15552

DY 4.9 Mon 12:15 H43

Memory effects and non-linear responses in colloidal depinning — Arthur V. Straube[1,2] and •Felix Höfling[2,1] — [1]Zuse-Institut Berlin — [2]Institut für Mathematik, Freie Universität Berlin

Particle transport in inhomogeneous environments is complex and typically exhibits non-Markovian responses. The latter can be quantified by a memory function within the framework of the linear generalised Langevin equation (GLE). Here, we exemplify the implications of steady driving on the memory of a colloidal model system for Brownian motion in a corrugated potential landscape, a prototypical set-up to study depinning and non-linear responses far from equilibrium [1,2]. Relying on exact solutions of the model, we show that the random force entering the GLE displays a bias far from equilibrium, which corroborates a recent more general prediction. Based on Brownian dynamics simulations, we show that already moderate driving accelerates the decay of the memory function by several orders of magnitude in time. Moreover in equilibrium, the memory persists much longer than suggested by the timescales of the mean-square displacement. Furthermore, the memory function changes from a monotonic decay to non-monotonic, damped oscillations, which can be understood from a competition of confined motion and depinning. The simulated transport process also is pronouncedly non-Gaussian, which questions the usual Gaussian approximation of the random force in the GLE.

[1] A. V. Straube & F. Höfling, J. Phys. A **57**, 295003 (2024).
[2] A. V. Straube & F. Höfling, Phys. Rev. E **110**, L06260x (2024).

DY 4.10 Mon 12:30 H43

Non-Gaussian random forces in the generalized Langevin equation — •Hélène A. Colinet and Roland R. Netz — Freie Universität Berlin

The generalized Langevin equation (GLE), derived by projection from a general many-body Hamiltonian, exactly describes the dynamics of an arbitrary coarse-grained variable in a complex environment. The complementary force term (typically called a random force) describes the interaction with the environment, and is characterized by its second moment, linking it to the time-dependent friction memory kernel. For practical applications, this complementary force is commonly modeled as a Gaussian stochastic process, thus neglecting higher-order moments, which can become a bad approximation for non-linear systems. Leveraging advanced GLE extraction and simulation techniques, we explore the limitations of the Gaussian assumption and examine the role of non-Gaussian random forces in protein folding and conformational changes.

DY 4.11 Mon 12:45 H43

Chemo-mechanical motility modes of partially wetting liquid droplets — •Florian Voss[1] and Uwe Thiele[1,2] — [1]Institute for Theoretical Physics, University of Münster, Germany — [2]Center for Nonlinear Science, University of Münster, Germany

We consider a simple thermodynamically consistent model that captures the interplay between an autocatalytic reaction of chemical species on the free surface of a droplet, the solutal Marangoni effect and the physics of wetting in the presence of chemical fuel [1]. We find that a positive feedback loop between the local reactions and the Marangoni effect induces surface tension gradients, allowing for self-propelled droplets. Besides simple directional motion, we find crawling, shuttling and randomly moving droplets. We study the occurring dynamics and show how the observed states generically emerge from (global) bifurcations. We speculate that our results may also be relevant to the study of cell crawling [2] and self-propelled biomolecular condensates [3].

[1] Voss, F., Thiele, U., J. Eng. Math. 149, 2024
[2] Ziebert, F., Swaminatahan, S., Aranson, I., J. R. Soc. Interface 9, 2012
[3] Demarchi, L., Goychuk, A., Maryshev, I., Frey, E., Phys. Rev. Lett 130, 2024

DY 5: Statistical Physics: General

Time: Monday 9:30–11:15 Location: H47

DY 5.1 Mon 9:30 H47

The scaling behaviour of localised and extended states in one-dimensional tight-binding models with disorder — •Luca Schaefer and Barbara Drossel — Technische Universität Darmstadt, Hochschulstraße 6, 64289 Darmstadt

We investigate two one-dimensional tight-binding models with disorder that have extended states at zero energy. We use the eigenmodes of the Hamiltonian and the associated participation ratios, and the transfer-matrix method to determine the localisation length. The first model has no on-site disorder, but random couplings. While the participation ratio remains finite at zero energy, the localisation length diverges logarithmically as the energy goes to zero. We provide an intuitive derivation of this logarithmic divergence based on the weak coupling of the two sublattices. The second model has a conserved quantity as the row sums of the Hamiltonian are zero. This model can be represented as a harmonic chain with random couplings, or as a diffusion model on a lattice with random links. We find, in agreement with existing analytical calculations, that the number of system-spanning eigenmodes increases proportionally to the square root of the system size, and we related this power law to other power laws that characterise the scaling behaviour of the eigenmodes, the participation ratio, the localisation length, and their dependence on energy and system size. When disorder is so strong that the smallest hopping terms can be arbitrarily close to zero, all these power laws change, and we show a crossover between the two scaling regimes. All these results are explained by intuitive arguments based on scaling.

DY 5.2 Mon 9:45 H47

How hidden free energy landscapes imprint on the time-ordering of observed states — •Francesco Malcangi and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Single molecule experiments, such as FRET, Plasmon Ruler, or optical tweezers, probe low (often one-) dimensional projections of high dimensional dynamics. Unless the unobserved, hidden degrees of freedom relax much faster than the observable, the projection induces memory effects. By accessing the information encoded in the time-ordering of projected states, we show in our work that opportunely chosen functionals of observed paths, in particular their fluctuations and correlations, may be used to infer the presence of hidden free-energy barriers, multiple pathways, and even irreversible drifts. These hidden features are found to display common manifestations upon projection, which together with the comparison with manifestly Markovian dynamics in the free energy landscape may be used as a diagnostic tool. We demonstrate our findings with illustrative examples.

DY 5.3 Mon 10:00 H47

Long-term behavior of master equations on a countable system — •Bernd Michael Fernengel[1], Thilo Gross[1], and Wolfram Just[2] — [1]HIFMB, Oldenburg, Germany — [2]University of Rostock, Rostock, Germany

Master equations play a crucial role in natural science, as they describe the time evolution of probability distributions of all systems that can be modeled as directed, weighted graphs. Despite their essential role, computing a solution is often avoided and authors refer to numerical methods or approximation techniques instead.

We present both a mathematically sound framework for master equations on a discrete, countable configuration space as well as sufficient conditions the generator of the master equation must have for the time limit t -> infinity to converge, which is not guaranteed on an infinite dimensional space.

We discuss the assumptions for the possibility of interchanging the thermodynamic limit and the time limit. This makes it possible to obtain the long-term behavior of an infinite system from a thermodynamic limit of stationary solutions of corresponding finite subnetworks.

Our method is demonstrated by a few examples of master equations on linear, infinitely long chains, with one- and two open ends.

DY 5.4 Mon 10:15 H47

Density Fluctuations, Solvation Thermodynamics and Coexistence Curves in Grand Canonical Molecular Dynamics Simulations — •Mauricio Sevilla, Luis A. Baptista, Kurt Kremer, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research

The physics of externally driven systems is a challenge as the complexity of the amount of effects involved, yet crucial to be understood as it is present in many biological systems. Aiming to build a computational method to deal with such situations, it is first needed to reproduce correctly the equilibrium statistics of open systems. However, open-boundary computational methods are scarce and often do not satisfy all the conditions imposed by reality. The system of interest (SoI) must be at thermodynamic and chemical equilibrium with an infinite reservoir of particles. The fluctuations of the SoI in equilibrium should sample the grand canonical ensemble. The local solvation thermodynamics, extremely sensitive to finite-size effects due to particle depletion, should be correctly described. The method should be robust enough to deal with phase transitions and coexistence conditions that might occur in the SoI. In this context, the adaptive resolution method (AdResS), where the system's atomistic and ideal gas representations coexist at constant thermodynamic and chemical equilibrium, emerges as a promising alternative. Indeed, in this talk, we demonstrate with prototypical liquid systems that AdResS, coupled with particle insertion/deletion steps, satisfies all these requirements, and it is thus a suitable method to perform simulations of open systems.

DY 5.5 Mon 10:30 H47

Optimal control of fluid transitions in a Lennard-Jones like system — •William D. Pineros and Etienne Fodor — Department of Physics and Material Science, University of Luxembourg, 162a, avenue de la Faïencerie, L1511, Luxembourg

We study optimal control transitions in a system of Lennard-jones like fluid via a linear-response framework whose solutions correspond to minimum dissipation protocols in a thermodynamic space. In particular, we investigate fluid-fluid transitions via changes in particle size and attraction strength both in the homogenous and phase separated state. We compute the underlying friction tensor, representing the ease of parameter change in this space, directly from simulations and compare against an analytical approximation for low density fluids at the continuum level.

DY 5.6 Mon 10:45 H47

Noether-constrained correlations and hyperforces in equilibrium liquids — •Sophie Hermann[1,2], Silas Robitschko[1], Florian Sammüller[1], and Matthias Schmidt[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]Sorbonne Université/CNRS, Paris, France

Noether's calculus of invariant variations in statistical mechanics yields exact identities ("sum rules") from functional symmetries. The invariance of spatial transformation of the underlying classical many-body Hamiltonian at first order in the transformation field Noether's theorem yields the local force balance. At second order three distinct two-body correlation functions emerge, namely the standard two-body density, the localized force-force correlation function, and the localized force gradient. An exact Noether sum rule interrelates these correlators. More generally exploiting invariance of a thermally averaged classical phase space functions results in hyperforce sum rules. These relate the mean gradient of a phase-space function to its negative mean product with the total force. As applications we investigate via computer simulations (including Lennard-Jones liquids, monatomic water and a colloidal gel former) the emerging one-body force fluctuation profiles in bulk and confined liquids. These local correlators quantify spatially inhomogeneous self-organization, demonstrate their fundamental role in the characterization of spatial structure and their measurement allows for the development of stringent convergence tests and enhanced sampling schemes in complex systems.

DY 5.7 Mon 11:00 H47

Hybrid particle-phase field model and renormalized surface tension in dilute suspensions of nanoparticles — •Alexandra Hardy, Abdallah Daddi-Moussa-Ider, and Elsen Tjhung — The Open University, Milton Keynes, UK

We present a two-phase field model and a hybrid particle-phase field model to simulate dilute colloidal sedimentation and flotation near a liquid-gas interface (or fluid-fluid interface in general). Both models are coupled to the incompressible Stokes equation, which is solved numerically using a combination of sine and regular Fourier transforms to account for the no-slip boundary conditions at the boundaries. The continuum two-phase field model allows us to analytically solve the equilibrium interfacial profile using a perturbative approach, demonstrating excellent agreement with numerical simulations. Notably, we show that strong coupling to particle dynamics can significantly alter the liquid-gas interface, thereby modifying the liquid-gas interfacial tension. In particular, we show that the renormalized surface tension is monotonically decreasing with increasing colloidal particle concentration and decreasing buoyant mass.

DY 6: Critical Phenomena and Phase Transitions

Time: Monday 11:30–13:00 Location: H47

DY 6.1 Mon 11:30 H47

The square lattice Ising model with quenched surface disorder — Luca Cervellera, Oliver Oing, Jan Büddefeld, and •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen

Using exact enumeration, the Casimir amplitude and the Casimir force are calculated for the square lattice Ising model with quenched surface disorder on one surface in cylinder geometry at criticality. The system shape is characterized by the aspect ratio $\rho = L/M$, where the cylinder length L can take arbitrary values, while the circumference M is varied from $M = 4$ to $M = 54$, resulting in up to 2^{54} numerically exact free energy calculations. A careful $M \to \infty$ extrapolation shows that quenched surface disorder is irrelevant in two dimensions, but gives rise to logarithmic corrections.

DY 6.2 Mon 11:45 H47

Partition Function Zeros of the Frustrated J_1-J_2 Ising Model on the Honeycomb Lattice — •Denis Gessert[1,2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Leipzig University, 04081 Leipzig, Germany — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, United Kingdom — [3]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

We study the partition function zeros in the complex temperature plane (Fisher zeros) and in the complex external field plane (Lee-Yang zeros) of a frustrated Ising model with competing nearest-neighbor ($J_1 > 0$) and next-nearest-neighbor ($J_2 < 0$) interactions on the honeycomb lattice. We consider the finite-size scaling (FSS) of the leading Fisher and Lee-Yang zeros as determined from a cumulant method and compare it to a traditional scaling analysis based on the logarithmic derivative of the magnetization $\partial \ln\langle|M|\rangle/\partial\beta$ and the magnetic susceptibility χ. While for this model both FSS approaches are subject to strong corrections to scaling induced by the frustration, their behavior is rather different, in particular as the ratio $\mathscr{R} = J_2/J_1$ is varied. As a consequence, an analysis of the scaling of partition function zeros turns out to be a useful complement to a more traditional FSS analysis. The scaling of the zeros convincingly shows that the system remains in the Ising universality class for $\mathscr{R}$ as low as -0.22, where results from traditional FSS using the same simulation data are less conclusive. The approach hence provides a valuable additional tool for mapping out the phase diagram of models afflicted by strong corrections to scaling.

DY 6.3 Mon 12:00 H47

Cluster percolation in the three-dimensional $\pm J$ random-bond Ising model — •Lambert Muenster and Martin Weigel — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

We study the relation between cluster percolation and ordering phenomena in the three-dimensional $\pm J$ random-bond Ising model with different fraction of ferromagnetic bonds by performing Monte Carlos simulations. In particular a certain type of two-replica clusters is studied [1,2]. The density of these clusters can be linked to the overlap. We start the analysis with the pure ferromagnet

and demonstrate that the percolation transition maps onto the ferromagnetic phase transition. Then, we continue our analysis with the frustrated disordered ferromagnet and finally consider the spin-glass system where half of all bonds are anti-ferromagnetic and point out differences as well as similarities between the cases.

[1] J. Machta, C. M. Newman, and D. L. Stein, *J. Stat. Phys.* **130**, 113 (2008).
[2] L. Münster and M. Weigel, *Phys. Rev. E* **107**, 054103 (2023).

DY 6.4 Mon 12:15 H47

Analysis of the Mpemba effect in magnetic systems — •Janett Prehl and Martin Weigel — Technische Universität Chemnitz, Chemnitz, Deutschland

The Mpemba effect, first discovered by Mpemba and Osborne for water [1], is observed when a hot sample cools faster than an initially colder one, when both are refrigerated in the same thermal reservoir. During the last years this effect has also been found to take place in the general context of magnetic phase transitions of different orders [2–4]. Here, we investigate and discuss the occurrence of this non-equilibrium process for different ferromagnetic models exhibiting a phase transition at a critical temperature T_c. We aim to analyze how different initial temperatures, structural properties or updating dynamics influence the time behavior of quantities such as energy per spin $\langle e \rangle$ or the average domain length ℓ for different system sizes L to get a deeper insight in the occurring mechanism of the Mpemba effect for the systems under consideration.

[1] E.B. Mpemba and D.G. Osborn, *Phys. Educ.* **4**:172 (1969)
[2] M. Baity-Jesi, et al., *PNAS*, **116**:15350 (2019)
[3] N. Vadakkayil, S.K. Das, *Phys. Chem. Chem. Phys.*, **23**:11186 (2021)
[4] A.K. Chatterjee, S. Takada, H. Hayakawa, *Phys. Rev. Lett.*, **131**:080402 (2023)

DY 6.5 Mon 12:30 H47

Relating phase transitions of confined materials and topology of pore network — Georgiy Baroncha[1], Rustem Valiullin[1], and •Eustathios Kikkinides[2] — [1]Leipzig University, Leipzig, Deutschland — [2]Aristotle University of Thessaloniki, Thessaloniki, Griechenland

Measuring adsorption/desorption and melting/freezing transitions in porous materials is a common route to obtain information about pore structure. To describe phase transition behavior we exploit statistical network models including cooperative effects. In this way, important properties such as pore size distribution can be deduced. By constructing statistically-disordered random-brunching Bethe lattices we show that the average pore connectivity can be assessed. However, phase transitions remain insensitive to fine details of pore network, namely its topology. Further we discuss the experimental approaches to probe pore network topology.

DY 6.6 Mon 12:45 H47

Study of the de Almeida-Thouless (AT) line in the one-dimensional diluted power-law XY spin glass — •Ramana Bharadwaj Vedula — IISER Bhopal, Bhopal, India

The behavior of finite-dimensional spin glasses at low temperatures has been debated for decades, with the replica symmetry breaking (RSB) and droplet pictures offering competing explanations. This work investigates the Almeida-Thouless (AT) line in the one-dimensional power-law diluted XY spin glass model, where interactions decay as $1/r^{2\sigma}$. Tuning σ emulates dimensional changes, bridging mean-field and non-mean-field regimes.

A novel heatbath algorithm was developed to efficiently equilibrate XY spins at low temperatures. Using this, we studied phase transitions for $\sigma = 0.6\ (< 2/3)$, where clear evidence for an AT line exists, and for $\sigma = 0.75,\ 0.85\ (> 2/3)$, where the evidence weakens. Interestingly, data for $\sigma = 0.75$ and $\sigma = 0.85$ suggest finite-size effects mimic RSB-like behavior, but analysis aligns with the droplet picture.

Unlike traditional approaches, we also varied the magnetic field at fixed temperature, providing unique insights into spin glass properties. Our results show that the AT line disappears as σ increases, favoring the droplet model for low-dimensional spin glasses.

DY 7: Active Matter II (joint session BP/CPP/DY)

Time: Monday 15:00–17:00 Location: H37

DY 7.1 Mon 15:00 H37

Emerging cellular dynamics from turbulent flows steered by active filaments — Mehrana Nejad[1,4], Julia Yeomans[2], and •Sumesh Thampi[2,3] — [1]Department of Physics, Harvard University, Cambridge, MA 02138 — [2]The Rudolf Peierls Centre for Theoretical Physics, Parks Road, Oxford OX1 3PU, UK — [3]Department of Chemical Engineering, Indian Institute of Technology, Madras, Chennai, India 600036 — [4]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Describing the mechanics of cell collectives and tissues within the framework of active matter, without resorting to the details of biology is an exciting area. We develop a continuum theory to describe the dynamics of cellular collectives, discerning the cellular force-generating active filaments from cells shape. The theory shows that active flows and straining part of the active turbulence can elongate isotropic cells, which form nematic domains. This is important as cell morphology is not only an indicator of diseases but it can affect the nucleus morphology, gene expression and other biochemical processes inside the cells. Our theory highlights the importance of distinguishing the roles of active filaments from cell shape and explains outstanding experimental observations such as the origin of cell-filament alignment patches. Further, we reconcile how the contractile forces generated by the cytoskeletal network makes the cells to exhibit flow behaviours similar to that of extensile active systems. Revealing the crucial role of activity and rheology to describe the dynamics of cellular layers, our study is in consonance with a number of experimental observations.

DY 7.2 Mon 15:15 H37

Defects in active solids: self-propulsion without flow — •Fridtjof Brauns[1], Myles O'Leary[2], Arthur Hernandez[3], Mark Bowick[1], and Cristina Marchetti[4] — [1]Kavli Institute for Theoretical Physics, Santa Barbara, USA — [2]Princeton University, Princeton, USA — [3]Leiden University, Leiden, the Netherlands — [4]University of California Santa Barbara, Santa Barbara, California 93106, USA

Topological defects are a key feature of orientational order and act as organizing centers of orientation fields. Self-propulsion of +1/2 defects has been extensively studied in active nematic fluids, where the defects are advected with the fluid through the flow field they generate. Here, we propose a minimal model for defect self-propulsion in a nematic active solid: a linear elastic medium with an embedded nematic texture that generates active stress and in turn is coupled to elastic strain. We show that such coupling gives rise to self-propelled +1/2 defects that move relative to the elastic medium by local remodeling of the nematic texture. This mechanism is fundamentally different from the fluid case. We show that this mechanism can lead to unbinding of defect pairs and stabilize +1 defects. Our findings might help explain how orientational order, e.g. of muscle fibers, is reconfigured during morphogenesis in solid-like tissues. For instance, motility and merging of +1/2 defects play a crucial role in setting up the body axis during Hydra regeneration.

DY 7.3 Mon 15:30 H37

Isovolumetric dividing active matter — Samantha R. Lish[1], Lukas Hupe[1], Ramin Golestanian[1,2], and •Philip Bittihn[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We introduce and theoretically investigate a minimal particle-based model for a new class of active matter where particles exhibit directional, volume-conserving division in confinement while interacting sterically, mimicking cells in early embryogenesis. We find that complex motion, synchronized within division cycles, displays strong collective effects and becomes self-similar in the long-time limit. Introducing the method of normalized retraced trajectories, we show that the transgenerational motion caused by cell division can be mapped to a time-inhomogenous random walk with an exponentially decreasing length scale. Analytical predictions for this stochastic process allow us to extract effective parameters, indicating unusual effects of crowding and absence of jamming. Robustness of our findings against desynchronized divisions, cell size dispersity, and variations in confinement hints at universal behavior. Our results establish an understanding of the complex dynamics exhibited by isovolumetric division over long timescales, paving the way for new bioengineering strategies and perspectives on living matter.

DY 7.4 Mon 15:45 H37

Tracking plankton-to-biofilm transition in phototrophic bacteria — •Anupam Sengupta — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — Institute for Advanced Studies, University of Luxembourg, Luxembourg

Phototrophic bacteria commonly inhabit natural aquatic and marine ecosystems, exhibiting both motile and sessile lifestyles [1]. Yet, how and when they switch between the two states has remained unknown. Using quantitative imaging, AFM and mathematical modeling, we track the conditions and phenotypic changes across multiple generations in Chromatium okenii, a motile pho-

totrophic purple sulfur bacterium [2]. Enhanced cell-surface adhesion together with changes in the cell shape and cellular mass distribution facilitate the motile-to-sessile shift. Our results, supported by cell mechanics model, establish a synergistic link between motility, mass distribution and surface attachment in promoting biofilm lifestyle. [1] T. Sommer et al., Geophys. Res. Lett. 44, 2017. [2] F. Di Nezio,.., & A. Sengupta, Plos one 19, e0310265, 2024.

15 min. break

DY 7.5 Mon 16:15 H37

How localized active noises influence the conformations and dynamics of semiflexible filaments — •Shashank Ravichandir[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Universität Augsburg, 86159 Augsburg, Germany

The structure and dynamics of active polymers have been recently studied in some detail. In these works all the monomers are considered to be active. However, in most biological systems non-equilibrium fluctuations manifest as activity only at isolated locations within the polymer. There have been only few studies of such polymers, in which the active monomers occur periodically along the polymer contour. We consider arbitrary active-passive copolymers and isolate the effects of the number and locations of active monomers on the conformational and dynamical properties of polymers. We use Langevin dynamics simulations to calculate the end-to-end distance, radius of gyration, and mean-squared displacement of such semiflexible filaments and classify the various states of these polymers based on their conformational properties. We also present preliminary results of polymers in which the location of active monomer moves dynamically along the chain contour. This is an idealized model of biopolymers such as DNA, during DNA transcription, and microtubules, which are driven by kinetic motors that traverse along its length.

DY 7.6 Mon 16:30 H37

Sequence-specific folding of partially active polymers — •Shibananda Das — Department of Physics, Indian Institute of Science, Bengaluru, India

Biological polymers like actin filaments and microtubules exhibit important physical properties due to their out-of-equilibrium behavior induced by ATP or GTP. In contrast, synthetic polymers rely on energy from their surrounding environment, often using local chemical, electrical, or thermal gradients to remain far from equilibrium. Theoretically, active polymers serve as minimal models for these systems, enabling systematic study of the competition between thermodynamic and active forces while they undergo conformational changes.

Using a combined analytical and numerical approach, we investigate an active polymeric chain composed of multiple self-avoiding units, representing good solvent condition in the absence of active forces. For partially active polymers without orientational constraints, we find that distribution of the active units in distinct sequences along the backbone can induce a significant collapse into folded, globular structures. Detailed analysis shows that this activity-dependent collapse is driven by a reduction in swim pressure of the monomers, linking the distribution of active forces along the polymer contour to its folded conformations.

DY 7.7 Mon 16:45 H37

Effect of interactions on the chemotactic response of active-passive chains — •Hossein Vahid[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[3] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of Augsburg, Augsburg, Germany

Living organisms, from single cells to populations, exhibit complex behaviors driven by the need to navigate toward favorable environments. These behaviors are often shaped by interactions within clusters or mixed populations, where collective dynamics play a crucial role in the characteristic properties of multicellular systems.

Chemotactic bacteria, found in diverse environments such as the gastrointestinal tract, plant surfaces, and aquatic ecosystems, demonstrate the significance of chemotaxis at the population level. While extensive research has focused on the properties of active polymers in spatially homogeneous activity fields, their behaviors in inhomogeneous fields remain less explored.

This study investigates the behavior of self-propelled polymers in activity gradients, emphasizing the effects of inter- and intra-chain interactions, such as steric and excluded volume effects, on chemotactic responses. These interactions give rise to distinct phases or collective behaviors that influence the stability and persistence of chemotaxis. Additionally, polymer density emerges as a critical factor impacting diffusion and the overall efficiency of chemotaxis. This work aims to study the dynamics of the active polymer populations in non-uniform environments systematically.

DY 8: Focus Session: Nonlinear Dynamics and Stochastic Processes – Advances in Theory and Applications II

Deterministic chaos and stochastic processes are often seen as opposites. However, not only do they share the aspect of being mechanisms for irregular temporal fluctuations, but more importantly, the theory of stochastic processes has helped to understand and quantify many aspects of chaos. Deterministic diffusion, intermittency, long-range temporal correlations can be generated by simple deterministic systems, but are conveniently characterized by concepts of stochastic processes. In both classes of systems, the inclusion of time delays in feedbacks through memory kernels has introduced additional phenomena, and more recently non-normalizable distributions have been found as causes of ageing. While a unified approach to chaos and stochastics is fascinating and satisfying from a theoretical point of view, it also has surprisingly strong application relevance. Examples include the study of turbulence, the nonlinear dynamics of wind turbines, industrial processes for metal milling and turning, laser dynamics, cardiac dynamics, and neuronal systems.

Organized by Robert Magerle (Chemnitz) and Holger Kantz (Dresden)

Time: Monday 15:00–18:30 Location: H43

Invited Talk DY 8.1 Mon 15:00 H43

Spatio-temporal pattern formation in time-delayed optical systems — •Svetlana Gurevich — Institute for Theoretical Physics, University of Münster, Germany

Control and engineering of complex spatio-temporal patterns in high-dimensional non-equilibrium systems has evolved as one of the central issues in applied nonlinear science. However, real-world complex systems can be strongly influenced by time delays due to unavoidable finite signal propagation speeds and time-delayed dynamical systems have proven to be a fertile framework for the modeling of nonlinear phenomena. Nonlinear laser dynamics is one of the fields where time-delayed system are frequently employed to model the arising complex dynamics. In this talk, we will explore time-delayed models to describe the behavior of ultrashort pulses in optical micro-cavities, highlighting their potential for the formation of spatio-temporal structures.

DY 8.2 Mon 15:30 H43

Thermo-optical excitations and mixed-mode oscillations in an injected Kerr microcavity — •Elias Koch[1], Julien Javaloyes[2], and Svetlana Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany — [2]Departament de Fisica, Universitat de les Illes Balears & IAC-3, Cra. de Valldemossa, km 7.5, E-07122 Palma de Mallorca, Spain — [3]Center for Nonlinear Science (CeNoS), University of Münster, Corrensstraße 2, 48149 Münster, Germany

We study the dynamics of a vertically emitting micro-cavity containing a Kerr nonlinearity that is subjected to detuned optical injection. To this end, we present an extended model that allows investigation of the influence of cavity heating, which shifts the microcavity resonance and thus the detuning on a slow time scale. As a consequence of this scale separation, we uncover a canard scenario featuring dark and bright excitations, as well as mixed-mode oscillations that can be manipulated by tuning the injection amplitude and frequency. When the microcavity is coupled to a long external feedback loop, subjecting it to strong time-delayed optical feedback, we can examine the additional influence of the time delay on excitability dynamics, as well as the impact of thermal effects on preliminary studies.

DY 8.3 Mon 15:45 H43

Back to the future: Fermi–Pasta–Ulam–Tsingou recurrence in a time-delayed system — •Jonas Mayer Martins[1], Elias Koch[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9 and Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, 48149 Münster, Germany — [2]Departament de Física and IAC-3, Universitat de les Illes Balears, C/ Valldemossa km 7.5, 07122 Palma de Mallorca, Spain

We demonstrate Fermi–Pasta–Ulam–Tsingou (FPUT) recurrence, a surprising quasi-periodicity of certain spatially extended systems, in a time-delayed system. Although the bi-Riccati system that we study is not integrable, we find in the long-delay limit that its normal form is a partial differential equation approximating the integrable Korteweg–de Vries (KdV) equation, prominently known to exhibit FPUT recurrence. Our results underscore the analogy between spatially extended and time-delayed systems.

DY 8.4 Mon 16:00 H43

Momentum space induced complex billiard dynamics — •Lukas Seemann, Jana Lukin, and Martina Hentschel — Institut für Physik, TU Chemnitz, Deutschland

While billiard models have always been a paradigm to study nonlinear dynamics, their class has been enriched by realistic models such as optical cavities, ballistic quantum dots, or graphene systems over the past decades. The originally hard billiard walls are replaced by confinement through total internal reflection of light or potential wells trapping electrons. They are well-known model systems in the field of mesoscopic physics, quantum chaos, and wave-ray correspondence exhibiting a broad range of dynamical behavior, ranging from regular and mixed to purely chaotic dynamics depending on their geometric shape. However, employing their material-specific properties allows one to influence and even control their complex dynamics in more ways. Using an anisotropy (as for electrons in bilayer graphene systems), one can induce chaotic motion even in a circularly shaped cavity [1]. We develop a ray tracing algorithm for anisotropic media and illustrate how anisotropy affects the billiards dynamics in real and phase space. In particular we show how deformation away from the circular shape in real and momentum space, changes the phase space structure and can be optimized to the formation of large stable island [2] that we quantify using Lyapunov exponents.

[1] L. Seemann, A. Knothe, M. Hentschel, Phys. Rev. B 107, 205404 (2023)
[2] L. Seemann, A. Knothe, M. Hentschel, NJP 26, 10 (2024)

DY 8.5 Mon 16:15 H43

Stochastic Properties of Musical Time Series: Measuring Musical Variability — Corentin Nelias and •Theo Geisel — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Music philosophers and psychologists have argued that emotions and meaning in music depend on an interplay of expectation and surprise. We aimed to quantify the variability of musical pieces empirically by considering them as correlated dynamical processes. Using a multitaper method we determined power spectral density (PSD) estimates for more than 550 classical compositions and jazz improvisations down to the smallest possible frequencies [1]. The PSDs typically follow inverse power laws ($1/f^{\beta}$-noise) with exponents near β=1 for classical compositions, yet only down to a cutoff frequency, where they end in a plateau. Correspondingly the pitch autocorrelation function exhibits slow power law decays only up to a cutoff time, beyond which the correlations vanish abruptly. We determined cutoff times between 4 and 100 quarter note units serving as a measure for the degree of persistence and predictability in music. They tend to be larger in Mozart's compositions than in Bach's, which implies that the anticipation and expectation of the musical progression tends to last longer in Mozart's than in Bach's compositions

[1] C. Nelias, T. Geisel, Nature Comm. 15, 9280 (2024)

15 min. break

Invited Talk DY 8.6 Mon 16:45 H43

Nonlinear dynamics and time delays in metal cutting — •Andreas Otto — Fraunhofer Institute for Machine Tools and Forming Technology IWU, Reichenhainer Str. 88, 09126 Chemnitz, Germany

Since products and consequently production processes in manufacturing industry becomes more and more individual, an agile and robust process design is important for minimizing costs while guaranteeing high product quality. A fundamental understanding of the underlying physics of the manufacturing processes is essential for finding sweet spots of high productivity with optimal quality of the produced part.

In this talk, we present some examples from metal cutting, where especially the complex behavior of mechanical vibrations also known as chatter lead to undesired noise, tool wear and scraped parts. We show that mechanical vibrations at machine tools can be described by nonlinear delay differential equations and in many situations the time delay is, in addition, distributed, time-varying or state-dependent. Some recent developments for the prediction of the stability of metal cutting processes with respect to chatter vibrations and applications for online chatter detection are presented.

DY 8.7 Mon 17:15 H43

Stability of power grids concerning strong perturbations - tropical cyclones and increasing resilience — •Jürgen Kurths — Potsdam Institute for Climate Impact Research, Telegraphenberg, 14473 Potsdam

The infrastructure of our modern society is efficient but also sensitive concerning strong perturbations, as terrorist attacks on the cybersystem or extreme climate events. An important part of modern infrastructure are power grids, which are characterized by multistability. For them, the strongly ongoing transition to distributed renewable energy sources leads to a proliferation of dynamical actors. The desynchronization of a few or even one of those would likely result in a substantial blackout. We discuss the concept of basin stability covering strong perturbations and identify most vulnerable motifs in power grids. To consider the vulnerability of power grids against extreme wind loads, we combine a detailed model of of extreme events, and a cascadable model of the transmission network to provide a holistic co-evolution model to consider wind-induced failures of transmission lines in the Texan electrical network.

DY 8.8 Mon 17:30 H43

Critical demand in a stochastic model of flows in supply networks — •Yannick Feld[1] and Marc Barthelemy[1,2] — [1]Université Paris-Saclay, CNRS, CEA, Institut de Physique Théorique, 91191 Gif-sur-Yvette, France — [2]Centre d'Analyse et de Mathématique Sociales (CNRS/EHESS) 54 Avenue de Raspail, 75006 Paris, France

Supply networks are essential to modern production, yet their critical properties remain understudied. This talk presents a stochastic model with random production capacities that allows us to investigate material flow to a root node, focusing on the network topology and buffer stocks. We examine the critical demand at the root, where unsatisfied demand diverges. Without stocks, minimal production governs behavior, and topology is mostly irrelevant. Buffer stocks introduce memory, significantly altering the dynamics. Now the topology is crucial, with local connectivity proving beneficial.

DY 8.9 Mon 17:45 H43

Generalizations of laminar chaos — •David Müller-Bender — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Laminar chaos was originally discovered in scalar dynamical systems with a large periodically time-varying delay [Phys. Rev. Lett. 120, 084102 (2018)]. This demonstrated how drastically a temporal modulation of the delay can change the dynamics of a system as laminar chaos is an extremely low-dimensional dynamics compared to turbulent chaos, which is observed in such systems with constant delay. In this talk, I give an overview of recent generalizations of laminar chaos to systems with quasiperiodic [Phys. Rev. E 107, 014205 (2023)], random and chaotic delay time modulation. Using a connection to spatially disordered circle maps [Phys. Rev. E 106, L012202 (2022)], it is found that short-time correlated random and chaotic delays lead to low-dimensional generalized laminar chaos in almost the whole delay parameter space spanned by the mean delay and the delay amplitude. This is in stark contrast to the case of a constant delay, where only high-dimensional turbulent chaos is found. Finally, an outlook on laminar chaos in systems with state-dependent delay is given. I acknowledge the contributions of the late Günter Radons to these results.

DY 8.10 Mon 18:00 H43

Chaotic Diffusion in Systems with Delay — •Tony Albers, David Müller-Bender, and Lukas Hille — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Chaotic Diffusion is a purely deterministic phenomenon occurring in nonlinear systems. While much is known about chaotic diffusion in low-dimensional dynamical systems such as iterated maps or Hamiltonian systems, there are only a few works dealing with chaotic diffusion in higher-dimensional systems. In this talk, we show that chaotic diffusion is also possible in dynamical systems with time delay, which raises the dimension of the problem formally to infinity. Moreover, we demonstrate that introducing a periodic modulation of the delay can increase the strength of the diffusion, as measured by the diffusion coefficient, by several orders of magnitude [1]. This phenomenon is counterintuitively related to a significant decrease of the Kaplan-Yorke dimension of the chaotic attractor due to the appearance of so-called laminar chaos [2], which is a recently discovered type of chaos that is not observed in systems with constant delay. We acknowledge the contributions of the late Günter Radons who initiated this work.

[1] Tony Albers, David Müller-Bender, Lukas Hille, and Günter Radons, Phys. Rev. Lett. **128**, 074101 (2022)
[2] David Müller, Andreas Otto, and Günter Radons, Phys. Rev. Lett. **120**, 084102 (2018)

DY 8.11 Mon 18:15 H43

Weak generalized synchronization in random neural networks and its impact on time series forecasting — •Hiromichi Suetani[1,2] and Ulrich Parlitz[3,4] — [1]Faculty of Science and Technology, Oita University, Oita, Japan — [2]International Research Center for Neurointelligence , The University of Tokyo, Tokyo, Japan — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [4]Institute for the Dynamics of Complex Systems, Universität Göttingen, Göttingen, Germany

Time series forecasting is one of the important issues in data science, and approaches based on reservoir computing (RC), have been attracting attention. Previous studies have often suggested that the hyperparameter region at the so-called "edge of chaos," provides optimal performance in time series forecasting. But this concept is problematic because generally a reservoir is a non-autonomous dynamical system driven by external inputs, it should be referred to as the "edge of conditional stability" rather than the edge of chaos.

In this study, we argue that this is not just a matter of terminology, and that the edge of conditional stability does not provide optimal performance. For this purpose, we clarify the relevance of the concept of "weak generalized synchronization (W-GS)." This study demonstrates that random neural networks driven by chaotic inputs exhibit W-GS and shows that the fractal nature of the GS function affects forecasting ability. We quantitatively compare the relationship between the characteristics of GS and those of RC, such as the information processing capacity, to elucidate the role of GS in RC.

DY 9: Statistical Physics far from Thermal Equilibrium

Time: Monday 15:00–18:30 Location: H47

DY 9.1 Mon 15:00 H47

Shear-driven diffusion with stochastic resetting — •Iman Abdoli, Kristian Stølevik Olsen, and Hartmut Löwen — Institut für Theoretische Physik II - Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Here, we explore the non-equilibrium dynamics that emerge from the interplay between linear shear flow and stochastic resetting. The particle diffuses with a constant diffusion coefficient while simultaneously experiencing linear shear and being stochastically returned to its initial position at a constant rate. We perturbatively derive the steady-state probability distribution that captures the effects of shear-induced anisotropy on the spatial structure of the distribution. We show that the dynamics, which initially spread diffusively, will at late times reach a steady state due to resetting. At intermediate timescales, the system approaches this steady state either by passing through a superdiffusive regime (in the shear-dominated case) or by exhibiting purely sub-diffusive behavior (in the resetting-dominated case). The steady state also gains cross correlations, a feature absent in simpler resetting systems. We also show that the skewness has a non-monotonic behavior when one passes from the shear-dominated to the resetting-dominated regime. We demonstrate that at small resetting rates, the energetic cost of maintaining the steady state becomes significantly higher due to the displacement caused by shear, a unique scaling not seen without shear. Surprisingly, if only the x-position is reset, the system can maintain a Brownian yet non-Gaussian diffusion pattern with non-trivial tails in the distribution.

DY 9.2 Mon 15:15 H47

Propulsion force and heat exchange for nonreciprocal nanoparticles — •Laila Henkes[1], Kiryl Asheichyk[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August-Universität — [2]Department of Theoretical Physics and Astrophysics, Belarusian State University

Nonreciprocity allows for interesting new phenomena in Casimir physics, such as propulsion forces pointing in translationally invariant directions, and persistent heat currents between objects of the same temperatures. To study these quantities, we derive general formulas for heat transfer and Casimir force involving a non-reciprocal point particle. These display how nonreciprocity of the particle couples to the nonreciprocity of the surrounding and also yield conditions for persistent heat current or propulsion force. Furthermore, we find a bound for the propulsion force acting on a point particle in terms of its heat exchange. This is, e.g., relevant for the efficiency of this arrangement when used as a heat engine.

DY 9.3 Mon 15:30 H47

Exponential change of relaxation rate by quenched disorder — •Jan Meibohm and Sabine H. L. Klapp — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstraße 36, 10623 Berlin, Germany

We determine the asymptotic relaxation rate of a Brownian particle in a harmonic potential perturbed by quenched Gaussian disorder, a simplified model for rugged energy landscapes in complex systems. Depending on the properties of the disorder, we show that the mean and variance of the asymptotic relaxation rate are non-monotonous functions of the parameters for a broad class of disorders. In particular, the rate of relaxation may either increase or decrease exponentially compared to the unperturbed case, implying that the effect of disorder is stronger than that associated with other, well-studied anomalous-relaxation effects. In the limit of weak disorder, we derive the probability distribution of the asymptotic relaxation rate and show that it is Gaussian, with analytic expressions for the mean and variance that feature universal limits. Our findings indicate that controlled disorder may serve to tune the relaxation speed in complex systems.

DY 9.4 Mon 15:45 H47

Mean back relaxation for position, densities and others — •Gabriel Knotz and Matthias Krüger — Institute for theoretical physics, Göttingen, Germany

Recently, a so-called mean back relaxation (MBR) has been introduced, which correlates a scalar observable at three time points. The deviation of its long-time value from 1/2 has been shown to be a marker for breakage of time-reversal symmetry for observables with finite mean. We have extended the discussion by introducing a cut off length when evaluating the MBR from trajectories. For Gaussian systems we can derive a relation between MBR and the mean squared displacement and demonstrate that the MBR can be easily applied to stochastic observables like positions and densities. We discuss the application of the density MBR to multi-particle systems.

[1] Gabriel Knotz and Matthias Krüger, Mean back relaxation for position and densities, Phys. Rev. E 110, 044137 (2024)

[2] Till M. Muenker, Gabriel Knotz, Matthias Krüger and Timo Betz, Accessing activity and viscoelastic properties of artificial and living systems from passive measurement, Nature Materials 23, pages 1283*1291 (2024)

Invited Talk DY 9.5 Mon 16:00 H47

Large-deviation simulations of non-equilibrium stochastic processes — •Alexander K. Hartmann — University of Oldenburg, Germany

Stochastic processes are investigated by obtaining the probability distributions $P(S)$ of relevant quantities S of interest. A full description is obtained, if $P(S)$ is known over its full range of support. Also the structure of the entities contributing to the different parts of $P(S)$ are of interest. Usually analytical calculations are not feasible, so most of the time one has to use numerical simulations. Unfortunately, most of the support, in particular in the tails, is not accessible by standard algorithms.

By applying special large-deviation algorithms, also the tails can be accessed, down to probabilities such as 10^{-200}, or even much smaller. Here, a very general *black-box* algorithm [1] is explained, which allows one to study rather arbitrary stochastic processes. Some application examples are shown, such as force-induced RNA unfolding [2], S being the physical work W; interface growth [3], S being the height H; fractional Brownian motion [4], S being the area A under the curve; or the spread of diseases [5], S being the number of infected.

[1] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)
[2] P. Werner and A.K. Hartmann, Phys. Rev. E **104**, 034407 (2021)
[3] A.K. Hartmann, P. Le Doussal, S.N. Majumdar, A. Rosso and G. Schehr, Europhys. Lett. **121**, 67004 (2018)
[4] A.K. Hartmann and B. Meerson, Phys. Rev. E **109**, 014146 (2024)
[5] Y. Feld and A.K. Hartmann, Phys. Rev. E **105**, 034313 (2022)

15 min. break

DY 9.6 Mon 16:45 H47

Dissipation bounds precision of current response to kinetic perturbations — •Krzysztof Ptaszyński[1,2], Timur Aslyamov[1], and Massimiliano Esposito[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland

The precision of currents in Markov networks is bounded by dissipation via the so-called thermodynamic uncertainty relation (TUR). We conjecture [1] and prove [2] a similar inequality that bounds the precision of the static current response to perturbations of kinetic barriers. Perturbations of such type, which affect only the system kinetics but not the thermodynamic forces, are highly important in biochemistry and nanoelectronics. Our inequality cannot be derived from the standard TUR, but rather implies it and provides an even tighter bound for dissipation. We also provide a procedure for obtaining the optimal response precision for a given model.

[1] Phys. Rev. Lett. 133, 227101 (2024); [2] arXiv:2410.17140

DY 9.7 Mon 17:00 H47

Theory of Nonequilibrium Responses for Markov Jump Processes — •Timur Aslyamov[1] and Massimiliano Esposito[2] — [1]University of Luxembourg, Luxembourg — [2]University of Luxembourg, Luxembourg

The theory of nonequilibrium responses in complex systems to parameter perturbations is fundamental, spanning disciplines from ecology to metabolic control and the design of low-noise devices. The framework of Markov jump processes is one of the most popular approaches for studying a broad range of nonequilibrium phenomena across various fields.

In recent papers [1, 2], we formulated a theory of static response for Markov jump processes under arbitrary parameterizations. Leveraging stochastic thermodynamics, we developed a novel approach based on simple linear algebra, enabling us to extend beyond previously known results. Through our analysis, we uncovered a novel fundamental property of Markov processes: the responses are constrained by specific linear combinations, which we term the Summation and Cycles Response Relations.

[1] Aslyamov, T., and Esposito, M. (2024). Nonequilibrium Response for Markov Jump Processes: Exact Results and Tight Bounds. Physical Review Letters, 132(3), 037101.

[2] Aslyamov, T., and Esposito, M. (2024). General Theory of Static Response for Markov Jump Processes. Physical Review Letters, 133(10), 107103.

DY 9.8 Mon 17:15 H47

How topologically distinct non-equilibrium currents imprint on projected observables — •Felix Tippner and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Almost all measurements track only a limited subset of degrees of freedom simultaneously. Mathematically, the higher-dimensional stochastic process governing a physical system (e.g., the dynamics of protein conformation) is accessible only through observables of projected dynamics, which, in practice, are constrained by strict experimental limitations. These projections not only introduce or amplify non-Markovian effects but also obscure features such as irreversible currents (e.g., driven versus non-driven systems) or barriers in the underlying energy landscape. In our work we investigate how topological and geometric properties imprint on projected dynamics that appear similar (i.e., those exhibiting the same observed steady state), both in and out of equilibrium. This is achieved by examining path-wise observables, such as empirical densities and currents inferred from projected trajectories, through a detailed analysis of their fluctuations and (cross-)correlations.

DY 9.9 Mon 17:30 H47

Slow relaxation in a facilitated trap model — •Gregor Diezemann — Department Chemie, JGU Mainz

Trap models have successfully been applied to understand a number of relaxation features of simulated and real-world supercooled liquids. A common choice for the transition rates is that the system leaves a trap and chooses the destination trap at random. Depending on the form of the prior distribution of trap energies, a broad the relaxation spectrum results. Recently, a facilitated trap model (FTM) in which each transition is accomponied by a small change in the energies of all traps equivalent to a diffusion of trap energies has been implemented. It has been shown that a strong asymmetry of susceptibilities can be obtained with reasonable assumptions regarding the model parameters(1).

In the present contribution, we present the numerical solution of the master equation for the FTM and discuss the relaxation behavior of various one-time and two-time quantities, both in equilibrium and in the particular non-equilibrium situation encountered after temperature jumps, such as in typical aging experiments. Using a model of random rotational jumps for the reorientational motion, the linear dielectic susceptibility in thermal equlibrium is found to be given as a convolution of a Debye-like response originating from the energy drift inherent in the FTM and the response of the original trap model.

(1) C. Scalliet, B. Guiselin, and L. Berthier, J. Chem. Phys. 155, 064505 (2021).

DY 9.10 Mon 17:45 H47

Nonequilibrium shortcuts and anomalous thermal relaxations: the Mpemba effect — •Gianluca Teza[1], John Bechhoefer[2], Antonio Lasanta[3], Oren Raz[4], and Marija Vucelja[5] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Simon Fraser University, Burnaby, Canada — [3]Universidad de Granada, Ceuta, Spain — [4]Weizmann Institute of Science, Rehovot, Israel — [5]University of Virginia, Charlottesville, USA

Most of our intuition about the behavior of physical systems is shaped by observations at or near thermal equilibrium. However, even a phenomenon as basic as a thermal quench leads to states far from any thermal equilibrium, where counterintuitive effects can occur. A prime example of anomalous thermal relaxation is the Mpemba effect, a phenomenon in which a hot system cools down faster than an equivalent colder one. Although originally witnessed in water, perspectives towards the design of optimal heating/cooling protocols and observations in a variety of systems pushed the development of a high-level characterization in the framework of nonequilibrium statistical mechanics. In this talk, I will review the phenomenology of this and related anomalous relaxation effects, in which nonmonotonic relaxation times act as the common denominator. With a focus on Ising systems, I will provide insight on the physical mechanisms that enable their emergence. I will show how they can survive arbitrarily weak couplings, highlighting the role played by equilibrium and dynamical features, as well as experimental observation of these effects in quantum simulators.

DY 9.11 Mon 18:00 H47

Power-Efficiency Trade-offs in Finite-Time Thermodynamics: From Minimal Model to General Principle — •Shiling Liang[1,2,3,4], Yu-Han Ma[5,6], Daniel Maria Busiello[4], and Paolo De Los Rios[1] — [1]EPFL, Lausanne, Switzerland — [2]Okinawa Institute of Science and Technology, Okinawa, Japan — [3]Center for Systems Biology Dresden, Dresden, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [5]Beijing Normal University, Beijing, China — [6]Graduate School of China Academy of Engineering Physics, Beijing, China

Thermodynamic systems operating in finite time face fundamental trade-offs between power output and efficiency. While conventional wisdom dictates that Carnot efficiency is only attainable in the quasi-static limit with vanishing power, we demonstrate theoretically that this constraint can be circumvented in finite-time operations. We present a minimal heat engine model incorporating intrinsic energy level degeneracy that achieves Carnot efficiency at maximum power in the thermodynamic limit. The enhanced performance originates from first-order phase transitions far from the linear response regime, enabled by collective effects in many-body systems. Our results reveal how collective advantages can fundamentally alter power-efficiency trade-offs and suggest new strategies for designing efficient heat engines operating at finite times far from equilibrium.

[1] Liang, S., Ma, Y. H., Busiello, D. M., & De Los Rios, P. (2023). A Minimal Model for Carnot Efficiency at Maximum Power. arXiv preprint arXiv:2312.02323.

DY 9.12 Mon 18:15 H47

Fluctuating diffusivity in living cells: Analog of Carnot engine — •Yuichi Itto — Aichi Institute of Technology, Japan — ICP, Universität Stuttgart, Germany

The diffusivity fluctuating over local areas of living cells is experimentally known to obey the exponential law for normal/anomalous diffusion. In Ref. [1], a formal analogy of the fluctuating diffusivity to thermodynamics has been studied. Remarkably, the exponential law is formally equivalent to the "canonical distribution": the diffusivity, which is proportional to local temperature of the cell in nonequilibrium stationary states [2], is identified with the analog of the system energy. Consequently, the analogs of the internal energy, the quantity of heat, work, and the Clausius inequality have been established.

Here, the analog of the heat engine is constructed for the fluctuating diffusivity [3]. This heat-like engine consists of processes realized by compression/expansion of the cell and the change of temperature, along which the average value of the diffusivity or local temperature is kept fixed. The efficiency of the engine in a cycle, which characterizes how much the diffusivity change as the analog of work is extracted, is found to formally take that of Carnot's. The result is expected to be useful, for example, for tuning the rates of biochemical reactions in cells, see, e.g., Ref. [4].

References [1] Y. Itto, Entropy, 23, 333 (2021). [2] Y. Itto and C. Beck, J. Royal Society Interface, 18, 20200927 (2021). [3] Y. Itto, in preparation. [4] N. Bellotto, J. Agudo-Canalejo, R. Colin, R. Golestanian, G. Malengo, and V. Sourjik, eLife, 11, e82654 (2022).

DY 10: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 16:15–17:15 Location: H34

See CPP 10 for details of this session.

DY 11: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 17:30–18:30 Location: H34

See CPP 14 for details of this session.

DY 12: Quantum Coherence and Quantum Information Systems (joint session TT/DY)

Time: Tuesday 9:30–13:15 Location: H31

See TT 15 for details of this session.

DY 13: Many-body Quantum Dynamics I (joint session DY/TT)

Time: Tuesday 9:30–13:00 Location: H37

DY 13.1 Tue 9:30 H37

Controlling Many-Body Quantum Chaos — •Lukas Beringer[1], Mathias Steinhuber[1], Juan Diego Urbina[1], Klaus Richter[1], and Steven Tomsovic[1,2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA USA

Controlling chaos is a well-established technique that leverages the exponential sensitivity of classical chaotic systems for efficient control. This concept has been generalized to single-particle quantum systems [1] and, more recently, extended to bosonic many-body quantum systems described by the Bose-Hubbard model [2]. In direct analogy to the classical paradigm, a localized quantum state can be transported along a specific trajectory to a desired target state. In the latter context, this approach reduces to time-dependent control of the chemical potentials, making it suitable for implementation in optical lattice experiments. Highlighted potential applications are rapid, customizable state preparation and stabilization of quantum many-body scars in one-, two-, and three-dimensional lattices. Recent progress includes potential applications to large time-crystal platforms and preparation protocols for entangled states, such as cat-like states.

[1] S. Tomsovic, J. D. Urbina, and Klaus Richter, Controlling Quantum Chaos: Optimal Coherent Targeting, PRL 130.2 (2023): 020201.

[2] L. Beringer, M. Steinhuber, J. D. Urbina, K. Richter, S. Tomsovic, Controlling many-body quantum chaos: Bose-Hubbard systems, New J. Phys (2024): 26 073002.

DY 13.2 Tue 9:45 H37

Exact spectral function and nonequilibrium dynamics of the strongly interacting Hubbard model — Ovidiu I. Pâțu[1], •Andreas Klümper[2], and Angela Foerster[3] — [1]Institute for Space Sciences, Bucharest-Măgurele, R 077125, Romania — [2]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [3]Instituto de Física da UFRGS, Av. Bento Gonçalves 9500, Porto Alegre, RS, Brazil

Analytical results on the correlation functions of strongly correlated many-body systems are rare in the literature and their importance cannot be overstated. We present determinant representations for the space-, time-, and temperature-dependent correlation functions of the strongly interacting one-dimensional Hubbard model in the presence of an external trapping potential. These representations are exact and valid in both equilibrium and nonequilibrium scenarios like the ones initiated by a sudden change of the confinement potential. In addition, they can be implemented numerically very easily significantly outperforming other numerical approaches. As applications of our results we investigate the single particle spectral functions of systems with harmonic trapping and show that dynamical quasicondensation occurs for both fermionic and bosonic spin-1/2 systems released from a Mott insulator state.

DY 13.3 Tue 10:00 H37

Quantum many-body scars beyond the PXP model in Rydberg simulators — Aron Kerschbaumer[1], Marko Ljubotina[1,2,3], Maksym Serbyn[1], and •Jean-Yves Desaules[1] — [1]Institute of Science and Technology Austria, Klosterneuburg, Austria — [2]Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Persistent revivals recently observed in Rydberg atom simulators have challenged our understanding of thermalization and attracted much interest to the concept of quantum many-body scars (QMBSs). QMBSs are non-thermal highly excited eigenstates that coexist with typical eigenstates in the spectrum of many-body Hamiltonians, and have since been reported in multiple theoretical models, including the so-called PXP model, approximately realized by Rydberg simulators. At the same time, questions of how common QMBSs are and in what models they are physically realized remain open.

In our work, we demonstrate that QMBSs exist in a broader family of models that includes and generalizes PXP to longer-range constraints and states with different periodicity. We show that in each model, multiple QMBS families can be found. Each of them relies on a different approximate su(2) algebra, leading to oscillatory dynamics in all cases. However, in contrast to the PXP model, their observation requires launching dynamics from weakly entangled initial states rather than from a product state. The new QMBSs we unveil may be experimentally probed using Rydberg atom simulator in the regime of longer-range Rydberg blockades.

DY 13.4 Tue 10:15 H37

Roughening dynamics of quantum interfaces — Wladislaw Krinitsin[1,2], •Niklas Tausendpfund[1,3], Matteo Rizzi[1,3], Markus Heyl[4], and Markus Schmitt[1,2] — [1]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, Jülich, Germany — [2]Faculty of Informatics and Data Science, University of Regensburg, Regensburg, Germany — [3]Institute for Theoretical Physics, University of Cologne, Köln, Germany — [4]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The roughening transition, known from three-dimensional classical spin systems, describes how fluctuations of interfaces transition from being bounded to being extensive when crossing the characteristic roughening temperature. We explore signatures of such phenomena in the dynamics of domain walls in the two dimensional quantum Ising model, where we observe pre-thermal steady states in their evolution well beyond the perturbative limit using Tree Tensor Networks. We formulate an effective model of the interface, which captures qualitative features of a roughening transition. Most notably, it exhibits a Berezinskii Kosterlitz Thouless quantum phase transition from smooth to rough interfaces, whose signatures extend to finite temperatures. These findings can be related to the observed slow thermalization in the full model, opening the way to a better understanding of pre-thermalization effects in interface dynamics, which can be easily implemented and tested in experimental setups such as Rydberg atom experiments.

DY 13.5 Tue 10:30 H37

Semigroup Influence Functionals for the Dynamics of Quantum Impurity Models — •Michael Sonner[1], Valentin Link[2], and Dmitry Abanin[3,4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — [4]Google Research, Brandschenkestrasse 150, 8002 Zürich, Switzerland

Quantum impurity models~(QIM) consist of a local interacting impurity which is coupled to baths of free fermions. These models exhibit a range of non-trivial phenomena such as the Kondo effect. and play a central role in the dynamic mean field theory (DMFT) approach to correlated matter. However, despite their importance, computing the real time dynamics of QIM remains a challenge. Recently, approaches based on matrix product states (MPS) representation of influence functionals (IF) have been proven effective approaches to this problem. These method work by capturing the, generically non-markovian dynamical effects of the quantum environments on the local impurity in a multi time object, which then is compressed as MPS. Taking explicit advantage of time-translation invariance of the model, we find an infinite MPS or semigroup representation of the IF. I will demonstrate how these ideas can be used to predict QIM dynamics for very long times as well as give direct access to stationary non-equilibrium states.

DY 13.6 Tue 10:45 H37

Quantum Fisher information of monitored random circuits — •Arnau Lira Solanilla, Xhek Turkeshi, and Silvia Pappalardi — Universität zu Köln

We characterize the multipartite entanglement structure of monitored random quantum circuits using the quantum Fisher information. We show that, despite the known phase transition in bipartite correlations, the multipartiteness is bounded. On the other hand, we generate a phase with extensive multipartite

entanglement under symmetry preserving random operations by introducing two-qubit measurements. We focus on the limit where no unitary operations are applied, but there is a competition between two noncommuting projective measurements. We exploit a map to bond percolation to precisely calculate the universal scaling of multipartite entanglement.

DY 13.7 Tue 11:00 H37

Entanglement in quantum circuits with SU(2) symmetry — •Tobias Dörstel and Michael Buchhold — Institute for Theoretical Physics, Cologne

Quantum circuits offer a robust framework for studying the out-of-equilibrium dynamics of quantum many-body systems. We investigate one-dimensional monitored quantum circuits with global SU(2) symmetry, serving as digital counterparts to the Heisenberg chain. These circuits consist of unitary qubit SWAPs and non-unitary SWAP-measurements. Entanglement in the chain is governed by the configuration of qubit singlet states, whose count is fixed by the symmetry sector. Varying the measurement rate, unitary operations, and singlet number reveals diverse entanglement behaviors, ranging from volume law to $\log^2(L)$ and $\log(L)$ scaling of half-chain entanglement. We explain these scaling regimes analytically using an SU(2)-symmetric "Page law" and a mapping to loop models with crossings.

15 min. break

DY 13.8 Tue 11:30 H37

Generalized dual-unitary circuits from biunitarity — •Michael A. Rampp, Suhail A. Rather, and Pieter W. Claeys — Max-Planck-Institut für Physik komplexer Systeme, Dresden

We present a general framework for constructing solvable lattice models of chaotic many-body quantum dynamics with multiple unitary directions using biunitary connections. We show that a network of biunitary connections on the Kagome lattice naturally defines a multi-unitary circuit, where three 'arrows of time' directly reflect the lattice symmetry. These models unify various constructions of hierarchical dual-unitary and triunitary gates and present new families of models with solvable correlations and entanglement dynamics. Using multilayer constructions of biunitary connections, we additionally introduce multilayer circuits with monoclinic symmetry and higher level hierarchical dual-unitary solvability and discuss their (non-)ergodicity. Our work demonstrates how different classes of solvable models can be understood as arising from different geometric structures in spacetime.

DY 13.9 Tue 11:45 H37

Magic spreading in doped Clifford circuits — •Jiangtian Yao and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems

We study the spreading of magic, or nonstabilizerness, in Clifford circuits with doping by non-Clifford gates. We characterize the spatial extent of magic in classes of Clifford circuits where the growth behavior of entanglement entropy and operator strings are known. The dynamics of magic spreading in such circuits is compared to that of entanglement entropy, and quantitative measures for longer-ranged magic are also explored.

DY 13.10 Tue 12:00 H37

One magnon magnetization dynamics for the kagome lattice antiferromagnet — Henrik Schlüter, •Jannis Eckseler, and Jürgen Schnack — Faculty of Physics, Bielefeld University, Bielefeld, Germany

We present aspects of the one-magnon dynamics of the antiferromagnetic kagome lattice as an example of flat-band dynamics extending the work of [1] to two dimensional systems. We illustrate how localized eigenstates also called localized magnons [2] influence the dynamics of excitations and possibly prevent the system from thermalization. To this end we introduce a $J_1 - J_2$-model for the kagome lattice which guarantees the stability of one out of three localized magnons and lets us distinguish the different flat bands.

[1] F. Johannesmann, J. Eckseler, H. Schlüter, and J. Schnack, Phys. Rev. B 108, 064304 (2023).

[2] J. Schnack, H.-J. Schmidt, J. Richter, and J. Schulenburg, Eur. Phys. J. B 24, 475 (2001).

DY 13.11 Tue 12:15 H37

Towards a Many-Body Generalization of the Wigner-Smith Time Delay — •Georg Maier[1], Carolyn Echter[2], Juan Diego Urbina[1], Caio Lewenkopf[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik Universität Regensburg, Regensburg, Germany — [2]Mathematische Fakultät Universität Regensburg, Regensburg, Germany — [3]Instituto de Física Universidade Federal Fluminense, Niterói RJ, Brazil

Many body systems with a large number of degrees of freedom are usually described by statistical physics on the theoretical side while experiments usually relay on scattering (e.g. particle physics). Is it possible to relate scattering and statistical physics, or to measure scattering-related observables which directly relate to quantities of statistical physics? At least for single particle systems a close relation exists between the well known Wigner-Smith delay time in scattering theory and the density of states of the scattering system.

I will present a novel ansatz relating a many-body version of dwell-/Wigner-Smith delay time and many body density of states based on the famous Birman-Krein-Friedel-Loyd formula connecting scattering theory and statistical observables in the many-body context. Due to the flexibility of this ansatz it can be used to investigate a wide variety of MB systems. I will discuss interesting scaling behaviors for different systems, like the harmonic trap[1] or the free particle together with the different behavior of bosons, fermions and indistinguishable particles.

[1] C. Echter et. al 2409.08696

DY 13.12 Tue 12:30 H37

Subleading logarithmic behavior in the parquet formalism — •Marcel Gievers[1,2], Richard Schmidt[3], Jan von Delft[1], and Fabian B. Kugler[4] — [1]Ludwig-Maximilians-Universität, München — [2]Max-Planck-Institut für Quantenoptik, Garching — [3]Universität Heidelberg — [4]CCQ, Flatiron Institute, New York

The Fermi-edge singularity in x-ray absorption spectra of metals is a paradigmatic case of a logarithmically divergent perturbation series. Prior work has thoroughly analyzed the leading logarithmic terms. Here, we investigate the perturbation theory beyond leading logarithms and formulate self-consistent equations to incorporate all leading and next-to-leading logarithmic terms. This parquet solution of the Fermi-edge singularity goes beyond the previous first-order parquet solution and sheds new light on the parquet formalism regarding logarithmic behavior. We present numerical results in the Matsubara formalism and discuss the characteristic power laws. We also show that, within the single-boson exchange framework, multi-boson exchange diagrams are needed already at the leading logarithmic level.

DY 13.13 Tue 12:45 H37

Ballistic transport in a disordered, boundary-driven XXZ spin chain. — •Johannes S Hofmann[1], Adam McRoberts[2], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]International Centre for Theoretical Physics, Strada Costiera 11, 34151, Trieste, Italy

Recent experiments on Google's sycamore NISQ device on spin transport realised ballistic transport in a edge-driven XXZ chain without disorder; and theoretical works on the classical variant demonstrated the survival of ballistic regime in the easy-plane upon the introduction of bond disorder. Here, we consider various generalisations of this set-up.

DY 14: Focus Session: Nonlinear Dynamics in Biological Systems I (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 9:30–12:30 Location: H43

Invited Talk DY 14.1 Tue 9:30 H43

Robust signal amplification and information integration via self-tuned proximity to bifurcation points — •Isabella Graf — Developmental Biology Unit & Theory Transversal Theme, EMBL Heidelberg, Germany

Many living systems demonstrate exquisite sensitivity to small input signals. A tempting hypothesis is that these systems operate close to bifurcation or critical points, where the system's response exhibits a diverging susceptibility to the control parameter and small signals are amplified into a large collective response. A common concern, however, is that proximity to such points requires fine-tuning of parameters, which seems impossible for noisy biological systems. Based on several distinct sensory systems, we have investigated a feedback motif that robustly maintains these systems close to their respective bifurcation point. The key ingredient is that the collective response feeds back onto the control parameter. To illustrate this idea, I will mention several examples ranging from snake thermosensing to mammalian hearing and discuss the functional benefits associated with being near-critical.

DY 14.2 Tue 10:00 H43

Exceptional Points and Stability in Nonlinear Models of Population Dynamics having PT symmetry — •Alexander Felski — Max Planck Institute for the Science of Light, Erlangen, Germany

Nonlinearity and non-Hermiticity, for example due to environmental gain-loss processes, are a common occurrence throughout numerous areas of science. For the latter, parity-time-reflection (PT) symmetry has played an eminent role in understanding exceptional-point structures and phase transitions in these systems. Yet their interplay has remained by-and-large unexplored. We analyze models governed by the replicator equation of evolutionary game theory and related Lotka-Volterra systems of population dynamics. These foundational nonlinear models offer a broad platform for non-Hermitian theory beyond physics. In this context we study the emergence of exceptional points in two cases: (a) when the governing symmetry properties are tied to global properties of the models, and, in contrast, (b) when these symmetries emerge locally around stationary states–in which case the connection between the linear non-Hermitian model and an underlying nonlinear system becomes tenuous. We outline further that when the relevant symmetries are related to global properties, the location of exceptional points in the linearization around coexistence equilibria coincides with abrupt global changes in the stability of the nonlinear dynamics. Exceptional points may thus offer a new local characteristic for the understanding of these systems.

DY 14.3 Tue 10:15 H43

Pattern selection and the route to turbulence in polar active fluids — Henning Reinken[1], Sebastian Heidenreich[2], •Markus Bär[2,3], and Sabine Klapp[3] — [1]OVGU Magdeburg, Germany — [2]Physikalisch-Technische Bundesanstalt, Germany — [3]TU Berlin, Germany

Active fluids, such as suspensions of microswimmers, are well known to self-organize into complex spatio-temporal flow patterns. An intriguing example is mesoscale turbulence, a state of dynamic vortex structures exhibiting a characteristic length scale. Here, we employ a minimal model for the effective microswimmer velocity field to explore how the turbulent state develops from regular, stationary vortex patterns when activity is increased. First, we demonstrate analytically that the system develops a stationary square vortex lattice in the absence of nonlinear advection. Subsequently, we perform an extended stability analysis and uncover a linear instability, above which the square vortex lattice becomes unstable. In numerical simulations, we confirm that this instability is predictive for the unset of turbulence. In addition, an extended region of hysteresis where turbulence and a stable vortex lattice coexist, is found Reference: H. Reinken, S. Heidenreich, M. Bär, S. Klapp, New J. Phys. 26 063026 (2024).

DY 14.4 Tue 10:30 H43

Likelihood-based inference for heterogeneous motile particle ensembles — •Jan Albrecht[1], Cristina M. Torres[1], Carsten Beta[1], Manfred Opper[2,3,4], and Robert Grossmann[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Faculty of Electrical Engineering and Computer Science, Technische Universität Berlin, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom — [4]Institute of Mathematics, University of Potsdam, 14476 Potsdam, Germany

The inherent complexity of biological agents often leads to motility behavior that appears to have random components. Robust stochastic inference methods are therefore required to understand and predict the motion patterns from time discrete trajectory data provided by experiments. In many cases second-order Langevin models are needed to adequately capture the motility. Additionally, population heterogeneity needs to be taken into account when analyzing data from multiple individual organisms. We present a maximum likelihood approach to infer stochastic models and, simultaneously, estimate the heterogeneity in a population of motile active particles from discretely sampled trajectories. To this end we propose a new method to approximate the likelihood for nonlinear second order Langevin models. We demonstrate that our approach outperforms alternative methods for heterogeneity estimation, especially for short trajectories, while also providing a measure of uncertainty for the estimates. We use the approach to investigate population heterogeneity in systems of ameboid cells.

DY 14.5 Tue 10:45 H43

Surviving the first "winter": Protocells with polymerization reactions protects against environmental fluctuations — •Xi Chen, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, Dresden, Germany

The origin of life has been a long standing question with various hypotheses describing the emergence of the first protocells. Phase separated condensates are promising candidates for protocells because they are compartments that enrich specific polymers and host nonequilibrium reactions that leads to growth and division. However, the ability of protocells to survive in an environment that has large fluctuations, such as temperature and composition, is poorly understood. We show with a mean-field model that condensates formed by polymers which undergo nonequilibrium polymerization/depolymerization reactions exhibit significant robustness to large environmental fluctuations.

This robustness occurs when the nonequilibrium polymerization reactions are faster inside condensate phases than outside. The first condensate does not form until environmental factors lead to strong enough reactions that polymers long enough to phase separate form. The effects of nonequilibrium polymerization is then fully realized because a condensate exists. From here, the condensate does not dissolve until the nonequilibrium reactions are diminished to significantly below when the condensate formed. Altogether, this forms a hysteretic loop with respect to the environmental factors that drive nonequilibrium reactions. We show this hysteretic loop prevents protocells from dying from environmental fluctuations.

DY 14.6 Tue 11:00 H43

How inter-particle interaction affects two species transport in nano-channels — •Wolfgang Bauer — Dept. of Internal Medicine I, UKW, Würzburg, Germany

Channel transport mechanisms of multiple species is essential for cell physiology and nanotechnology. Here, we present a model maintaining spatial correlations of two species, moving away from mean field approaches. The spatial occupations of the channel give the state space, where local flux and entropy production

determine channel transport and its thermodynamic efficiency. Optimal transport coupling between species occurs in an attractive empty channel and strong repulsive forces between particles of the same species. This confines state space to a circular topology with concentration gradients of the two species acting as thermodynamic driving forces in series. For opposing gradients, the species with the stronger gradient produces positive entropy, while the other negative entropy. Attenuating the repulsive force within one species and maintaining that of the other adds a bypass path on the circular topology in state space. This enables a leak flow of the less repulsive species parallel to its gradient, generating local positive entropy on the bypass. For a certain range of opposing gradients, both species can produce positive overall entropy simultaneously. However, the rectifying potential of the concentration gradient of the species with bypass option is diminished, i.e. it cannot rectify flow of the other species above a threshold of the latter's opposing gradient. Vice versa the flow of the species with bypass option may always be rectified parallel to the concentration gradient of the other.

15 min. break

Invited Talk DY 14.7 Tue 11:30 H43

Beyond the connectionist view: (De-)synchronizing neural networks via cell-intrinsic dynamics — •Susanne Schreiber — Humboldt-Universität zu Berlin, Institute for Theoretical Biology, Berlin, Germany

Neural computation is thought to arise from the connectivity among neurons. Accordingly, we are often more than happy to ignore seemingly unimportant and potentially overwhelming biological detail, for example, related to the properties of the neurons themselves. In this talk, however, I will highlight how cell-intrinsic dynamics, namely the biophysics of action-potential generation, can have a decisive impact on network behaviour. Recent work of my lab shows that, among regularly firing neurons, the somewhat unattended homoclinic type (characterized by a spike onset via a saddle homoclinic orbit bifurcation) particularly stands out: First, spikes of this type foster specific network states - synchronisation in inhibitory and splayed-out/frustrated states in excitatory networks. Second, homoclinic spikes can be easily induced in by changes in a variety of physiological parameters (like temperature, extracellular potassium, or dendritic morphology). As a consequence, small changes in these parameters can suffice to induce drastic switches in network states. I will discuss functional consequences of homoclinic spikes for the design of pattern-generating motor circuits in Drosophila as well as for mammalian pathologies like febrile seizures. Our work predicts an interesting role for homoclinic action potentials as an integral part of brain dynamics in both health and disease.

DY 14.8 Tue 12:00 H43

Transient spatiotemporal chaos in cardiac excitable media — •Melvin Dix[1,2], Thomas Lilienkamp[1,3], Stefan Luther[1,4,5], and Ulrich Parlitz[1,2,5] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Faculty for Applied Mathematics, Physics, and General Science, Computational Physics for Life Science, Nuremberg Institute of Technology Georg Simon Ohm, Nürnberg, Germany — [4]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [5]German Center for Cardiovascular Research (DZHK), Partner Site Göttingen, Göttingen, Germany

Life-threatening cardiac arrythmia such as ventricular fibrillation have been linked to spatiotemporal chaotic dynamics governed by scroll or spiral waves. It has been observed in vivo and in vitro that these dynamics can be transient, e.g. abruptly stop. Using simulations with different numerical models we investigate the effects of factors such as heterogeneities, motivated by the complexity of the heart. We show that these perturbations can (significantly) prolong the duration of chaotic transients and may also lead to persistent chaos or stable periodic wave patterns [1].

[1] Melvin Dix et al. Physical Review E 110(4), 044207 (2024).

DY 14.9 Tue 12:15 H43

Nonlinear dynamics of heart and brain — •Irene Pellini[1,2], Simon Bauer[1], Johannes Zierenberg[1,3], Philip Bittihn[1,3], and Viola Priesemann[1,3] — [1]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany — [2]Max Planck School Matter to Life, Heidelberg, Germany — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The core function of the heart and brain arises from the coordinated interaction of their cells. Both organs rely on excitable units – cardiomyocytes and neurons – that propagate electrical signals when a specific threshold is exceeded. Despite this similarity, the two organs exhibit opposed collective behavior due to marked differences in intercellular dynamics and network topology. In the heart, localized electrical connectivity through reciprocal gap junctions generates local synchronization and traveling waves, ensuring efficient pumping function with low entropy. In the brain, long-range connectivity via delayed, non-reciprocal chemical synapses promotes asynchronous dynamics with high entropy, supporting information processing.

Using coupled FitzHugh-Nagumo oscillators, we showcase that characteristic non-linear dynamics for the heart and brain can be related to the network structure, which places both systems on opposite sides of a synchronization phase transition. Crossing this phase transition would lead to pathological conditions, e.g., heart arrhythmia or brain seizures, quantifiable via entropy measures. Our joint view on heart and brain dynamics may foster new perspectives on the function and pathology of both organs.

DY 15: Active Matter III (joint session DY/BP/CPP)

Time: Tuesday 9:30–13:00 Location: H47

DY 15.1 Tue 9:30 H47

From micro to macro: systematic coarse-graining of active particle models and implications on phase separation — •Sumeja Burekovic[1], Filippo De Luca[2], Cesare Nardini[1,3], Ananyo Maitra[4,5], and Michael E. Cates[2] — [1]CEA, Paris-Saclay, France — [2]DAMTP, University of Cambridge, UK — [3]LPTMC, Sorbonne Université, France — [4]LPTM, CY Cergy Paris Université, France — [5]LJP, Sorbonne Université, France

Significant insights into collective phenomena of active systems, such as phase separation, have been obtained through minimal field theories developed in a top-down manner. In contrast, the bottom-up approach seeks to link these continuum models to the microscopic dynamics of active particles, often formulated as Langevin equations for their position and orientation. This connection is typically achieved via explicit coarse-graining and allows active field theories to be expressed in terms of physically meaningful parameters. A major challenge in coarse-graining is the consistent elimination of irrelevant fast degrees of freedom to derive closed equations for the hydrodynamic variables or order parameters, such as the density field. We propose a systematic extension of standard homogenization/projection-operator techniques. As we show in minimal examples with few degrees of freedoms, our technique allows to go beyond the state of the art of homogenization in the mathematical literature. We then discuss the predictions of our coarse-graining methods for the large-scale phenomenology of non-aligning active particles, including cases in which microphase separation - rather than full phase separation - emerges due to activity.

DY 15.2 Tue 9:45 H47

Active Quadrupolar Dumbbells — •Margaret Rosenberg[1], Marco Musacchio[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf — [2]Università di Roma Sapienza, P.le Aldo Moro 2, 00185 Rome, Italy

The field of Active Matter has thrived in recent years, driven both by the insight that it underlies fundamental processes in nature, and by its vast potential for applications. Although the self-propulsion mechanisms of Active Matter allow us to consider and control a wide range of motions, there is - by default - no obvious control over the orientation and rotation of the particles. One approach to resolve this is the use of anisotropic particles and interactions. This contribution presents a computational study of a novel system composed of active, quadrupolar dumbbells, the phase behavior of which is determined by the competition between active motion and the orthogonal alignment favored by quadrupolar attraction. We explore the novel phase behavior unlocked by these anisotropic interactions, and discuss options for experimental realizations and applications.

DY 15.3 Tue 10:00 H47

Order by disorder in a swarm with obstacles — Pradeep Kumar[1], Sanjay Puri[1], and •Martin Weigel[2] — [1]School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067, India — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Simple models of swarming and active matter such as the Vicsek model [1] have been studied in detail, and the phase diagram as a function of noise strength and particle density is by now well understood. Real active systems are usually affected by impurities and random disorder, however. The presence of a quenched distribution of disc-like obstacles in the domain of the Vicsek model

is observed to have a dramatic effect on the ordering behavior [2]: in contrast to the model without obstacles, where the strongest alignment is observed for the lowest noise, as soon as obstacles are added only the presence of a certain amount of noise leads to a global alignment of particles. This order by disorder phenomenon for active systems is traced back to the interplay of multiple length scales in the system: the typical inter-obstacle distance, the typical cluster size, and the resulting mean-free-paths of cluster-obstacle and cluster-cluster collisions. We present scaling arguments explaining these connections and provide an outlook towards similar phenomena in related systems.

[1] T. Vicsek, Phys. Rev. Lett. 75, 1226 (1995).
[2] O. Chepizhko, E. G. Altmann, and F. Peruani, Phys. Rev. Lett. 110, 238101 (2013).

DY 15.4 Tue 10:15 H47

Autonomous navigation in synthetic microswimmers: solving mazes with chemical echolocation — •Aritra K. Mukhopadhyay[1], Linhui Fu[2], Kai Feng[2], Ran Niu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems.

We propose and experimentally demonstrate a mechanism enabling synthetic microswimmers, such as autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, creating echoes that carry structural information about the environment. Remarkably, these echoes invoke automatic responses, such as synthetic chemotaxis, enabling the swimmers to avoid dead ends and autonomously find paths through complex mazes.

Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities, which could be useful for developing self-navigating micromachines with potential applications in targeted drug delivery and environmental sensing.

DY 15.5 Tue 10:30 H47

Active Particles in Tunable Colloidal Environments — •Abhimanyu Nowbagh[1], Venkata M.S.G. Tanuku[2], Thomas Palberg[2], and Ivo Buttinoni[1] — [1]Institute of Experimental Colloidal Physics, Heinrich-Heine University, 40225 Düsseldorf — [2]Institute of Physics, Johannes-Gutenberg University, 55128 Mainz

Active colloids are microscopic particles which propel through aqueous media by converting the externally available energy into directed motion. Using non equilibrium thermodynamics to understand biological systems: interactions of active colloids with crowded systems, and emergent phenomena of ensembles of active particles, remain an important and open question.

In this work, we investigate the dynamics of active particles in crowded environments subjected to alternating-current (AC) electric fields. The AC electric field is used to control: i) the velocity of active particles and ii) the inter-particle interaction between passive colloids. As we increase electric field strength, the velocity of active particles increases and the inter-particle interaction between passive colloids becomes stronger. We study the behaviour of active particles as a function of: i) the frequency of the applied AC electric field, ii) the area fraction of the passive crowd, iii) the active to passive particle number ratio, and iv) the velocity of the active particles.

Our experimental findings show that the active particles reorient faster with an increasing electric field strength. With an increase in the active to passive particle ratio, we show that cluster formation is non-monotonically sensitive to the passive crowd density.

Invited Talk DY 15.6 Tue 10:45 H47

Beyond spheres - active matter in new shapes — •Juliane Simmchen — University of Strathclyde, Cathedral street 295, Glasgow UK

Surface minimisation for a given volume is energetically favourable on the small scale - this is why most colloidal particles are spherical. In active matter they have the added advantage of facilitating comparison between experiment and theory, one of the reasons why spherical Janus particles dominate the field.

However, broadening the range of materials has led to interesting discoveries - behaviour that would not have been observable in the spherical regime. This talk will give an overview of the intriguing behaviour of non-spherical active materials at the microscale - from plates to truncated bipyramids and rods.

15 min. break

DY 15.7 Tue 11:30 H47

Modeling Filamentous Cyanobacteria — •Elias Fischer and Holger Stark — Institute Of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet, both in the present and the past. They triggered the great oxygenation event about 2.5 billion years ago, generating the atmospheric oxygen of our planet while contributing large parts of our fossil fuel record.

Filamentous cyanobacteria exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood. Furthermore, the gliding of cyanobacteria is strongly affected by external cues, most importantly light. They aggregate in regions with the highest light intensity, which means best environmental conditions for photosynthesis.

Following recent advances in understanding the self-organization of cyanobacteria, we present a novel approach for modeling the mechanical and behavioral aspects of individual cyanobacteria filaments, including force synchronization and response to light. Each filament is modeled as a bead-spring chain in 3D with bending and torsional elasticity, as well as a hard-core repulsion between the filaments. Notably, the propulsion forces that drive the individual parts of the filament forward are only considered locally where the filament comes into contact with another surface. First results on the 3D bending and twisting motion of a filament and its reaction to light are presented.

DY 15.8 Tue 11:45 H47

Self-assembly and control of active and passive triblock Janus colloids — •Juri Franz Schubert, Salman Fariz Navas, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Triblock Janus colloids belong to the family of patchy particles, interacting with hydrophobic attraction at opposite poles and electrostatic repulsion in the equatorial region. They are known to self-assemble into a colloidal kagome crystal from experiments [1] and theory [2,3,4]. However, investigating the self-assembly of such systems via Brownian Dynamics can result in timescales inaccessible to brute force simulations, often requiring complex sampling techniques [3]. Recently, it has been shown that introducing self-propulsion can significantly accelerate self-assembly and enhance the Kagome yield [4]. Here, we study the model introduced in [4] and further investigate the self-assembled structures in active and passive systems. Using simple time-dependent activity protocols, we are able to sample a temperature-density state diagram of the passive system. Our results closely match with earlier studies [2,3], where different triblock models and sampling techniques were used.

[1] Q. Chen, S. C. Bae, S. Granick, Nature 469, 7330 (2011).
[2] F. Romano, F. Sciortino, Soft Matter 7, 12 (2011).
[3] K. Bahri, H. Eslami, and F. Müller-Plathe, JCTC 18, 1870 (2022).
[4] S. A. Mallory, A. Cacciuto, JACS 141, 6 (2019).

DY 15.9 Tue 12:00 H47

Enhanced Diffusion and Universal Rouse-like Scaling of an Active Polymer in Poor Solvent — Suman Majumder[1], Subhajit Paul[2], and •Wolfhard Janke[3] — [1]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India — [2]Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India — [3]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

By means of Brownian dynamics simulations we study the steady-state dynamic properties of a flexible active polymer in a poor solvent condition. Our results show that the effective diffusion constant of the polymer D_{eff} gets significantly enhanced as activity increases, much like in active particles. The simulation data are in agreement with a theoretically constructed Rouse model of active polymer, demonstrating that irrespective of the strength of activity, the long-time dynamics of the polymer chain is characterized by a universal Rouse-like scaling $D_{\text{eff}} \sim N^{-1}$, where N is the chain length. We argue that the presence of hydrodynamic interactions will only have an insignificant effect on the observed scaling behavior.

DY 15.10 Tue 12:15 H47

A Pulsating Active Solid — •Umang A Dattani[1], Francesco Serafin[1], Jonas Ranft[2], and Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institut de Biologie de l ENS, Ecole Normale Superieure, CNRS

Active matter has garnered significant attention in recent decades due to its numerous parallels with biological systems. Inspired by recent studies of biological tissues, such as cardiac cells, where constituent cell sizes periodically vary, a new form of activity termed "pulsating active matter" has been introduced recently. We propose a model of a pulsating active solid, consisting of size-changing particles linked by a triangular spring network. Despite the fixed connectivity, our model exhibits a variety of patterns and topological phase defects, akin to previous studies. Additionally, we explore the elastic continuum limit, which success-

fully predicts several essential features of the microscopic model. We conclude by highlighting intriguing properties of this system and its different potential parallels.

Invited Talk DY 15.11 Tue 12:30 H47

Emergent correlations and boundary fluctuations in epithelial cell sheets — •Silke Henkes — Lorentz Institute, Leiden University, Leiden, The Netherlands

In soft active materials, the driving motion of individual constituents competes with their mechanical interactions, giving rise to active liquids, solids or glasses. An especially important example of this are epithelial cell sheets, which form a barrier function in the body and where the active crawling motion of cells over the substrate acts against cell-cell adhesion and repulsion.

I will show that a minimal model of cell sheets with uncorrelated activity, based on active Brownian dynamics and a vertex model, is a good quantitative match to data from two experiments on corneal and MDCK cell sheets. Its core feature is an emergent correlation length, arising from the diffusive spread of active forces through an elastic solid. This is a very general result that emerges in many active solids.

The boundary of such cell sheets exhibits a 'fingering instability' where the initially straight boundary develops large, spatiotemporally correlated fluctuations. Despite previous interpretations within many frameworks as an instability, I will show that it can be fully explained as arising from the active correlations of the cell sheets driving the boundary.

DY 16: Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)

Time: Tuesday 14:00–15:30 Location: H37

DY 16.1 Tue 14:00 H37

Power-law banded random matrices as models for quantum many-body Hamiltonians — •Wouter Buijsman[1], Masudul Haque[2,1], and Ivan M. Khaymovich[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]TU Dresden, Institute of Theoretical Physics, Dresden, Germany — [3]Nordita, Stockholm, Sweden

Hamiltonians of one-dimensional, disordered single-particle sytems with long-range hoppings can naturally be modeled by power-law banded random matrices. In this picture, the phase diagram of power-law banded random matrices show an ergodic, weakly ergodic, and localized phase. Motivated by modern developments on ergodicity breaking and localization in interacting quantum many-body systems, we study many-body interpretations of such random matrices. We discuss a number of ways to label the basis states with many-body configurations, and compare the physical properties of the resulting Hamiltonians. Specifically, we study the scaling of the many-body entanglement entropy with system size for eigenstates at both the bulk and the edge of the spectra. Using a scaling analysis on the full sets of eigenstates, we subsequently provide a quantitative picture of the phase diagram. We elaborate on the physical relevance of this interpretation of random matrix models for quantum many-body systems.

DY 16.2 Tue 14:15 H37

Escaping the Krylov space during reorthogonalization — •Max Pieper, Jannis Eckseler, and Jürgen Schnack — Universität Bielefeld

Krylov complexity [1] is often used as a measure of complexity in quantum many-body-systems. During its calculation, the Lanzcos algorithm is used to construct an operator basis. Due to the poor orthogonality of the resulting basis reorthogonalization is often employed [2]. We investigate how using reorthogonalization causes the Lanczos algorithm to accumulate non-Krylov basis elements. We suspect this to negatively affect the Krylov algorithm.

[1] D. E. Parker et al. Phys. Rev. X 9, 041017 (2019)
[2] E. Rabinovici et al. JHEP 06, 062 (2021)

DY 16.3 Tue 14:30 H37

An estimate of the equilibration time based on the operator growth hypothesis — •Merlin Füllgraf, Jiaozi Wang, and Jochen Gemmer — Universität Osnabrück

We study the equilibration times T_{eq} of local observables in quantum chaotic systems by considering their auto-correlation functions. Based on the recursion method, we suggest a scheme to estimate T_{eq} from the corresponding Lanczos coefficients. We numerically find that, if an observable follows the *operator growth hypothesis*, a finite number of Lanczos coefficients is sufficient for a reasonable estimate of the equilibration time. This implies that equilibration occurs on a realistic time scale much shorter than the life of the universe. The numerical findings are further supported by analytical arguments.

DY 16.4 Tue 14:45 H37

Effects of chaos in Bose-Hubbard systems with few degrees of freedom. The smallest possible heat engine? — •Viviane Bauer, Nico Fink, and James Anglin — Physics Department and Research Center OSCAR, RPTU Kaiserslautern-Landau

Microscopic engines are a research focus in both biochemistry and nanotechnology. While other forms of engines besides heat engines are also being considered, the fully microscopic limit of a heat engine is a fundamentally important problem in physics. What happens to thermodynamics when not only the working fluid and mechanism of a heat engine, but even the hot and cold reservoirs are microscopic?

To realize such microscopic heat baths, we turn to the process of chaotic ergodization, studied in Bose-Hubbard dimers and trimers.

One realization we currently study is based on two Bose-Hubbard trimers, which allow energy and particle transport between them. The particle transport is furthermore coupled to a mass, so our engine works against a force to lift it. Moreover, we have identified a dynamic mechanism which can stabilize this lifting process. The result is a system which operates just like a heat engine, except for being fully microscopic. The structure of coupled chaotic subsystems both supports and requires an understanding of the fully microscopic heat engine in terms of open-system control.

DY 16.5 Tue 15:00 H37

Impurity coupled to the SYK bath — •Anastasia Enckell and Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

System-plus-bath models play an important role in addressing fundamental questions in condensed matter physics. One challenging aspect is modelling the bath, which is often approached using free-particle or open quantum system frameworks. Here, we explore the Sachdev-Ye-Kitaev (SYK) model as a new kind of quantum bath with unique properties, including the absence of quasiparticles, maximal chaos, and non-integrability, which make it a valuable framework for studying system-plus-bath interactions. We study the time evolution of the occupation of an impurity coupled to the SYK bath following a quench. From the Kadanoff-Baym equations for a noninteracting impurity, we see that the only relevant property for the impurity occupation is a combination of hybridisation and density of states of the bath. These parameters can be adjusted in order to model the impurity coupled to any bath of interest. Using this approach, we can study the impurity dynamics coupled to the SYK bath by making suitable changes to the hybridisation in impurity plus Fermi bath setting, which significantly simplifies the task. We observe oscillatory dynamics of the impurity at zero temperature, with the oscillations decreasing as the temperature increases. This behaviour contrasts with that of a free-particle bath and suggests interesting underlying physics.

DY 16.6 Tue 15:15 H37

Thermal-relaxation asymmetry in fluctuating hydrodynamics — •Felipe Pereira-Alves and Aljaž Godec — Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

It was theoretically predicted and recently experimentally confirmed that small systems, such as trapped colloidal particles quenched far from equilibrium, heat up faster than they cool down. The phenomenon was coined thermal-relaxation asymmetry. The proposed physical explanation of the asymmetry instigated intriguing questions about its existence in the thermodynamic limit. Here we investigate thermal relaxation dynamics in far-from-equilibrium temperature quenches on the level of fluctuating hydrodynamics of short- and long-range (logarithmically) interacting many-body systems. We prove the existence of a strict asymmetry for any temperature quench for both, short- and long-range interactions. Remarkably, in contrast to small systems, there is no "close-to-equilibrium" regime of quenches for which heating and cooling are symmetric. Notably, we find that relaxation is self-similar up to the relaxation time, and uncover intricate differences between short- and long-range interactions.

DY 17: Focus Session: Nonlinear Dynamics in Biological Systems II (joint session DY/BP)

Nonlinear dynamics play a central role for biological systems to achieve remarkable complexity and adaptability. They underlie processes where small changes cascade into large effects, critical thresholds drive transitions, and feedback mechanisms maintain intricate balances. Biological systems are often far from equilibrium, exhibiting behaviors shaped by competing forces, stochastic fluctuations and emergent behavior. From the amplification of sensory signals near bifurcation points to the development of turbulence, concepts from nonlinear dynamics provide a unifying framework for studying patterns, stability, and collective behavior in living systems. This focus session explores the richness of nonlinear dynamics across biological scales, from molecular circuits to population-level phenomena, spanning vastly different fields from cardiac dynamics, embryogenesis and cell motility to active fluids, condensates and origin of life. Through theoretical models, experimental insights, and computational approaches, the talks illustrate how nonlinear-dynamics principles unravel the mechanisms driving function and complexity in biology, offering new perspectives across disciplines.

Organized by Philip Bittihn (Göttingen), Stefan Klumpp (Göttingen), and Carsten Beta (Potsdam)

Time: Tuesday 14:00–15:15 Location: H43

Invited Talk DY 17.1 Tue 14:00 H43

Mechanistic origins of temperature scaling in the early embryonic cell cycle — •Lendert Gelens — Laboratory of Dynamics in Biological Systems, Department of Cellular and Molecular Medicine, KU Leuven, Herestraat, 49, Leuven, Belgium

Temperature profoundly impacts organismal physiology and ecological dynamics, particularly affecting ectothermic species and making them especially vulnerable to climate shifts. Even though complex physiological processes usually involve dozens of enzymes, empirically it is found that the rates of these processes often obey the Arrhenius equation, which was originally derived for single enzyme-catalyzed reactions. Here we have examined the temperature scaling of the early embryonic cell cycle, with the goal of understanding why the Arrhenius equation approximately holds, and why it breaks down at temperature extremes.

Using experimental data from different frog, fish, fly, and worm species, we find that the apparent activation energies for the early embryonic cell cycle for diverse ectotherms are all similar. Computational modeling and experiments with frog egg extracts show that the non-Arrhenius scaling can be accounted for by biphasic temperature scaling in critical individual components of the cell cycle oscillator circuit, in combination with imbalances in the activation energies for different partially rate-determining enzymes. These findings provide mechanistic insights into the dynamic interplay between temperature and complex biochemical processes, and into why biological systems fail at extreme temperatures.

DY 17.2 Tue 14:30 H43

Reshaping morphogen gradients through porous tissue architecture — •Diana Khoromskaia[1,2] and Zena Hadjivasiliou[1,2,3] — [1]Francis Crick Institute, London, United Kingdom — [2]University College London, London, United Kingdom — [3]London Centre for Nanotechnology, London, United Kingdom

The morphogenesis of tissues during embryonic development is controlled by concentration gradients of morphogens – signalling molecules whose readout determines cell fate decisions. How the spread of morphogens is affected in tissues with complex geometry and spatially heterogeneous architecture is not well understood. To address this question, we introduce a porous vertex model, by explicitly considering the network of extracellular spaces between the cells. Morphogens produced by source cells disperse through the tissue via three modes of transport: extracellular diffusion, membrane-bound diffusion, and cell-based transport through recycling. With this model we investigate numerically and analytically how cell-scale geometry, such as cell size, cell shape anisotropy, and cell distance, influences effective diffusion and degradation of morphogens at tissue-scale. We further show that a non-linear coupling between cell packing and morphogen concentration renders the morphogen gradient robust to perturbations, for instance by locally buffering fluctuations in the production. Our characterisation of tissues as active porous materials provides new insights into how morphogenesis and cell fate determination may interact during embryonic development.

DY 17.3 Tue 14:45 H43

Active viscoelastic condensates provide controllable mechanical anchor points — •Oliver Paulin[1], Luise Zieger[2,3], Júlia Garcia-Baucells[5], Alexander Dammermann[5], Sebastian Aland[2,3,4], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]TU Bergakademie Freiberg — [3]HTW Dresden — [4]Center for Systems Biology, Dresden — [5]Max Perutz Labs, University of Vienna

Many biological materials must couple mechanical strength with the ability to rapidly self-assemble at a specific location. In particular, biomolecular condensates readily self-assemble via phase separation, but may also need to anchor external forces to fulfil their function. Spatial localisation of condensate formation can be controlled by active cores that preferentially drive the production of condensate material at a particular point, while resistance to external forces can be facilitated by viscoelastic material properties. Here, we develop a continuum model of viscoelastic growth around an active core, and investigate the results in a spherically symmetric geometry. We find that viscoelastic stresses restrict condensate growth, but also impart resistance to deformation. We investigate the effect of varying different mechanical properties on condensate growth and strength, and also study how strain-dependent material incorporation may limit the maximum rate of growth. Finally, we compare the predictions of our model to experimental data from centrosomes in C. elegans embryos, identifying a parameter regime in which rapid growth can be combined with appropriate mechanical strength.

DY 17.4 Tue 15:00 H43

Modelling cell crawling on different substrate stiffness — Sohei Nakamura and •Mitsusuke Tarama — Kyushu University, Fukuoka, Japan

Crawling cells sense the mechanical properties of the underlying substrate and change their dynamics accordingly. This ability called durotaxis is of great importance in various biological processes including development and homeostasis. In order to understand how intracellular chemical reactions and cellular mechanics give rise to durotaxis, we constructed a simple model from reaction diffusion equations for intracellular chemical compounds and force balance equations for the intracellular mechanics including the effect of the substrate stiffness. We found that within the model, the cell speed and diffusion coefficient change non-monotonically with the substrate stiffness, indicating the existence of an optimal substrate stiffness for migration. This non-monotonic behavior of the cell speed is consistent with experimental observations and can be understood to be caused by the competition between substrate adhesion and cell shape deformation. We further discuss cell migration on a patterned substrate.

DY 18: Pattern Formation

Time: Tuesday 14:00–15:30 Location: H47

DY 18.1 Tue 14:00 H47

Amplitude and envelope equation for the conserved-Hopf bifurcation — •Daniel Greve[1] and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Universität Münster, Münster, Germany — [2]Center for Nonlinear Science (CeNoS), Münster, Germany

Nonreciprocal interactions and conservation laws both play an important role in out-of-equilibrium pattern formation processes, e.g., in biochemical systems.[1,2] The generic large-scale oscillatory instability in such systems – the conserved-Hopf instability – is a central organizing element for such processes.[3,4] After classifying this instability within an extension of the Cross-Hohenberg[5] scheme, we use weakly nonlinear multi-scale analysis to obtain aclosed form (but nonlocal) slow time evolution equation for the spatiotemporal dynamics of the amplitude of fast time oscillations for thee example of two-species nonreciprocal Cahn-Hilliard models. Analytical results then reveal

a universal coarsening suppression in oscillatory phase separation. Finally, we demonstrate the agreement of the two levels of description in a comparison of numerical results for the reduced and full model.

[1] A. Dinelli, J. O'Byrne, A. Curatolo, Y. Zhao, P. Sollich, and J. Tailleur, Nat. Commun. 14, 7035 (2023). [2] F. Brauns and M. C. Marchetti, Phys. Rev. X 14, 021014 (2024). [3] A. Förtsch and W. Zimmermann, (2023), talk, DPG Spring Meeting, Dresden, and A. Förtsch, Ph.D. thesis, Bayreuth (2023). [4] T. Frohoff-Hülsmann and U. Thiele, Phys. Rev. Lett. 131, 107201 (2023). [5] M. C. Cross and P. C. Hohenberg, Rev. Mod. Phys. 65, 851 (1993).

DY 18.2 Tue 14:15 H47

Wavelength selection mechanism for turbulent superstructures in Rayleigh Bénard convection — •Fabián Alvarez-Garrido and Michael Wilczek — University of Bayreuth, Bayreuth, Germany

Large-scale flow patterns coexist with small-scale turbulence in high-aspect-ratio Rayleigh-Bénard cells. These flow patterns, known as turbulent superstructures, are significantly larger than convection rolls that emerge at the onset of convection. Direct numerical simulations of the Oberbeck-Boussinesq equations reveal that the size of these structures increases with the Rayleigh number. However, the mechanism behind this increase has not been elucidated.

Small-scale turbulence plays an important role in the redistribution of heat across the system. Motivated by how the background temperature gradient profile varies between the boundary layers and the bulk, we formulate effective equations for the large scales introducing a height-dependent turbulent thermal diffusivity. A sharp increase in the diffusivity renders the boundary layers effectively thermally insulating boundaries, fundamentally modifying how the fluid exchanges heat with its surroundings. A linear stability analysis of our model shows that this change in boundary conditions goes along with a change of the type of instability, which then leads to an increased wavelength of the flow patterns. These findings provide a mechanism to understand the increasing size of turbulent superstructures.

DY 18.3 Tue 14:30 H47

Turbulence-like behavior of spot patterns mediated by defects in the context of the liquid crystal light valve experiment — •Simon Navia[1], Marcel Clerc[2], and Pedro Aguilera[2] — [1]University of Münster, Münster Germany — [2]University of Chile, Santiago, Chile

The liquid crystal light valve experiment (LCLV) with optical feedback consists of a liquid crystal cell stimulated by a voltage and a photodiode that is coupled to the intensity of the light reaching the cell, thereby creating the optical feedback loop. This experiment exhibits a variety of complex spatiotemporal phenomena. This talk presents the experimental results of the observed formation of aperiodic spatiotemporal patterns in a quasi-one-dimensional channel, characterized by power-law scaling in the temporal and spatial-spectral density of the measured light intensity, as well as in the pseudo-envelope and pseudo-phase. Moreover, theoretically, the system is locally described as being near nascent bistability and spatial instability, from which a simplified model could be derived. We performed numerical simulations of this simplified model which show chaotic spatiotemporal patterns and spectral densities with exponents similar to those observed in the experiment.

[1]Aguilera-Rojas PJ, Clerc MG, Navia S. Opt Lett. 2024 doi: 10.1364/OL.522830.

[2]Verschueren N, Bortolozzo U, Clerc MG, Residori S. Phys Rev Lett. 2013 doi: 10.1103/PhysRevLett.110.104101.

DY 18.4 Tue 14:45 H47

Efficient formation of Turing patterns using physical interactions — •Cathelijne ter Burg, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organisation, Am Fassberg 17, Gottingen 37077, Germany

Turing patterns arise when an activating and an inhibitory component drive local activation and global inhibition of their production. Physical interactions between the components can facilitate such patterns. Using a thermodynamically-consistent version of such a model, we show that physical interactions lower the energetic requirements for forming patterns of a given length scale. Stronger physical interactions thus permit pattern formation for systems that are less active. However, we also found a dynamic regime where structures of well-defined length scales evolve chaotically for very strong physical interactions. This regime emerges from an interplay of coarsening and spinodal decomposition of bulk phases. We conclude that physical interactions of intermediate strength are energetically optimal for forming stationary patterns of a well-defined length scale.

DY 18.5 Tue 15:00 H47

Numerical and Experimental Analysis of Multi-Soliton Interactions in Ultrafast Lasers — •Julia Lang and Georg Herink — Universität Bayreuth

Ultrafast lasers are excellent platforms for experimentally observing multi-soliton solutions of the nonlinear Schrödinger equation in real-time. Interactions between solitons are often neglected in common pulse propagation models. However, they generate a variety of nonlinear dynamics, which manifest in distinct soliton trajectories observed via real-time spectral interferometry. Here, we report on soliton interactions in two different classes of widely established laser systems, namely Kerr-lens mode-locked Ti:sapphire [1] and SESAM mode-locked Er:fiber [2] lasers. Laser system-specific components result in virtually opposite behaviour, i.e., in soliton attraction, repulsion and/or binding. We discuss their representations in the generalized Schrödinger equation and present one-to-one correspondences between experiment and theory.

[1] A Völkel et al. Intracavity Raman scattering couples soliton molecules with terahertz phonons. Nat Commun. 2022;13(1):2066.

[2] J. A. Lang et al. Controlling intracavity dual-comb soliton motion in a single-fiber laser. Sci Adv. 2024;10(2):eadk2290.

DY 18.6 Tue 15:15 H47

Self-similarity in 1 and 2-dimensional cellular automata — •Jens Christian Claussen — University of Birmingham, UK

Cellular automata with a localized single seed initial condition can exhibit deterministic time series with power-law scaling, which led us numerically to the identification of two universality (sub)classes within the Wolfram class IV cellular automata [1], where rule 90 (Sierpinski) and rule 150 are representatives of these classes. The generated time series can be analytically described by a tensorial Fibonacci iteration [2]. An exploration of 2-dimensional outer-totalistic cellular automata showed that fractals with more general one- or two-step self-similarity may exist, including a rule providing a triple replication, and generating a 2-dim spatial Sierpinski pattern. Here we also consider the more general question what variety of universality classes can be found, eventually extending the dynamics to more general algebraic structures. We show that in the 1-dimensional ECA case of a mod 2 dynamics indeed only the two self-similarity cases represented by rule 90 and rule 150 exist.

[1] J. Nagler and J.C.Claussen (2005) $1/f^{\alpha}$ spectra in elementary cellular automata and fractal signals, Phys. Rev. E 71, 067103 (2005) [2] Time evolution of the rule 150 cellular automaton activity from a Fibonacci iteration, J. Math. Phys 49, 062701 (2008)

DY 19: Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)

In this joint focused session of the divisions DY, HL, and TT, we bring together two dynamic areas of research: semiconductor quantum emitters and chaotic cavities. While quantum emitters in cavities represent an established building block for quantum information technologies, chaotic microcavities may promise novel design routes towards optimized cavity performance parameters. Experts from both fields will provide an overview of the current state of research, exploring the potential of chaotic and unconventional microcavities to enhance the emission of quantum states.

Organized by Sonja Barkhofen (University of Paderborn) and Christian Schneider (University of Oldenburg).

Time: Wednesday 9:30–12:15 Location: H17

Invited Talk DY 19.1 Wed 9:30 H17

From complex internal dynamics to emission characteristics control in quantum billiards — •Martina Hentschel — 1 Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

The field of mesoscopic physics has given access to new classes of fascinating model systems ranging from ballistic quantum dots via microcavity lasers to graphene billiards over the past decades. Their rich internal dynamics, subject to quantum chaos and often successfully accessed employing wave-particle correspondence in real and phase space, is directly related to their emission properties. Here, we illustrate this close connection for various examples and system classes. For optical microcavities, we vary the internal dynamics by changing the geometric shape of the resonator and explain how the far-field emission charac-

teristics is determined by the underlying steady probability distribution and a possibility to achieve directional emission required for microlasing devices with the Limaçon geometry. Placing sources into the cavity will affect the internal dynamics of the cavity by, taking the particle point-of-view, effectively changing the set of initial conditions, as observed for optical cavities as well as for graphene billiards in the form of Dirac fermion optics. A further way to change the dynamics of a system is the existence of anisotropies that can either be intrinsically present such as in bilayer graphene in the form of trigonal warping [1], or can be induced to a given system by, for example, applying a mechanical strain. [1] L. Seemann, A. Knothe, and M. Hentschel, New J. Phys. 26, 103045 (2024).

Invited Talk DY 19.2 Wed 10:00 H17

Positioning of microcavities around single emitters — •Tobias Huber-Loyola — Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Single emitters in solids are great sources of single and entangled photons for usage in quantum information technologies. Many emitters possess high internal quantum efficiency, majority of the emission into the zero-phonon line and controllable single charge spins that can be used as quantum memories or as resource to generate chains of entangled photons. However, due to their solid-state host, which usually comes with a high refractive index, the outcoupling of photons requires the use of nanophotonic structures such as waveguides or microcavities. In this talk, I will show how we place microcavities around pre-registered quantum dots using hyperspectral imaging and e-beam lithography and I will give an overview of how placement accuracy has different effects on the emitted photons' properties based on the type of cavity.

Invited Talk DY 19.3 Wed 10:30 H17

Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities — •Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, Germany

Optical microcavities play a fundamental role in many fields of basic and applied research in physics. A chaotic microcavity is a type of cavity where the light ray dynamics is (partially) chaotic [1]. This can occur in a microdisk cavity with a deformed boundary shape. Chaotic microcavities are ideal for studying ray-wave correspondence, or wave chaos, in open systems, allowing direct comparisons with experiments [2]. These cavities can also exhibit non-Hermitian phenomena such as reflectionless scattering modes [3] and exceptional points [4].

The light emission from chaotic microcavities has been studied exclusively within the classical domain. The effects of electromagnetic field quantization, including phenomena like entanglement, single-photon states, and squeezed light, remain unexplored in this context. In this talk, I will review my group's recent efforts to investigate classical emission from chaotic microcavities and quantum emission from semiconductor quantum dots embedded in conventional microcavities. Additionally, I will discuss the prospects for achieving genuine quantum emission from chaotic microcavities.

[1] H. Cao and J. Wiersig, Rev. Mod. Phys. 87, 61 (2015)
[2] X. Jiang et al., Science 358, 344 (2017)
[3] X. Jiang et al., Nat. Phys. 20, 109 (2023)
[4] C.-H. Yi et al., Phys. Rev. Lett. 120, 093902 (2018)

15 min. break

Invited Talk DY 19.4 Wed 11:15 H17

Correlations and statistics in cavity embedded quantum dot sources of quantum light — •Ana Predojevic — Stockholm University, Stockholm, Sweden

Single quantum dots coupled to photonic cavities are established emitters of single photons and entangled photon pairs. The cascaded generation of photon pairs intrinsically contains temporal correlations that negatively affect the ability of such sources to perform two-photon interference, hindering applications. I will show how such correlation interacts with decoherence and temporal postselection, and under what conditions temporal postselection could improve two-photon interference visibility. Our study identifies crucial parameters of the source and shows the way to achieve optimal performance. The single photons emitted by a quantum dot exhibit quantum statistics, which is usually verified in an autocorrelation measurement. Single photons can be subjected to more extensive tests of quantum nature, such as non-Gaussianity. However, there is little evidence that such a measurement can be made on pairs of photons. I will show that pairs of photons exhibit strongly non-classical properties that can be quantified. Our result is applicable to a wide range of quantum light sources and measurement methods.

Invited Talk DY 19.5 Wed 11:45 H17

Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum — •Dario Ballarini — CNR-NANOTEC, Lecce, Italy

Exciton-polaritons in semiconductor microcavities have demonstrated remarkable collective behaviors and nonlinear interactions. In this work, we introduce an alternative platform to study strong light-matter interactions within a waveguide configuration. Among other interesting phenomena and applications, such as dispersion engineering of waveguide exciton-polaritons or exciton tuning through the Stark effect [1,2], we highlight the demonstration of parametric nonlinearities, polariton lasing from bound-in-the-continuum (BIC) states, and the recent realization of polariton BICs operating at room temperature in 2D materials [3-5].

[1] Electrically controlled waveguide polariton laser, Optica 7, 1579 (2020). [2] Reconfigurable quantum fluid molecules of bound states in the continuum, Nature Physics 20, 61 (2024). [3] Polariton Bose-Einstein condensate from a bound state in the continuum, Nature 605, 447 (2022). [4] Emerging supersolidity from a polariton condensate in a photonic crystal waveguide, arXiv:2407.02373 (2024). [5] Strongly enhanced light-matter coupling of monolayer WS2 from a bound state in the continuum, Nature Materials 22, 964 (2023).

DY 20: Many-body Quantum Dynamics II (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: H37

DY 20.1 Wed 9:30 H37

The Sound of Entanglement — •Benjamin Orthner[1], Clemens Wenger[5], Johannes Kofler[2], Richard Küng[2], Enar de Dios Rodríguez[3], Martin Ringbauer[4], Alexander Ploier[2], and Philipp Haslinger[1] — [1]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Vienna, Austria — [2]Johannes Kepler University Linz, Austria — [3]Internationale Forschungszentrum Kulturwissenschaften, Kunstuniversität Linz, Austria — [4]University of Innsbruck, Austria — [5]Universität für Musik und darstellende Kunst Graz, Austria

This contribution presents *The Sound of Entanglement*, a project at the intersection of quantum physics, music, and visual art. At its core lies a Bell experiment setup, where polarization-entangled photon pairs are generated through spontaneous parametric down-conversion in a β-BBO crystal. The experiment acts as a quantum conductor, utilizing the quantum correlations between the photons to coordinate and influence the choices of live musicians in real-time, creating a performance guided by principles beyond classical physics.

This work seeks to make these abstract concepts more accessible and engaging to broader audiences by transforming them into tangible, sensory experiences. By combining live music with a dynamic light show, both controlled by the experiment, this project illustrates how advancements in technology, like those shaping the second quantum revolution, can redefine artistic expression and bridge the gap between science and art.

DY 20.2 Wed 9:45 H37

A Solvable Model for Full Eigenstate Thermalization — •Felix Fritzsch and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The Full Eigenstate Thermalization Hypothesis (Full ETH) aims to characterize thermalization in many-body quantum systems in terms of the dynamics of higher-order spatiotemporal correlation functions, going beyond the current standard ETH paradigm. In this talk, we introduce a solvable random matrix model for many-body quantum dynamics in which the asymptotic dynamics of generalized out-of-time-order correlation functions can be exactly obtained in the thermodynamic limit. The dynamics of this model naturally maps to dynamics on the lattice of non-crossing partitions, combinatorial structures underlying the mathematics of Free Probability and Full ETH. We demonstrate how local observables approach asymptotic freeness at late times and explicitly characterize all relevant time scales. We confirm our analytical results with numerical simulations performed directly in the thermodynamic limit.

DY 20.3 Wed 10:00 H37

Scrutinizing the Mori memory function for transport scenarios — •Scott Daniel Linz, Jiaozi Wang, Robin Steinigeweg, and Jochen Gemmer — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

Diffusion is a phenomenological hydrodynamic transport behavior that holds over a wide range of materials. Within condensed matter physics there is the opinion that as long as the area under the current-current correlation function

converges in time, one has a criterion for diffusive behavior of the corresponding spatiotemporal density dynamics. Attempts to derive this statement are notoriously challenging. We will first demonstrate that it is possible to construct correlation functions of some local density, where the area under a current-current correlation function converges, but the system is not diffusive. After this is demonstrated, we shall introduce a method based on the recursion method and the Mori memory formalism, that yields insight into whether or not a process is truly diffusive. The only disadvantage of this strategy is that one would have to know the behavior infinitely many Lanczos coefficients, whereas in practice one can only calculate a finite number of them in most cases. In the cases examined in this talk, however, the convergence or lack thereof becomes apparent to the naked eye with the finite amount of coefficients that were calculated.

DY 20.4 Wed 10:15 H37

Long-time Freeness in the Kicked Top — •Elisa Vallini and Silvia Pappalardi — University of Cologne, Köln, Germany

Recent work highlighted the importance of higher-order correlations in quantum dynamics for a deeper understanding of quantum chaos and thermalization. The full Eigenstate Thermalization Hypothesis, the framework encompassing correlations, can be formalized using the language of Free Probability theory. In this context, chaotic dynamics at long times are proposed to lead to free independence or "freeness" of observables. We investigate these issues in a paradigmatic semiclassical model - the kicked top - which exhibits a transition from integrability to chaos. Despite its simplicity, we identify several non-trivial features. By numerically studying 2n-point out-of-time-order correlators, we show that in the fully chaotic regime, long-time freeness is reached exponentially fast. These considerations lead us to introduce a large deviation theory for freeness that enables us to define and analyze the associated time scale. The numerical results confirm the existence of a hierarchy of different time scales, indicating a multifractal approach to freeness in this model. Our findings provide novel insights into the long-time behavior of chaotic dynamics and may have broader implications for the study of many-body quantum dynamics.

DY 20.5 Wed 10:30 H37

Periodically and aperiodically Thue-Morse driven long-range systems: from dynamical localization to slow dynamics — •VATSANA TIWARI — Indian Institute of Science Education and Research Bhopal, Bhopal, India

In this talk, I will discuss the impact of time-periodic and aperiodic field on power-law random banded matrix (PLRBM) model where variation in the power-law exponent yields a delocalization-to-localization phase transition. We investigate the periodically driven PLRBM model with the help of the static measures such as level spacing ratio and generalized inverse participation ratio and report the drive-induced multifractal to localization transition. The transport study of the periodically driven system demonstrates the transition from diffusive to logarithmically slow relaxation at dynamical localization point. Extending our analysis to the aperiodic Thue-Morse driving, we find that specific driving parameters leads to the *exact dynamical localization* in a disordered-free long-range model regardless of the long-range parameter. In the disordered case, the localized phase exhibits a long prethermal plateau followed by diffusion to an infinite temperature state, while the delocalized phase shows immediate diffusion. Additionally, we compare this with a quasi-periodic model that also undergoes a localization-delocalization transition, noting that, unlike the delocalized side of the disordered long-range model, it features a prolonged plateau followed by diffusion to the infinite temperature state.

DY 20.6 Wed 10:45 H37

Symmetry-Resolved Out-of-Time-Order Correlators with Projected Matrix Product Operators — •Martina Gisti, David Luitz, and Maxime Debertolis — Institute of Physics, University of Bonn, Nußallee 12, 53115 Bonn, Germany

Out-of-Time-Order Correlators (OTOCs) are key measures of quantum many-body chaos and information spreading. We systematically analyse OTOCs as a function of particle number for interacting spinless fermions in one dimension. With the concept of generalized operator charge, we develop a formalism for the time evolution of symmetry-projected matrix product operators, which we use to resolve the scrambling behaviour by particle number sector. Our results reveal a crossover from ballistic to diffusive dynamics at early times and a saturation regime at late times.

DY 20.7 Wed 11:00 H37

Revealing ultrafast phonon mediated inter-valley scattering through transient absorption and high harmonic spectroscopies — •Kevin Lively[1], Shunsuke Sato[2,3], Guillermo Albareda[2,4], Angel Rubio[2], and Aaron Kelly[2] — [1]Deutsches Zentrum für Luft- und Raumfahrt — [2]Max Planck Institute for the Structure and Dynamics of Matter — [3]University of Tsukuba — [4]Ideaded

Processes involving ultrafast laser driven electron-phonon dynamics play a fundamental role in the response of quantum systems in a growing number of situations of interest, as evinced by phenomena such as strongly driven phase transitions and light driven engineering of material properties. To show how these processes can be captured from a computational perspective, we simulate the transient absorption spectra and high-harmonic generation signals associated with valley selective excitation and intraband charge-carrier relaxation in monolayer hexagonal boron nitride. We show that the multitrajectory Ehrenfest dynamics approach, implemented in combination with real-time time-dependent density-functional theory and tight-binding models, offers a simple, accurate, and efficient method to study ultrafast electron-phonon coupled phenomena in solids under diverse pump-probe regimes which can be easily incorporated into the majority of real-time ab initio software packages.

15 min. break

DY 20.8 Wed 11:30 H37

Chiral basis for qubits and decay of spin-helix states — •Frank Göhmann — Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

In a recent cold-atom experiment by the Ketterle group at MIT one-dimensional spin-helix states could be prepared and their time evolution induced by the XXZ Hamiltonian could be observed. The experiment allows to adjust the anisotropy parameter of the latter. For the special case of the XX model we describe the spatio-temporal decay of a transversal spin helix explicitly. The helix pattern stays stable in space, but has a non-trivial time-dependent decay amplitude which is of scaling form and is governed by a universal function that can be represented as a semi-infinite determinant related to the discrete Bessel kernel. This representation is valid for all times, is numerically utterly efficient and allows us to obtain the long-time asymptotics of the function. Our work is a rare example of a quench that has been experimentally realized and for which the full time dependence could be calculated exactly.

V. Popkov, X. Zhang, F. Göhmann and A. Klümper, *Chiral basis for qubits and spin helix decay*, Phys. Rev. Lett. **132** (2024) 220404 (5pp)

DY 20.9 Wed 11:45 H37

Towards the chaotic melting at low energies in large systems — •Mathias Steinhuber[1], Jonas Rigo[2], Juan Diego Urbina[1], Klaus Richter[1], and Markus Schmitt[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), Jülich, Germany

Thinking in a classical phase space picture, a many-body ground state should be localized around the minimum of the classical mean-field energy landscape with stable integrable features. But here, we investigate many-body ground states on chaotic features, as the phase space picture is actually fragile if we increase the system size and keep the quantum scale (the effective Plank constant $\hbar_{\text{eff}}$) fixed. With the new degrees of freedom, we disturb the energy landscape in the classical limit more and more such that classical chaos is present even for low energies. We show this phenomenon, called 'chaotic melting' [1,2], is indeed happening in the Bose-Hubbard system with disorder. By using neural quantum states we can push quantum calculations for ground states to large systems and find signatures of chaos at the ground state. An intriguing application for these large systems is that the Bose-Hubbard Hamiltonian with disorder is an effective model for transmon arrays which are a prime candidate for quantum computer hardware. Therefore we also gain access to quantum states describing a possible quantum computer with chaotic features.

[1] S.-D. Börner, et al. Phys. Rev. Research 6, 033128 (2024)
[2] J. Chávez-Carlos, et al. arXiv: 2310.17698 (2024)

DY 20.10 Wed 12:00 H37

Period n-tupling in driven two level systems — •Dhruv Deshmukh and Joachim Ankerhold — Institute for complex quantum systems, Ulm University, Germany

This talk presents the necessary and sufficient conditions for realizing period n-tupling phenomena in periodically driven two-level systems. For the specific case of a two-level system driven linearly by a sinusoidal drive, we numerically identify the drive parameters that enable period n-tupling. Experimental results verifying period doubling in an NV centre driven by a microwave drive, are given. Further, we show that period quadrupling drives yield pulses which are much faster than the standard (Rabi) $\pi/2$ and π pulses built from weak drives. These stronger and faster pulses can be utilized for qubit manipulation, enabling faster gates and more efficient pulse sequences. Moreover, they inspire a new strategy for constructing efficient pulses using a Floquet theory approach to optimal control. Furthermore, the drive parameters could also be set to achieve period-1 (stroboscopic) dynamical freezing. The fragility of such phenomena can be exploited for sensing applications, as illustrated with an example in magnetometry.

DY 20.11 Wed 12:15 H37

Efficient computation of cumulant evolution and full counting statistics: application to infinite temperature quantum spin chains — •Angelo Valli[1,2], Cătălin Pascu Moca[2,3], Miklós Antal Werner[1,4], Márton Kormos[1,2], Žiga Krajnik[5], and Tomaž Prosen[6] — [1]Budapest University of Technology

and Economics, Muegyetem rkp. 3., 1111 Budapest, Hungary — [2]HUN-REN BME Quantum Dynamics and Correlations Research Group — [3]University of Oradea, 410087, Oradea, Romania — [4]HUN-REN Wigner Research Centre for Physics, P.O. Box 49, 1525 Budapest, Hungary — [5]New York University, 726 Broadway, New York, NY 10003, USA — [6]University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia

We propose a numerical method to efficiently compute quantum generating functions (QGF) for a wide class of observables in one-dimensional quantum systems at high temperature. We obtain high-accuracy estimates for the cumulants and reconstruct full counting statistics from the QGF. We demonstrate its potential on spin S=1/2 anisotropic Heisenberg chain, where we can reach time scales hitherto inaccessible to state-of-the-art classical and quantum simulations. Our results are in excellent agreement with a recent Google Quantum AI experiment [2] and challenge the conjecture of the Kardar-Parisi-Zhang universality for isotropic integrable quantum spin chains.

[1] A. Valli et al. arXiv:2409.14442 (2024)
[2] E. Rozenberg et al. Science 384, 48-53 (2024)

DY 20.12 Wed 12:30 H37

Machine learning approach to study the properties of ground and excited states in the 1D Bose-Hubbard model — •Yilun Gao[1], Alberto Rodríguez González[2,3], and Rudolf A. Römer[1] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL — [2]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain — [3]Instituto Universitario de Física Fundamental y Matemáticas (IUFFyM), Universidad de Salamanca, E-37008 Salamanca, Spain

Many-body quantum interacting systems continue to play a key role in theoretical developments of modern condensed matter physics. Various numerical techniques have been used to explore the features of these many-body systems. Exact diagonalization methods, which most results going beyond ground state properties are based on, can only deal with small system sizes $L \lesssim 15$ because the Hilbert dimensions grow exponentially in L. Recently, deep learning has emerged as a numerical technique that uses strategies of artificial intelligence to predict the physics of such systems. Here we focus on the Bose-Hubbard chain and use HubbardNet [1] to investigate the physics of ground and excited states. We show that the energies and wavefunctions predicted by HubbardNet agree well with the ones calculated by exact diagonalization over a broad range of interaction strengths. We investigate the properties of the eigenstates via their finite-size generalized fractal dimensions. [1] Ziyan Zhu, et al., HubbardNet: Efficient predictions of the Bose-Hubbard model spectrum with deep neural networks, Phys. Rev. Res., **5**, 043084 (2023)

DY 20.13 Wed 12:45 H37

Entanglement Transitions in Quantum Games through Reinforcement Learning — •Giovanni Cemin[1], Marin Bukov[1], and Markus Schmitt[2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Regensburg, Regensburg, Germany — [3]Forschungszentrum Jülich, Institute of Quantum Control, Jülich, Germany

In this research, we investigate the dynamics of entanglement in Cliord circuits by employing a reinforcement learning (RL) algorithm in competition with a random agent. The RL agent is designed to strategically place gates that decrease entanglement, while the random agent aims to increase entanglement. This interaction between the two agents results in an entanglement transition, the nature of which is induced by the level of information accessible by the RL agent. By systematically varying the information provided to the RL agent, we analyze its impact on the transition characteristics. Our findings provide new insights into the interplay between entanglement manipulation and information constraints, shedding light on the fundamental mechanisms governing quantum circuit dynamics.

DY 21: Granular Matter

Time: Wednesday 9:30–11:30 Location: H43

DY 21.1 Wed 9:30 H43

Coarsening dynamics of ferrogranular networks for different granular temperatures — •Ali Lakkis[1], Matthias Biersack[1], Oksana Bilous[2], Pedro A. Sanchez[2], Sofia S. Kantorovich[2], and Reinhard Richter[1] — [1]University of Bayreuth, Experimental Physics 5, Universitätsstr. 30, 97440 Bayreuth, Germany — [2]University of Vienna, Faculty of Physics, Kolingasse 14-16, 1090 Vienna, Austria

We are exploring in experiments the aggregation process in a shaken granular mixture of glass and magnetized steel beads, filled in a horizontal vessel. After the shaking amplitude is suddenly decreased, the magnetized beads form a transient network that coarsens in time into compact clusters [1]. Recently it has been quantified how a homogeneous magnetic field B oriented in vertical direction impedes the emergence and growth of the networks [2,3], where the mean degree $\bar{k}$ of a node serves as an order parameter. Here we explore the impact of the acceleration amplitude Γ onto the velocity distribution of the particles, their granular temperature, and the coarsening dynamics of the network, i.e. $\bar{k}(\Gamma)$.

[1] A. Kögel, R. Maretzki, E. S. Pyanzina, P. A. Sánchez, S. S. Kantorovich, R. Richter *Soft Matter*, 14 (2018) 1001.
[2] M. Biersack, A. Lakkis, R. Richter, O. Bilous, P. A. Sánchez, S. S. Kantorovich *Phys. Rev. E*, 108 (2023) 054905.
[3] A. Lakkis, M. Biersack, O. Bilous, S. S. Kantorovich, R. Richter, *J. Magn. Magn. Mater* 589 (2024) 171620.

DY 21.2 Wed 9:45 H43

Decoding diffusion: insights into ferrogranulate dynamics under competing interactions — •Oksana Bilous[1], Kirill Okrugin[1], Pedro A. Sánchez[1], Ali Lakkis[2], Matthias Biersack[2], Reinhard Richter[2], and Sofia Kantorovich[1] — [1]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria — [2]Experimental Physics 5, University of Bayreuth, Bayreuth, Germany

Granulates with magnetic and non-magnetic particles exhibit unique diffusion behaviors, challenging conventional models. Using experiments and Langevin dynamics simulations, we studied their dynamics under varying magnetic fields and particle compositions.

In steady states, entropic, dipolar, and field-induced forces create distinct distributions: single particles, cluster-bound particles, and migrating particles transitioning between these states. Sub-diffusion occurs exclusively in magnetic particles within clusters, independent of external fields or concentrations. Glass particles remain non-aggregated.

Velocity distributions in high-shaking experiments validate the use of Langevin dynamics, revealing an effective temperature that links structural separations to thermodynamic scaling laws. These findings deepen our understanding of diffusion and force interactions in complex granular systems.

DY 21.3 Wed 10:00 H43

Advances and challenges in experiments with granular gases of rod-like particles — •Dmitry Puzyrev[1], Torsten Trittel[2,1], Kirsten Harth[2,1], Mahdieh Mohammadi[2], Raul Cruz Hidalgo[3], and Ralf Stannarius[2,1] — [1]Otto von Guericke University, Magdeburg, Germany — [2]Brandenburg University of Applied Sciences, Brandenburg an der Havel, Germany — [3]Univerisity of Navarra, Pamplona, Spain

Granular gases, i.e., ensembles of free-moving macroscopic particles which collide inelastically, demonstrate fascinating dynamical effects like unusual cooling properties, violation of energy equipartition, clustering, and spontaneous collective movement. Our investigation is focused on 3D microgravity experiments with ensembles of rod-like particles [1] and their mixtures. With the help of machine learning methods, we have obtained various statistical properties for the mixture of thinner and thicker rods [2]. Kinetic energy partitions and collision numbers were extracted for both vibrational heating and homogeneous cooling regimes. The systems in question pose some conundrums, such as cooling rates larger that theoretically predicted or accumulation of kinetic energy in rotational DOF which is hard to observe in the experiment. Currently, the granular gas mixture of shorter and longer rods is under analysis. Our studies are funded within by the DLR projects VICKI, EVA-II, JACKS, and KORDYGA (50WM2252, 50WK2348, 50WM2340, and 50WM2242). [1] K. Harth et al., Rev. Lett., 120, 214301 (2018) [2] Puzyrev et al., npj Microgravity, 10, 36 (2024)

DY 21.4 Wed 10:15 H43

Force networks in granular experiments: From topology to dynamics — •Lou Kondic — Department of Mathematical Sciences, NJIT, Newark, NJ, USA

We will discuss force networks that spontaneously form in particulate-based systems. These networks, most commonly known as 'force chains' in granular systems, are dynamic structures of fundamental importance for revealing the underlying causes of many physical phenomena involved in the statics and dynamics of particulate-based systems. While these networks emerging from discrete element simulations have been analyzed extensively, the analysis of networks found in physical experiments is far less developed. The presentation will focus on applications of algebraic topology, particularly persistent homology (PH) to analysis of such networks. PH allows for a simplified representation of complex interaction fields in both two and three spatial dimensions in terms of persistent diagrams (PDs) that are essentially point clouds. These point clouds could be compared meaningfully, allowing for the analysis of the underlying systems' static and dynamic properties. The presentation will focus on applications of topological data analysis of such networks found in photoelastic experiments involving an intruder moving in a stick-slip fashion through a 2D granular domain. We will particularly focus on exploring the predictability potential of the considered topological measures.

DY 21.5 Wed 10:30 H43

Crystallization dynamics in a dense sphere system — •Frank Rietz and Matthias Schröter — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen

When balls are thrown into a box and subsequently agitated, they tend to arrange themselves in a denser configuration, as observed in numerous experiments. However, a barrier is typically present at random close packing, which occupies approximately 64% of the available space. The spheres remain in their densest amorphous state and do not undergo a phase transition to a denser crystalline structure with a space-filling ratio of 74%. In our experiment, we successfully surmounted this barrier and observed the emergence of crystallization events from the disordered phase [1].

Initially, we observed the formation of groups of a few spheres that fluctuated between a disordered and a nucleated state. In rare instances when the balls remained in the ordered state, further investigation was conducted into their preceding conditions. This approach enables us to address the question of why the majority of precursors are not stable, while a few of them undergo growth to become part of the larger crystals of FCC and HCP structures that never dissolve.

[1] F. Rietz, C. Radin, H. L. Swinney, M. Schröter: Nucleation in sheared granular matter, Phys. Rev. Lett. 120, 055701 (2018)

DY 21.6 Wed 10:45 H43

Vibro-fluidized beds: A systematic dynamics study utilizing Diffusing Wave Spectroscopy — •Marlo Kunzner, Christopher Mayo, Matthias Sperl, and Jan Philipp Gabriel — Deutsches Zentrum für Luft- und Raumfahrt, Köln, Deutschland

Using a granular vibration fluidised bed, we demonstrate how our granular model system of polystyrene spheres becomes denser over time through different excitation amplitudes and how the heterogeneous dynamics of the system can be resolved with diffusing wave spectroscopy(DWS) measurements. We extract mean-square displacements from the DWS correlation functions of the sinusoidal excited system and model the excitation to extract the ballistic and diffusive time constants, as well as caging sizes, depending on applied acceleration and excitation time. At low excitations we observe a sub-diffusion power law behaviour of the MSD indicating potentially a glassy system.

DY 21.7 Wed 11:00 H43

Simulation of Spherical Particles as a Granular Gas in Microgravity: A Comparison with Experimental Results — •Mahdieh Mohammadi[1], Torsten Trittel[1], Rau'l Cruz Hidalgo[2], Dmitry Puzyrev[3], Ralf Stannarius[1], and Kirsten Harth[1] — [1]Department of Engineering, Brandeburg University of Applied Sciences, Magdeburger Str. 50, 14770 Brandenburg an der Havel,Germany — [2]Departamento de Física y Matemática Aplicada, Facultad de Ciencias , Universidad de Navarra, Pamplona, Spain — [3]MTRM, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Simulation of a Granular Gas of Frictional Spherical Particles in Microgravity: A Comparison with Experimental Results

We investigate dilute granular ensembles (granular gases) of rough spheres in Microgravity, both in experiment and simulation. The experiment examines the time scale (Haff time) for energy dissipation in an initially excited granular gas, the collision statistics, and the distribution of angular and translational velocities. We aim to determine how well the experimental results can be reproduced by a DEM simulation. A variety of criteria were tested, including different restitution coefficients. One goal of the simulation is to analyze the effect of different collision parameters on the statistical properties of a granular gas. Second, we aim demonstrate how the model can effectively replicate the experimental data, with a strong correlation between the translation energy in the model and experimental data.

We thank DLR for funding in grants 50WM2242 / 50WM2340.

DY 21.8 Wed 11:15 H43

Aerodynamic origin of aeolian mineral dust emission — Sandesh Kamath[1,2], Yaping Shao[2], and •Eric Parteli[1] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Institut für Geophysik und Meteorologie, Universität zu Köln

Atmospheric dust aerosol particles exert a substantial impact on climate, radiation balance, and various other components of the Earth's system. However, state-of-the-art climate models rely on empiric parameterization schemes for the vertical dust flux at emission. While such schemes are derived from wind-tunnel simulations on flat granular beds, environmental soils are often characterized by a spatial distribution of non-erodible elements and crusts. Indeed, the vertical flux predicted by the various schemes often differs from observations by orders of magnitude. Here we develop a numerical tool for the particle-based simulation of wind-blown transport of granular particles in the atmospheric boundary layer. Our model accurately reproduces the observed minimal threshold wind shear velocity for direct fluid entrainment over the entire broad range of particle diameters from dust to gravel particles. However, we show that a topographic effect in polydisperse beds and soils with large non-erodible elements lowers the minimal threshold for dust entrainment substantially. This finding challenges our understanding that dust is mainly ejected at sand grain-bed collisions, rather than being directly entrained by wind. Our simulations show that dust can be emitted as single grains, as dust agglomerates, or coated on the surface of sand grains, depending on dust grain size.

DY 22: Poster: Statistical Physics

Time: Wednesday 10:00–12:00 Location: P3

DY 22.1 Wed 10:00 P3

Adaptive Quasi-Monte Carlo Quadrature for Concentrated Distributions in Bayesian Inference — •Jinyi Zhou and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

By its probabilistic formulation, Bayesian inference cures many of the problems of the traditional parameter-fitting approach, such as potential ill-posedness and the lack of reliable uncertainty estimates. However, for highly nonlinear and sensitive models, the Bayesian posterior distribution can become complex and is often concentrated in a small fraction of the parameter space. This challenges established sampling approaches, which typically perform well only for smooth distributions. We address this challenge with a novel adaptive Quasi-Monte Carlo (aQMC) quadrature method. This approach combines the highly uniform coverage of Quasi-Monte Carlo with a greedy iterative subdivision algorithm, concentrating the sampling in subdomains where the quadrature error is expected to be largest. In addition to testing on benchmark functions, we demonstrate our approach on a kinetic model from the field of catalysis. In this field, concentrated distributions are expected because, even with the best priors derived from quantum chemical calculations, uncertainties can span several orders of magnitude for the predicted catalytic response, whereas experimental data is highly accurate in comparison.

DY 22.2 Wed 10:00 P3

A novel mathematical model for the coupled binary-fluid surfactant system — •Alexandra Hardy, Steven McDonald, Abdallah Daddi-Moussa-Ider, and Elsen Tjhung — The Open University, Milton Keynes, UK

We propose a new binary-fluid surfactant mathematical model derived from modeling the surfactant molecules as dumbbells. By explicitly taking into account the molecules alignment, we gain new field variable p(r,t); the average orientation of surfactants. Combined with standard phase-field theory for binary fluids gives the system equations, which we both solve numerically and analytically. We employ a hybrid finite difference (FDM) and spectral method for the simulations. Whereas regular perturbation theory is used for the equilibrium solutions, facilitated by assuming weak coupling between surfactant and fluid. Three investigations are presented, firstly we demonstrate excellent agreement between simulation and the analytical solutions for a planar water-oil interface. Second, we prove that our model accurately predicts the decrease in surface tension with increasing surfactant concentration, in line with experiments and related theory. Finally, we show that our model is capable of preventing surfactant-laden droplet coalescence due to the added polarization field p(r,t).

DY 22.3 Wed 10:00 P3

Nonequilibrium mixture dynamics: a model for mobilities and its consequences — •Maryam Akaberian[1], Filipe C Thewes[1,3], Peter Sollich[1,2], and Matthias Krüger[1] — [1]University of Goettingen — [2]King's College London — [3]Max plank institute

extending the famous model b for the time evolution of a liquid mixture, we derive an approximate expression for the mobility matrix that couples the different mixture components. this approach is based on a single component fluid with particles that are artificially grouped into separate species labelled by "colors". The resulting mobility matrix depends on a single dimensionless parameter, which can be determined efficiently from experimental data or numerical simulations, and includes existing standard forms as special cases. we identify two distinct mobility regimes, corresponding to collective motion and interdiffusion, respectively, and show how they emerge from the microscopic properties of the fluid. as a test scenario, we study the dynamics after a thermal quench, providing a number of general relations and analytical insights from a gaussian theory. specifically, for systems with two or three components, analytical results for the time evolution of the equal time correlation function compare well to results of Monte Carlo simulations of a lattice gas. a rich behavior is observed, including the possibility of transient fractionation.

DY 22.4 Wed 10:00 P3

Transport in classical systems with fractionally charged excitations — •Jannis Waldmann, Malte Grunert, Max Grossmann, and Erich Runge — Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Interacting systems of charged particles can show fractionally charged excitations, as is well known from the Fractional Quantum Hall Effect of electrons in a magnetic field. Fractionally charged excitations in the absence of magnetic fields have also been predicted for certain lattices with geometric frustrations, e.g. for quantum mechanical models of spinless fermions on the criss-crossed checkerboard lattice [1,2]. Here, we present result on transport properties of classical particles with nearest-neighbor repulsion on a Kagome lattice. Using Monte Carlo simulations, we study the transition from classical hopping at high temperatures to transport dominated by half-charged quasi-particles for special filling factors at low temperatures. Furthermore, we provide evidence for a residual entropy at zero temperature and Andreev-like reflection at interfaces to 'normal', i.e. not frustrated systems.

[1] Fulde et al., Ann. Phys. (Leipzig) 11 (2002) 12, 892-900
[2] Pollmann et al., J. Magn. Magn. Mater. 310 (2007), 966-968

DY 22.5 Wed 10:00 P3

Diffusion and order in mixed lattice gas of hard squares — •Piotr Nowakowski[1], Niklas Raake[2], and Ana-Sunčana Smith[2,1] — [1]Institut Ruđer Bošković, Zagreb, Croatia — [2]Friedrich–Alexander–Universität Erlangen–Nürnberg, Erlangen, Germany

We study the diffusion in a crowded environment using a model system of a lattice gas composed of hard square particles of 1×1 and 2×2 size (measured in lattice constant units) undergoing a Brownian motion on a two-dimensional square lattice. For the whole range of concentrations of both types of particles, we numerically test the accuracy and efficiency of an approximation of the motion by a persistent random walk with one or two step memory. A good agreement is observed for very low and very high concentrations of particles.

Additionally, we look at the second order phase transition from a gas phase for low densities of 2×2 particles to a columnar phase. Surprisingly, it seems that the density of large particles at which the transition occurs is not affected by the presence of smaller particles. Moreover, in columnar phase the diffusion constant can be approximated by studying a one-dimensional system.

DY 22.6 Wed 10:00 P3

The bath *remembers*: how many time-scales can we probe through recoil? — •Rupayan Saha[1], Niloyendu Roy[2], Debankur Das[1], Clemens Bechinger[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Göttingen 37073, Germany — [2]Fachbereich Physik, Universität Konstanz, Konstanz 78457, Germany

Recoil experiments, where one studies the transient dynamics of a colloidal particle after driving it externally, are of particular importance to gain insight into the non-Markovian properties prevalent in visoelastic solvents such as micellar suspensions. In an earlier experimental study by Félix Ginot et al. [*New J. Phys. 24.12 (2022): 123013*], the *translational* recoil was found to be governed by a small number of distinct time scales, reproduced by a microscopic model using a small number of so-called bath particles. In this contribution, we investigate *orientational* recoil of such a colloidal probe in a viscoelastic fluid, which, in contrast, appears to exhibit a large number of time scales. In collaboration with experiment, we develop microscopic models to account for such observations, and develop driving protocols to dissect the various time scales involved in this process.

DY 22.7 Wed 10:00 P3

Large-deviation simulation of the coupling time distribution for the CFTP method applied to the heat bath Ising process — •Mathis Groenhagen, Alexander K. Hartmann, and Peter Werner — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Coupling from the past (CFTP), introduced by Propp and Wilson [1], is a version of the Markov-chain Monte Carlo method, which is capable of generating exact samples from a finite set with a particular distribution. The performance of the CFTP method for a given application can be characterized by the distribution of the CFTP method's random running time, the *coupling time* τ, for this application.

A large-deviation Monte Carlo algorithm, as described for example in [2], is used to sample these coupling times for the application of the CFTP method to a single-spin-update heat-bath process for the ferromagnetic two-dimensional square lattice Ising model without an external field. This yields the coupling time distributions over a wide range of coupling times τ down to probability densities of 10^{-80} for different lattice sizes L and temperatures T. These results give additional numerical evidence for the analytical results shown in [3].

[1] J. Propp, D. Willson, Random Struct. Algorithms **9**, 223-252 (1996).
[2] A. K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[3] A. Collevecchio, E.M. Elçi, T.M. Garoni et al., J Stat Phys **170**, 22-61 (2018).

DY 22.8 Wed 10:00 P3

Large-deviation simulations of non-equilibrium stochastic processes — •Chinmay Chandratre — Heinrichstr. 16, 26131 Oldenburg

For N non-interacting diffusing particles in a harmonic trap where the stiffness is switched randomly between μ_1 and μ_2, the joint distribution of particle positions has been exactly computed [1]. This allowed the computation, in the limit of $N \to \infty$, of the distribution of the position M_k of the k-th rightmost particle. It is governed by a universal scaling function with finite support and tunable shape. However, the behaviour for finite numbers of particles, where the large-deviation corrections become relevant, is analytically not known. Numerically, standard algorithms fail to access the majority of the support, particularly in the tails. Here, special large-deviation algorithms [2] are used to access the tails of the distribution, reaching probabilities as small as 10^{-200} or even smaller. This includes a highly general *black-box* algorithm suitable for studying a wide range of stochastic processes.

[1] Biroli, Marco and Kulkarni, Manas and Majumdar, Satya N. and Schehr, Grégory, Phys. Rev. E **109**, 032106 (2024)
[2] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 22.9 Wed 10:00 P3

Residual entropy of ice: A study based on transfer matrices — •De-Zhang Li[1], Yu-Jie Cen[2], Xin Wang[3], and Xiao-Bao Yang[4] — [1]Quantum Science Center of Guangdong-Hong Kong-Macao Greater Bay Area — [2]Institute of Materials Chemistry, Vienna University of Technology — [3]Department of Physics, City University of Hong Kong — [4]Department of Physics, South China University of Technology

The residual entropy of ice systems has long been a significant and intriguing issue in condensed-matter physics and statistical mechanics. This study focuses on two typical realistic ice systems: hexagonal ice (ice Ih) and cubic ice (ice Ic). We present a transfer-matrix description of the number of ice-ruled configurations for these systems. A transfer matrix M is constructed for ice Ic, where each element represents the number of ice-ruled configurations of a hexagonal monolayer under certain conditions. The product of M and M^T corresponds to a bilayer unit in the ice Ih lattice, thus forming an exact transfer matrix for ice Ih. Utilizing this, we show that the residual entropy of ice Ih is not less than that of ice Ic in the thermodynamic limit, first proved by Onsager in the 1960s. Additionally, we introduce an alternative transfer matrix M' for ice Ih based on a monolayer periodic unit. Various interesting properties of M, MM^T and M' are analyzed, including the sum of all elements, the element in the first row and first column, and the trace. Each property corresponds to the residual entropy of a certain 2-d ice model. This work provides an effective description, based on transfer matrices, for the residual entropies of various 2-d ice models.

DY 22.10 Wed 10:00 P3

Beyond mean-field kinetic theory of nematic self-propelled particles — •Benjamin Kohler, Horst-Holger Boltz, and Thomas Ihle — Institute for Physics, University of Greifswald, 17489 Greifswald, Germany

We present Landau kinetic theory and direct simulation results for systems of self-propelled particles with alignment interactions of higher-order symmetry with a particular focus on nematic couplings. Systematically expanding the BBGKY-hierarchy approximation beyond the mean-field contributions, we employ the one-sided molecular chaos assumption and an diagrammatic approach to account for higher order correlations. Our calculations yield predictions with no free parameters that are in quantitative agreement with direct agent-based simulations without being restricted to low densities.

DY 22.11 Wed 10:00 P3

Barrier crossing and rare fluctuations of active Brownian particles — •Rafael Diaz Hernandez Rojas[1], Karthik Cheruvary[1,2], and Peter Sollich[1] — [1]University of Göttingen — [2]IISER Pune

Understanding noise-induced transitions is crucial for modelling complex systems where random fluctuations can affect both the local stability and the global behaviour of a system. Noise-activated escape processes are a key instance, and were solved by Kramers long ago for barrier crossing driven by thermal noise. A natural question is how different noise sources might change the picture, in particular those postulated in active matter models. Here we study the escape problem for the paradigmatic case of an Active Brownian Particle, where the direction of the self-propulsion velocity rotates randomly on a timescale known as persistence time. Using a path integral formalism in the weak thermal noise limit. We map the problem of finding the most likely escape trajectory to the minimisation of an appropriate action. We show that optimal trajectories always consist of an initial relaxation in a tilted potential, beyond which the escape becomes genuinely activated. We apply our approach to convex potentials (to study barrier climbing by rare fluctuations) as well as potentials with multiple minima (to analyse barrier crossing). We highlight the effects of directionality induced by the self-propulsion and its non-trivial interplay with the shape of the potential. A key result is that, for potentials with a symmetry axis along the line between two minima, activity can generate optimal escape paths that break this symmetry.

DY 22.12 Wed 10:00 P3

Rarefied gas transport in a narrow channel induced by an asymmetric wall geometry — •Constantin Rein[1], Klaus Kroy[1], and Viktor Holubec[2] — [1]Brüderstr. 16, D-04103 Leipzig — [2]V Holešovičkách 747/2, Praha 8, Czech Republic

Since the work of Knudsen on gas transport in a narrow channel, it is known that gases in the dilute limit, where the mean free path is larger than the characteristic length scale, behave different as compared to the well known finite density regime[1]. So-called Knudsen pumps use temperature differences along channel walls to induce gas particle transport along the channel[2]. Inspired by the working principle of our recently introduced active Brownian ratchet[3], we investigate numerically and analytically the gas transport phenomenon appearing in a narrow channel with specular walls, except for a diffusively reflecting triangle that protrudes into the channel from one of the walls. Despite the absence of a variation in the wall temperature, a flow emerges. It arises solely from an asymmetry of the incoming and outgoing orientational distribution. The magnitude, direction and flow pattern of the induced transport is discussed.

[1] Knudsen, M. Eine revision der Gleichgewichtsbedingung der Gase, Thermische Molekularströmung. Ann. Phys. 336,205*229 (1909). [2] Wang, X., Su, T., Zhang, W., Zhang, Z. & Zhang, S. Knudsen pumps: a review. Microsyst Nanoeng 6, 26 (2020). [3] Rein, C., Kolář, M., Kroy, K. & Holubec, V. Force-free and autonomous active Brownian ratchets(a). EPL 142, 31001 (2023).

DY 22.13 Wed 10:00 P3

Dielectric response and fluctuation-dissipation-theorem for moving bodies — •Daniele Gamba, Philip Rauch, and Matthias Krüger — Georg-August University, Göttingen

Casimir forces operate at microscopic scales and are integral to phenomena such as gecko adhesion and functionality of nano-devices. Recent research has unveiled new effects, arising from thermal and mechanical non-equilibrium, such as levitation or propulsive forces capable to driving heat engines, or novel effects tied to optically non-reciprocal materials [1,2]. In this contribution we formulate scattering theory for objects in respective motion. Specifically, we find the dielectric response and the fluctuation-dissipation theorem for arbitrary moving bodies. The dielectric response of a moving body is found to be nonlocal in space, optically non-reciprocal, and can also appear as being active. Conversely, it is possible to design an active medium that appears optically passive when in motion. Finally, we derive closed expressions for Casimir forces and heat transfer between moving bodies using scattering theory.

1. Krüger et al., Physical Review B, 2012.
2. Gelbwaser-Klimovsky et al., Physical Review Letters, 2021.

DY 22.14 Wed 10:00 P3

Criticality in non-reciprocal spin modells — •Max Hässler and Martin Weigel — TU Chemnitz, Chemnitz, Deutschland

Equilibrium statistical physics is based on symmetric, Hamiltonian interactions fulfilling Newton*s Third Law. On the other hand, active matter like bacteria or other self-propelled particles such as bird flocks violates time-reversal symmetry and is often characterized by non-reciprocal interactions. Simple models are of interest for exploring fundamental features of such systems. We examine classical spin systems including the Ising model with non-reciprocal interactions, using Monte Carlo simulations to study criticality in such models. For several systems we determine critical exponents and compare the observed universality classes to those of the corresponding reciprocal, equilibrium models.

DY 22.15 Wed 10:00 P3

Harnessing finite-size effects to gauge aging in the $2D$ Ising model — •Dustin Warkotsch[1,2], Malte Henkel[2,3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019), Université de Lorraine, Nancy, France — [3]Centro de Física Teórica e Computacional, Universidade de Lisboa, Lisbon, Portugal

The finite-size effects in a $2D$ Ising model with nearest-neighbor interactions are investigated at low temperature with respect to the two-time autocorrelation function $C(t,s)$, where t is the observation and s the waiting time. Using a finite-size scaling ansatz established for the spherical model linking the resulting plateaus in $C(t,s)$ to waiting time s and lattice size L, a precise and reproducible estimation for the autocorrelation exponent λ and dynamical exponent z is developed.

DY 22.16 Wed 10:00 P3

Theoretical and Experimental Advances in Non-Equilibrium Statistical Physics — •Anton Zizenko — Bolshaya Semenovskaya 38

Research helps to understand how complex systems behave when they are far from equilibrium, such as in cases of anomalous transport or phase transitions. Main achievements: Relaxation and fluctuations: Describing the behavior of systems after external influence. Critical phenomena: Studying changes in systems out of equilibrium. Entropy production: Connection with energy loss processes and irreversibility. Applications: Development of materials with new properties, improvement of thermal conductivity, and optimization of processes in chemistry and biology.

DY 22.17 Wed 10:00 P3

Frustrated Self-Assembly — •Andrey Zelenskiy and Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France

Biomolecular self-assembly lies at the very heart of the function of living cells, where it organizes individual components into functional biological machines. The macromolecular sub-units typically correspond to proteins, whose shapes have been optimized over millions of years of evolution to ensure a proper functionality of the self-assembled structures. However, in pathological cases, proteins fail to achieve the optimal folding, which often leads to complex ill-fitting shapes. This produces geometrical incompatibility, which leads to frustrated interactions between the sub-units. Surprisingly, despite a huge variability in protein structure, such misfolded units tend to robustly self-assemble into aggregates with well-defined morphologies. Interestingly, these structures display a clear preference for slimmer topologies, such as fiber aggregates. This emergent principle of dimensionality reduction suggests that the aggregation of irregular components derives from the generic physical principles, rather than the microscopic details of the interactions.

Inspired by this idea, we model the frustrated self-assembly of ill-shaped proteins as coarse-grained anisotropic particles, whose interactions depend on their relative orientations and positions in space. This simple model successfully reproduces a hierarchy of aggregate morphologies and gives pointers to the origins of dimensionality reduction.

DY 22.18 Wed 10:00 P3

Topological and thermodynamic inference in Markov networks with observed and hidden transitions — •Alexander M. Maier[1], Udo Seifert[1], and Jann van der Meer[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Kyoto University, Graduate School of Science, Division of Physics and Astronomy, Oiwakecho 145-10, Kyoto 606-8224, Japan

The number of observable degrees of freedom is typically limited in experiments. Here, we consider discrete Markov networks in which an observer has access to a few visible transitions. We present what information, locally and globally, of such a Markov network can be inferred from the observed data. In particular, we shed light on operationally accessible information about the topology of shortest paths between visible transitions in the underlying graph and show a rule that allows us to identify potential clusters of states or exclude their existence. Moreover, we show how to estimate entropy production along an observable, coarse-grained path. Combining this with further inferable information, we propose two strategies to reconstruct a graph that is compatible with the observations and part of the original graph underlying the Markov network. This approach highlights how much information waiting-time distributions contain while also paving the way to infer thermodynamically consistent models of observed partially accessible systems.

DY 22.19 Wed 10:00 P3

Stroboscopic measurements in Markov networks: Thermodynamic inference vs. exact generator reconstruction — •Malena Thea Bauer[1], Udo Seifert[1], and Jann van der Meer[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Kyoto University, Graduate School of Science, Division of Physics and Astronomy, Oiwakecho 145-10, Kyoto 606-8224, Japan

A major goal of stochastic thermodynamics is to estimate the inevitable dissipation that accompanies particular observable phenomena in an otherwise not fully accessible system. Quantitative results are often formulated as lower bounds on the total entropy production, which capture a part of the total dissipation that can be determined based on the available data alone. In this work, we discuss the case of a continuous-time dynamics on a Markov network that is observed stroboscopically, i.e., at discrete points in time in regular intervals. We compare the standard approach of deriving a lower bound on the entropy production rate in the steady state to the less common method of reconstructing the generator from the observed propagators by taking the matrix logarithm. Provided that the timescale of the stroboscopic measurements is smaller than a critical value that can be determined from the available data, this latter method is able to recover all thermodynamic quantities like entropy production or cycle affinities and is therefore superior to the usual approach of deriving lower bounds. We conclude the comparison of both methods with numerical illustrations and a discussion of the requirements and limitations of both methods.

DY 22.20 Wed 10:00 P3

Brownian particles for unconventional computing — •Alessandro Pignedoli, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanoin- tegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

Brownian particles naturally explore a system's configuration space offering an energy efficient approach to optimisation problems [1]. We demonstrate that

interacting Brownian particles can solve optimisation problems [2,3] more efficiently than individual particles acting alone. This collective efficiency arises from their local interactions, which mimic the principles of swarm intelligence, where the whole systems emergent behaviour outperforms the sum of its individual components [4].

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982); [2] German Patent Application DE 10 2023 131 171, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023); [3] German Patent Application DE 10 2023 131 706, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023); [4] Bonabeau, et al, Oxford University Press (1999).

DY 22.21 Wed 10:00 P3

Investigating hydrogen isotopologues at cryogenic temperature in the gas, liquid, and solid phase with the T2ApIR experiment — •Alexander Marsteller, Dominic Batzler, Beate Bornschein, Lutz Bornschein, Tobias Falke, Florian Hanss, Joshua Kohpeiss, Bennet Krasch, Simone Wadle, and Robin Grössle — Karlsruher Institut für Technologie, Karlsruhe, Deutschland

Cryogenic hydrogen is of interest for a wide range of research topics such as fundamental phyiscs of liquids, astrophysics or energy storage. Tritium, the radioactive isotope of hydrogen, is of particular use as an electron source for neutrino mass measurement, and also the most promising contender for fuel in nuclear fusion for power generation. In spite of this, literature on the material properties of tritium is sparse. To improve upon this, the Tritium Absorption InfraRed Spectroscopy 2 (T2ApIR) Experiment has been designed and built at the Tritium Laboratory Karlsruhe (TLK), and is currently in its scientific commissioning phase. The main focus of this experiment is to enable the investigation of the properties of all six hydrogen isotopologues and their mixtures in the gaseous, liquid, and solid phase. This is achieved using infrared absorption spectroscopy, a polariscope setup, Raman spectroscopy, as well as a temperature and pressure measurement. On this poster I will present the T2ApIR setup as well as some of the first measurements performed with it.

DY 22.22 Wed 10:00 P3

GEANT4 based design to measure the solubility of tritiated molecules in dual phase xenon — •J.R. Braun[1], V. Aures[2], D. Forck[1], R. Grössle[1], and M. Röllig[1] — [1]Tritium Laboratory Karlsruhe, Eggenstein-Leopoldshafen, Germany — [2]Technische Universität München, Garching bei München, Germany

Detection of trace amounts of tritium is a challenging task that can be tackled using scintillation. Liquid xenon is an excellent scintillator for this purpose. A fundamental property in designing analytical systems for tritium detection is the solubility of tritiated molecules. Trace detection of tritium is critical for experiments aimed at the detection of rare physical interactions, such as the direct detection of dark matter, where naturally occurring tritium background is a challenge to overcome. Consequently, systems for both detection and removal of tritium are required. The aim of the "Tritium in Xenon" (TriXe) experiment is to determine the Henry solubility and the diffusion constant of tritiated hydrogen, water and methanes in dual-phase xenon in thermal equilibrium. TriXe employs a dual-phase chamber in which the xenon is present at operating conditions of DARWIN. By detecting VUV scintillation light with photomultipliers, the concentration of the tritiated molecules in each phase can be determined, as the concentration is proportional to the counting rate. Together with the second diffusion law, the diffusion constant can be deduced from the change in the count rate over time. The results of TriXe can be used to make qualitative and quantitative suggestions for changes in background reduction and direct tritium monitoring by cryogenic distillation.

DY 22.23 Wed 10:00 P3

Precise Estimation of the Liquid-Gas Critical Point of Water — •Mayank Sharma and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz

We perform Molecular Dynamics simulations to investigate the liquid-gas critical point for the TIP4P water model. In the canonical (NVT) ensemble, density fluctuations are quantified and analyzed using a recently developed method [1] based on cumulant crossings. Complementary simulations in the isothermal-isobaric (NPT) ensemble yield density and energy distributions, which are mapped onto the universal 3D Ising master curve via histogram reweighting. The critical points determined by the two approaches exhibit very good agreement, highlighting the robustness of this methodology. This work establishes a reliable framework for accurately locating the critical point which is applied to test the influence of ionic conditions on the latter.

[1] J.T. Siebert et al., Phys. Rev. E (R) 98, 030601 (2018).

DY 22.24 Wed 10:00 P3

Linking Local and Macroscopic Transport Properties in Confined Electrolyte Systems: Molecular Dynamics Simulations of Water Swollen Hectorite — •Bastian Füsser, Aqsa Nisar, and Michael Vogel — Technische Universität Darmstadt, Darmstadt, Germany

In this work, we study the structural and dynamic properties of water and ions in hectoriete slit confinements using molecular dynamics simulations. Our goal is to develop a detailed understanding of the relationship between local interactions and macroscopic ion transport.

This study is part of a collaboration aiming to bridge experimental observations and theoretical models. Initially, we simulate hectorite systems as realistically as possible to compare the simulation results with experimental results. Subsequently, we investigate artificial systems to systematically analyze the role of specific parameters, such as layer charge. In doing so, we vary the interlayer spacing, solvent composition, and ion concentration.

Our goal is to develop an understanding of the relation between local interactions and dynamics with the long-range transport in confined electrolyte systems. These insights provide valuable contributions to the development of more efficient electrochemical systems, e.g., devices for energy storage and conversion.

DY 22.25 Wed 10:00 P3

Phase transitions in mesoporous solids with structural disorder — •Ali Alzaidi[1], Georgiy Baroncha[1], Dirk Enke[1], Eustathius Kikkinides[2], and Rustem Valiullin[1] — [1]Leipzig University, Leipzig, Germany — [2]Aristotle University of Thessaloniki, Thessaloniki, Greece

Phase transitions within the pore spaces of structurally disordered porous solids exhibit complex behavior with many aspect remaining poorly understood. This complexity arises from cooperative effects emerging during first-order phase transitions in pore networks. Building on the microscopic mechanisms of phase transitions occurring in single pores and between neighboring pores, we propose a statistical thermodynamic model to describe phase transitions in pore networks driven by two competing mechanisms: invasion and nucleation. We solve this model for two types of statistically disordered pore networks, linear pore chains and Bethe lattices, and correlate the results with experimental data on gas-liquid and solid-liquid equilibria in disordered porous glasses.

DY 22.26 Wed 10:00 P3

Cluster Formation and Phase Transitions Induced by Non-Reciprocal Interactions — •Thomas Richard Ullmann and Klaus Kroy — Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany

The emergence of cluster formation in a two-dimensional lattice spin system driven by non-reciprocal interactions (NRI) is investigated. The development of a novel phase, characterized by clusters distinct from the quasi-long-range order (QLRO) state of the conventional XY model, is unveiled through the use of a tunable non-reciprocal parameter. Cluster formation is shown to result from particular local spin alignment due to non-reciprocal coupling, which dynamically reshapes the stability landscape of defects and topological structures. The stability of the system is analyzed using nearest-neighbour interactions and stochastic dynamics, and critical points are identified indicating phase transitions associated with clustering. The stability and evolution of defects and structures within this regime are further examined, providing insights into the interplay between non-reciprocity and the dynamics of spin textures. Broader implications for understanding collective behaviour in non-equilibrium systems are suggested, offering a framework for exploring non-reciprocity-induced phases and their stability in both physical and biological contexts.

DY 22.27 Wed 10:00 P3

Criticality and Percolation in the Off-Lattice XY Model — •Manthan Chattopadhyay, Thomas Richard Ullmann, and Klaus Kroy — Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany

We investigate the critical behavior of the 2D XY model with quenched positional disorder by distributing spins randomly via a spatial Poisson point process. This off-lattice approach allows us to study how quenched disorder affects phase transitions and critical phenomena, with the primary focus being the critical power-law scaling between the Kosterlitz-Thouless transition temperature T_c and the mean spin density $\langle\rho\rangle$. Using both a homogeneous coarse-graining method and percolation theory, we derive predictions for the scaling $T_c \propto (\langle\rho\rangle - \langle\rho_c\rangle)^{\zeta}$. By considering the fractal nature of the spin network near the percolation threshold, characterized by the fractal dimension D_f, the exponent is estimated. Simulation results confirm the existence of a percolation threshold with an exponent obtained from simulations similar to those of our analytic work, aligning closely with theoretical prediction. The fractal nature of the spin network near $\langle\rho_c\rangle$ is validated through the box-counting method, which is consistent with the value for 2D percolation. At high densities well above the percolation threshold, critical exponents approach expected values of the XY universality class, and the magnetization exponent β conforms to empirical observations in ultrathin magnetic films.

DY 22.28 Wed 10:00 P3

The random-field Ising model and two-phase flow in disordered media — •Peter Henning and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Two-phase flow in disordered media exhibits a rich phenomenology of behaviors with manifold applications for example in oil extraction [1]. A simplified model for such flows might be provided by the zero-temperature dynamics of the random-field Ising model (RFIM) that exhibits interfaces between the pure

phases that propagate through avalanches and show a roughening transition as a function of disorder strength. In the present study we focus on several properties of the interface between the phases such as its fractal geometry which can be characterized by critical exponents [2]. Furthermore we investigate abrupt changes in the propagation of the interface also known as crackling noise. By applying the RFIM to this problem we hope to gain insights into the underlying mechanisms of two-phase flow in disordered media and to provide a framework for interpreting experimental observations.

[1] R. Holtzman, M. Dentz, R. Planet and J. Ortin, *Commun Phys.* **3**, 222 (2020).
[2] B. Drossel and K. Dahmen, *Eur. Phys. J. B* **3**, 485 (1998)

DY 22.29 Wed 10:00 P3

Relating Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Previous studies on 2D non-network glass formers utilized the million-fold acceleration of Swap Monte-Carlo and potential energy landscape (PEL) analysis to establish a connection between deviations from Gaussian behavior of the inherent structure (IS) density function, Fragile-to-Strong-Crossover [1] and a low-energy depletion regime. In recent work [2] a specific low-temperature behavior for thermodynamical (IS-energy) and dynamical (apparent activation energy) observables could be observed with basically the same onset temperature. To understand the physical background we investigate various model IS distributions in a trap-like picture and their derived dynamic and thermodynamic properties. Indeed, for different realizations of non-Gaussianity in the PEL strong correlations between the respective onset temperatures are observed as well, suggesting indeed a strong correlation between thermodynamics and dynamics. These results contribute to our understanding of the PEL picture of glass formers.

[1] A. Heuer, *J. Condens. Matter Phys.* **2008**, 20, 373101
[2] A. D. S. Parmar, A. Heuer, **2023** *arXiv preprint arXiv:2307.10143*

DY 23: Poster: Active Matter, Soft Matter, Fluids (joint session DY/CPP)

Time: Wednesday 10:00–12:00 Location: P3

DY 23.1 Wed 10:00 P3

Enhanced stability and chaotic condensates in multi-species non-reciprocal mixtures — •Laya Parkavousi[1], Navdeep Rana[1], Ramin Golestanian[1,2], and Suropriya Saha[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), D-37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Random non-reciprocal interactions between a large number of conserved densities are shown to enhance the stability of the system towards pattern formation. The enhanced stability is an exact result when the number of species approaches infinity and is confirmed numerically by simulations of the multi-species non-reciprocal Cahn-Hilliard model. Furthermore, the diversity in dynamical patterns increases with increasing number of components and novel steady states such as pulsating or spatiotemporally chaotic condensates are observed. Our results may help to unravel the mechanisms by which living systems self-organise via metabolism.

DY 23.2 Wed 10:00 P3

Non-reciprocal Model B and the role of mobilities and non-reciprocal interfacial forces — •Bibhut Sahoo[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Mathematics, King's College London, London

Recently the effects of non-reciprocal interactions have been widely studied in the Cahn-Hilliard model for phase separation, which is based on a magnetic analogy. Here we explore the corresponding nonreciprocal model B, as the continuum theory for non-reciprocal particle mixture. We focus on the effect of mobility matrix on topology of the phase diagram and find that changing mobility can change stability of a homogeneous state, which for reciprocal interactions would be impossible. We study spinodal dynamics in regions of instability, where static or travelling spinodal patterns can occur. This aspect is as in non-reciprocal Cahn-Hilliard but, the transitions between these instabilities are novel: they occur not via exceptional points, but via first order transitions in the length scale of the dominant unstable modes. At transition, a static and a travelling spinodal pattern with two different scales coexist. We show that more complicated transitions involving coexistence of three length scales can also occur. We finally argue, based on a nonreciprocal version of Dean's equation, that coarse graining into a model B description should lead to non-reciprocal interface terms, rather than only in the bulk as assumed in theories to date. We show that such interfacial terms can significantly enlarge the travelling spinodal regions in the phase diagram.

DY 23.3 Wed 10:00 P3

Mixed active fluids of two kinds — •Astik Haldar — Universität des Saarlandes, Saarbrücken 66123, Germany

We explore here the polar active fluids of two types, characterizing by their different aligning and propulsion strengths. We example here the fluids as the collections of moving living creatures, which could fuel itself through chemical reactions in their body . We called this system as active system, and consider their brilliant interactions. We here try to model those through considering some parameters and physically observable quantities. We find the parameters region where they have their oriented flocking as parallel or antiparallel, ordered rotating phase coherently meaning chiral phase. Our study finds the transition between the phases as saddle node as well as pitchfork bifurcation in mean field theory scheme. We find different kind of pattern formed states appear through the analytical as well as numerical study.

DY 23.4 Wed 10:00 P3

Verification, efficiency analysis and extension of the kinetic Event-Chain Algorithm — •Nico Schaffrath, Tobias Kampmann, and Jan Kierfeld — TU Dortmund, Dortmund, Germany

The novel cluster kinetic Monte-Carlo algorithm, which is based on the event-chain Monte-Carlo method, is specifically designed to simulate systems of two-dimensional self-propelled hard particles. We verify this algorithm from scratch by analysing various single-, two- and many-body systems, as well as some algorithm-specific quantities. To gain insight about the applicability of the algorithm, we compare its performance to that of an Event-Driven Brownian-Dynamics simulation. Finally, we investigate the possibility to simulate particles with soft interaction energies as well as an extension to three-dimensional systems. Regarding the latter, the phase diagram of self-propelled hard spheres is calculated.

DY 23.5 Wed 10:00 P3

AMEP: Analyzing Active Matter Simulations in Python — Kay-Robert Dormann[1], Lukas Hecht[1], Kai Luca Spanheimer[2], Aritra K. Mukhopadhyay[1], Mahdieh Ebrahimi[1], Suvendu Mandal[1], and •Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany

The **A**ctive **M**atter **E**valuation **P**ackage (AMEP)[1] is an easy-to-use Python library for analysing simulation data of particle-based and continuum simulations. It provides a powerful interface for handling complex analysis of large data sets from different simulation software such as LAMMPS, HOOMD-blue, GROMACS and others. A plethora of methods to calculate observables and visualise results make AMEP suitable to calculate complex observables not only for beginners but also for advanced studies of active and soft matter. AMEP is written in pure Python and leverages powerful and well-known libraries such as NumPy, SciPy and Matplotlib. Computationally expensive methods are parallelized to run on laptops and workstations as well as high-performance computing clusters.

The methods range from order parameters, cluster methods, spatial and time correlation functions to thermodynamic properties and coarse-graining methods. More information and examples are available at https://amepproject.de. AMEP can be installed via conda and pip.

[1] L. Hecht et al., arXiv:2404.16533 [cond-mat.soft]

DY 23.6 Wed 10:00 P3

Fluctuation induced network patterns in spatially correlated noise — •Sebastian Fehlinger[1], Kai Cui[2], Arooj Sajjad[1], Heinz Koeppl[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Institut für Physik Kondensierter Materie, Hochschulstraße 8, 64289 Darmstadt — [2]Technische Universität Darmstadt, Selbstorganisierende Systeme, Merkstraße 25, 64283 Darmstadt

Fluctuations play an important role in many fields of physics, from quantum electrodynamics to statistical mechanics. In active matter physics, so far, most works have focused on active particles that are subject to thermal fluctuations caused by the surrounding solvent. Here, we explore the collective behaviour of active particles under the influence of spatially correlated noise, that can arise, e.g., from fluctuating external fields. Therefore, we introduce a minimal model which describes the dynamics of (chiral) active particles with alignment interactions in a time-dependent Gaussian random field, that features a characteristic spatial correlation length, but no temporal correlations. Using Brownian dynamics simulations, we find, that the active particles aggregate to system spanning,

percolated networks. These structures are (i) fluctuation-induced, (ii) feature local alignment of the contained particles, but no global alignment, and (iii) hardly show any coarsening. We systematically characterize the emerging patterns with tools from topological data analysis (persistence diagrams, Vietoris-Rips complexes and Betty numbers).

DY 23.7 Wed 10:00 P3

Reconfiguring hydrodynamic flow fields of active particles by light — Lisa Rohde, Tom-Hannes Hemann, Gordei Anchutkin, and •Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Microscopic active particles propel themselves via localized energy conversion, generating hydrodynamic flow fields that govern their boundary interactions and collective behaviour. The long-range behaviour of the flow patterns classifies them as either pushers, which expel fluid along their swimming axis, or pullers, which draw fluid inward. In nature, some microorganisms can adaptively switch between pusher and puller modes in response to their environment. However, synthetic active particles are currently limited to a fixed pusher or puller configuration during fabrication, constraining our ability to study their dynamic responses to environmental cues. Here, we present a self-thermophoretic active particle that can reconfigure its flow field on demand during the experiment. This is achieved by illuminating the particle with an inhomogeneous light field shaped by a spatial light modulator. The illumination patterns create surface temperature fields inducing thermo-osmotic flow fields that propel the particle and shape the hydrodynamic interactions. By using gold nanoparticles, we trace and characterize the hydrodynamic flow field of the active particle. The ability to dynamically alter the propulsion characteristics will enable us to investigate and control their interactions and collective dynamics.

DY 23.8 Wed 10:00 P3

Brainbots as smart autonomous active particles with programmable motion — •Isa Mammadli[1], Martial Noirhomme[2], Nathan Vanesse[2], Jayant Pande[3], Ana-Sunčana Smith[1], and Nicolas Vandewalle[2] — [1]PULS, Institute for Theoretical Physics, FAU Erlangen-Nürnberg, 91058, Erlangen, Germany — [2]GRASP, Institute of Physics B5a, University of Liege, B4000 Liege, Belgium — [3]Department of Physical and Natural Sciences, FLAME University, Pune, India

We introduce an innovative robotic device designed to enable controlled motion for the study of active matter. Motion is driven by an internal vibrator, powered by a compact rechargeable battery. The system integrates acoustic and magnetic sensors alongside a programmable microcontroller. Unlike conventional vibrobots, this device employs a motor that generates horizontal vibrations, producing cycloidal trajectories that have been thoroughly characterized and optimized. Specific segments of these trajectories can be harnessed to create tailored motion patterns. As a proof of concept, we demonstrate how this versatile system can be used to develop active particles exhibiting diverse dynamics, ranging from ballistic motion to run-and-tumble diffusive behavior. Based on experimental data, we provide a simulation routine capable of replicating these trajectories, enabling the generation of extended datasets and the exploration of various input velocity configurations. This approach facilitates the determination and prescription of optimized input parameters for applications such as enhanced search strategies and precise path following.

DY 23.9 Wed 10:00 P3

Fundamental Measure Theory for active hard discs — •Jonas Buba and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The behavior of active soft particles has been studied extensively and provides a good model for many active matter systems [1]. However, some systems might be described more accurately by considering hard particles instead. While active soft particles have been described with a Phase Field Crystal approach (e.g., in [2]), a similar description of active hard particles is still lacking. In our approach we use Fundamental Measure Theory [3] to model hard discs and add activity. We expect to gain further insight into the role that the particle type can play in dynamical pattern formation.

[1] Marchetti M C, Joanny J F, Ramaswamy S, Liverpool T B, Prost J, Rao M and Simha R A. Hydrodynamics of soft active matter. Rev. Mod. Phys. 85 1143, 2013. [2] Arold D and Schmiedeberg M. Mean field approach of dynamical pattern formation in underdamped active matter with short-ranged alignment and distant anti-alignment interactions. J. Phys.: Condens. Matter 32 315403, 2020. [3] Roth R, Mecke K, and Oettel M. Communication: Fundamental measure theory for hard disks: Fluid and solid. The Journal of Chemical Physics, 136(8):081101, 2012.

DY 23.10 Wed 10:00 P3

Many-Body Dynamics of actively rolling fibers — •Alex Arnold[1], Falko Ziebert[1,2], and Igor M Kulic[3,4] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany — [3]Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg, France — [4]Institute Theory of Polymers, Leibniz-Institute of Polymer Research, D-01069 Dresden, Germany

Fiberboids are active filaments, capable of self-propulsion, whose dynamics were recently described in [A. Bazir, A. Baumann, F. Ziebert, I. M. Kulić, Soft Matter 2020]. So far, only single and simple 2-body dynamics of fiberboids were described.

In this work we will take a first look at the many-body dynamics. Specifically, we analyze a system of multiple nylon-rods, which when heated from below display self-propelled rolling motion. Confining the rods to roll on a single axis only, implements a simple realization of an 1D active gas. We analyze the experiments concerning clustering and nonequilibrium fluctuations and rationalize the system by simple lattice models.

DY 23.11 Wed 10:00 P3

Pumping currents and formation of flocks in 1D Ising model — •Adrian Morais Cabral and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Non equilibrium systems create phenomena that are not observed in equilibrium counterparts, such as long range order in two or less dimensions and breaking of detailed balance.

We use an effective description of coupled Langevin equations to study a 1D system where an Ising order parameter is coupled to a charge density. Our assumption is that the charge current has a contribution proportional to the order parameter for the driven system. The formation of domain walls leads to a source of dynamical frustration for the charge. Driving disallows the formation of domain walls and creates flocking blob like states in addition to constant ordered and disordered states and a non moving spike phase. These solutions are studied numerically in 1D for $T \geq 0$.

At $T = 0$, we characterize existing flocking solutions and compare analytical predictions to numerical simulations which agree well with only one fitting parameter.

At finite temperatures we find new dynamics for the flocking state such as reversals similar to the active Ising model and (quasi) crossings. However, we have not yet been able to answer whether the existing ordered phase is stable in 1D.

DY 23.12 Wed 10:00 P3

Statistical Field Theory for Vicsek-type models — •Carsten Littek, Falko Ziebert, and Matthias Bartelmann — Institut für Theoretische Physik, Universität Heidelberg, Germany

Dry, aligning, dilute active matter systems display a wide range of emergent phenomena such as collective, orientationally ordered motion and phase separation. The self-propelled particles in such systems undergo noisy aligning interactions with their neighbours, but they do not exchange momentum with their surrounding. While microscopic and hydrodynamic descriptions, whose connection involves approximations, exist, their predicted behaviour - such as scaling exponents - do not match.

Here we present a microscopic statistical field theory for active Brownian particles inspired by Mazenko (2010). In our formulation we interpret the particles' two-dimensional positions and their direction of motion as Martin-Siggia-Rose (MSR) fields to obtain a path integral representation of the N-particle partition function. The MSR action is augmented by a two-particle interaction that aligns particle directions either ferromagnetically as in the Vicsek model or nematically. Similar to quantum many-body theory the benefit of our field theoretic formulation of Vicsek-type models is that it allows for developing a self-consistent perturbation theory and using renormalization techniques. Our aim is the calculation of density and velocity correlation functions in the homogeneous ordered phase and the transition into the ordered phase.

DY 23.13 Wed 10:00 P3

Coupling reaction-diffusion and locomotion in vegetative cells — •Blaž Ivšić[1], Piotr Nowakowski[2], Igor Weber[2], and Ana Sunčana Smith[3,2] — [1]Institut za fiziku, Zagreb, Croatia — [2]Institut Ruđer Bošković, Zagreb, Croatia — [3]Friedrich-Alexander- Universität, Erlangen, Germany

Cellular locomotion involves the dynamic interplay between signaling molecules, cytoskeletal activity, and membrane deformation. We present a computational model coupling protein Rac1 reactiondiffusion dynamics to cell locomotion to study vegetative state of amoeba Dictyostelium discoideum. Rac1 regulates actin polymerization via effectors like WASP and Arp2/3, while GAP modulates its activity. The model captures Rac1 dynamics on a deforming membrane, reproducing experimentally observed spatiotemporal patterns.

Cell shape is modeled using a Level-set method to track membrane dynamics, driven by forces linked to Rac1 concentration. Specifically, surface tension and normal forces (due to interaction of the cell with the substrate) proportional

to Rac1 concentration influence membrane movement. The dynamics are conveyed through a fluid velocity field obtained by solving a time-dependent Stokes equation.

Our model replicates Rac1 activity patterns seen in live-cell imaging and links these patterns to cell motility. By bridging Rac1 reactiondiffusion dynamics with membrane mechanics, the model provides insights into the mechanisms of actin-driven locomotion in vegetative cells.

DY 23.14 Wed 10:00 P3

Numerical Simulation of Microplastic Permeation in Soil: from Solutes to Particles — •Hao Liu[1], Yifan Lu[2], Christina Bogner[2], Martin Lörder[1], and Stephan Gekle[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]University of Cologne, Cologne, Germany

Microplastics have become significant environmental pollutants, raising concerns about their accumulation and distribution across ecosystems. Although terrestrial environments, particularly soils, often exhibit high levels of microplastic contamination, they remain relatively understudied. Microplastic transport in soil involves complex interactions among particle properties, soil structure, and fluid dynamics. Understanding mechanisms such as permeation, aggregation, and degradation is essential for effective environmental risk assessments and strategies to control microplastic pollution.

This study aims to simulate and predict soil hydraulic conductivity in microplastic-laden flows. Challenges include modeling behaviors of microplastic particles as they transport in soil with complex porous structures. High-resolution μCT scans of soil samples will provide the necessary porous media data, and simulations will be conducted using FluidX3D software. The research progresses in two phases: first, disregarding particle size and shape to analyze solute transport mechanisms; second, incorporating detailed particle properties to study transport and accumulation in pores. The goal is to model microplastic dynamics for accurate predictions of microplastic distribution in soil systems.

DY 23.15 Wed 10:00 P3

Thermo-Osmotic Flows via Anti-Stokes Cooling — •akshay kallikkunnath[1], kamil bruchal[2], pawel karpinski[2], and frank cichos[1] — [1]Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Germany — [2]Faculty of Chemistry, Institute of Advanced Materials, Wroclaw University of Science and Technology, Poland

Fluidic manipulation has gained huge interest over time especially with the studies on metal nanoparticles as optically controlled heat sources generating temperature gradients. With recent developments in the synthesis of lanthanide doped crystals which can be cooled by anti- stokes cooling, we try to bring laser cooling of microcrystals to the field of fluidics. In this work, we optically trap and cool ytterbium doped NaYF4 crystals by means of anti-stokes cooling. Temperature measurements for such microscale cooled crystals are done using a technique which utilizes the phase transition of liquid crystals. With such a thermal gradient created using cold sinks in liquid, we study and provide for the first time experimental and numerical results for flows generated at solid-liquid boundary, i.e., thermo-osmotic flows. The results will provide further scope for studying dipolar thermo-osmotic and corresponding thermo-electric fields in an electrolyte solution generated by arranging optically heated and cooled particles together. Our findings can have direct implications on the study of temperature-dependent biochemical processes which inhibit with lower temperature or on response of a biological specimen to low temperature stress or may even find application in local cryotherapy.

DY 23.16 Wed 10:00 P3

Thermodynamically consistent coarsening model of crossover placement in meiosis — •Marcel Ernst[1,2] and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Universität Göttingen, Germany

Crossovers play an important role in meiosis, ensuring correct segregation of homologous chromosomes and increasing genetic variability. A recently proposed model suggests that crossover placement is determined by biomolecular condensates that coarsen by exchange and diffusion of a protein along chromosomes, consistent with experiments. We here present an extended model including exchange with the nucleoplasm based on thermodynamic principles. We study theoretically and numerically the initial protein loading onto the chromosome, the droplet growth regime, the coarsening regime, and the final equilibrium. We derive scaling laws for the number of crossovers analogous to Lifshitz-Slyozov-Wagner theory in different limits. Finally, we investigate the effect of protein exchange with the nucleoplasm on crossover placement and compare the results with empirical data from several species. In conclusion, our model allows us to explain key features of meiotic crossover placement in wild type and several mutants.

DY 23.17 Wed 10:00 P3

A lattice Boltzmann approach to electrolytic multiphase flows — •Alexander Reinauer and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

Simulating electrolytic multiphase flow presents significant challenges, often requiring either the detailed modeling of large numbers of particles or solving complex, nonlinear partial differential equations, such as the Navier-Stokes and Nernst-Planck equations. While particle-based simulations provide molecular details, continuum-scale approaches, including the Navier-Stokes and Nernst-Planck equations, enable the study of larger systems relevant to applications in oil recovery, biological processes, and waste treatment.

In this work, we extend the Lattice Boltzmann Method using a Color-Gradient approach to simulate immiscible two-phase flow, coupled with a custom Nernst-Planck solver for the transport of dissolved charged species. This coupling allows to incorporate the preferential solubilities of chemical species.

Our implementation, based on the pystencils/lbmpy framework, generates highly optimized code for both CPU and GPU architectures. To validate the model, we performed simulations of freely suspended liquid droplets subjected to an external electric field. Additionally, we explored contact angle models and initiated studies on applying the approach to porous media under varying conditions.

DY 23.18 Wed 10:00 P3

Coarsening of chemically active droplets — •Stefan Köstler[1,2], Yicheng Qiang[1], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Droplets formed by phase separation play an important role in cellular organization and are widely used in the design of synthetic cells and lab-on-chip devices. Droplet emulsions typically coarsen due to surface tension and hydrodynamic effects, which generally prevents precise control over droplet sizes. While coarsening can be suppressed by active chemical reactions, it is unclear how these reactions affect the coarsening dynamics and control droplet sizes. To elucidate this, we numerically simulate a binary mixture that phase separates and undergoes reactions. We find three different dynamical regimes: Small droplets are dominated by coalescence due to hydrodynamic advection, then transition to an Ostwald ripening regime dominated by diffusion, and finally exhibit size control by active chemical reactions. We predict the transition from ripening to size control analytically, and we validate our analytical estimate of the final size using a numerical minimization of a surrogate equilibrium free energy. Our theory provides an improved understanding of coarsening mechanisms, allowing to achieve greater control of emulsions.

DY 23.19 Wed 10:00 P3

Zetapotential of Gold Surfaces in a Flow Cell — •Mattis Rasenat, Peter Vogel, Marcus Witt, and Thomas Palberg — Johannes gutenberg Universität Mainz

We present a case study on the zeta-potential of gold surfaces in a continuous flow cell. The charge of dielectric surfaces is of high interest for technological applications. Therefore, we measure the zeta potential of polymer particles in a custom-made electrokinetic flowthrough cell with exchangeable sidewall. The zeta potential is measured with a super-heterodyne light scattering setup.

DY 23.20 Wed 10:00 P3

Use of molecular CO_2 for surface charge regulation — Peter Vogel[1], Markus U. Witt[1], David Beyer[2], Christian Holm[2], Muhammad Navaz Qaisrani[3], Marialore Sulpizi[4], and •Thomas Palberg[1] — [1]Inst. of Physics, JGU, Mainz, Germany — [2]Inst. of Computational Physics (ICP), U Stuttgart, Stuttgart, Germany — [3]MPI for Polymer Research, Mainz, Germany — [4]Dept. of Physics, RU Bochum, Bochum, Germany

In deionized water CO_2 forms carbonic acid which partially dissociates. Such 'realistic' salt free systems contain a significant background electrolyte concentration and a pH of 5.5. Both lowers the effective charge of dielectric surfaces. Surprisingly, the remaining molecular CO_2 causes an additional drastic decharging effect, even to complete decharging in water equilibrated against pure CO_2. Molecular CO_2 acts directly on the degree of dissociation and thus lowers the bare charge, while effective charges merely follow suit. MD simulations show the formation of a diffusely adsorbed monolayer of CO_2, which locally lowers the dielectric constant. Based on this we suggested dielectric charge regulation as novel decharging mechanism. If then salts are added to the carbonized surfaces, one finds recharging by co-ion adsorption. This process is favoured by hydrophobicity, by co-ion size and, most important, also by the amount of adsorbed CO_2. Given the ubiquity of dielectric surfaces in contact with aqueous electrolytes, this very general charge regulation processes appear to be of great fundamental and practical importance.

DY 24: Focus Session: Broken Symmetries in Statistical Physics - Dynamics of Odd Systems

In recent years, the effect of broken microscopic symmetries on emergent mesoscopic and macroscopic behavior has gained significant attention in non-equilibrium statistical physics. For example, breaking Newton's third law leads to so-called "non-reciprocal interactions" among species and gives rise to odd transport coefficients. These are primarily investigated in active systems. However, even with Newton's third law valid, odd transport can emerge, and even in equilibrium systems. In both cases, many novel phenomena have been reported over the last years, such as asymmetric clustering, oscillatory phase behavior, crowding-enhanced diffusion in in- and out-of-equilibrium systems, as well as off-diagonal correlation functions, topologically protected edge flows, and many more. With this symposium, we bring together the communities working on odd transport systems in the context of (non)equilibrium statistical physics, to stimulate discussions about the physical background and implications of such broken symmetries in transport-related phenomena.

Organized by Erik Kalz (Potsdam), Ralf Metzler (Potsdam), and Abhinav Sharma (Augsburg)

Time: Wednesday 15:00–18:30 Location: H43

Invited Talk DY 24.1 Wed 15:00 H43

Dynamics of odd and chiral active systems — •Hartmut Löwen — Heinrich-Heine-Universität Düsseldorf

After a brief introduction into "odd" systems characterized by odd viscosity, odd elasticity or odd diffusivity, we focus on *odd diffusive dynamics*. For normal diffusive systems, repulsive interactions typically reduce the dynamics as signalled by a reduction of the long-time self-diffusion coefficient. Contrarily, in odd-diffusive systems, collisions can enhance the self-diffusion due to a mutual rolling effect. We further address *active chiral particles* which break the discrete left-right symmetry in their motion. Examples include spinners, circle swimmers and particles moving on helical trajectories. We explore phase separation, glassy dynamics as well as crystallization and polymerisation in these chiral systems. New phenomena absent for achiral objects are observed including active surfactants, rotating crystallites, self-wrapping of chiral polymers and a hammering effect in supercooled fluids. Also the realization of such odd systems in granular or colloidal experiments is discussed.

DY 24.2 Wed 15:30 H43

A route from force to velocity autocorrelation in over-damped odd dynamic and its applications to the study of diffusion — Filippo Faedi and •Abhinav Sharma — University of Augsburg, Augsburg, Germany

In this work we present a derivation of the relation between the velocity and force autocorrelation in over-damped dynamic starting from the underdamped Langevin equation. Time reversal symmetries are used to simplify the noise force autocorrelation and this procedure can be applied both in the presence and in the absence of magnetic field. Thanks to these relation we can prove that off diagonal element of the force autocorrelation matrix contribute to the self diffusion coefficient in the presence of a magnetic field. In addition the result is applied to study the dynamics of two odd dimers with same and opposite charges.

DY 24.3 Wed 15:45 H43

A model collective system made of spinning micro-disks: from fundamentals to microrobot swarms — •Gaurav Gardi — Max Planck Institute fort Intelligent Systems, Stuttgart, Germany

Collective systems such as bird flocks and fish schools in nature and colloidal and robotic artificial collectives, display order in their spatiotemporal patterns. Although they are inherently out-of-equilibrium systems, the order in their patterns may share similarities with well-understood phases of matter in equilibrium and thus may be characterized by similar metrics. These phases also contain information, which is embedded in their spatiotemporal structures and can be quantified by information entropy. Although order and information are connected fundamentally in thermodynamics, their relation in collective systems is seldom explored. Here we combine the approaches of statistical mechanics and information sciences to demonstrate the order and the information in the phases of a two-dimensional (2D) small-scale robotic collective system consisting of hundreds of spinning micro-disks at the air-water interface. We design and control the balances of local interaction forces between micro-disks so that distinct globally ordered phases emerge. We relate the order and information in the global phases using concepts from statistical physics and information theory. Lastly, we design experiments to demonstrate the diverse self-organised behaviours of our system and its ability to transition to non-reciprocal regime. Overall, this talk highlights our system's capability to act as an adaptable and versatile model system for dynamic self-organisation and for development of versatile microrobot collectives.

DY 24.4 Wed 16:00 H43

Active pattern formation emergent from single-species nonreciprocity — Zhi-Feng Huang[1], •Michael te Vrugt[2], Jonas Mayer Martins[3], Raphael Wittkowski[3,4], and Hartmut Löwen[5] — [1]Department of Physics and Astronomy, Wayne State University, Detroit, Michigan 48201, USA — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany — [3]Institut für Theoretische Physik, Universität Münster, 48149 Münster, Germany — [4]Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany — [5]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

Nonreciprocal interactions violating Newton's third law are common in a plethora of nonequilibrium situations ranging from predator-prey systems to the swarming of birds and effective colloidal interactions under flow. Here (arXiv:2404.10093), we systematically derive a field theory for the basic case of a single-component system breaking the *actio* and *reactio* equality of force within the same species from the microscopic particle dynamics, leading to a generic continuum model termed *Active Model N*. One particular new characteristic pattern found in this model is an interwoven self-knitting "yarn" structure with a unique feature of simultaneous development of micro- and bulk phase separations. The growth dynamics of a "ball-of-wool" active droplet towards these self-knitted yarn or branched states exhibits a crossover between different scaling behaviors.

DY 24.5 Wed 16:15 H43

Dance of odd-diffusive particles: A Fourier approach — •Amelie Langer[1], Abhinav Sharma[2,3], Ralf Metzler[4], and Erik Kalz[4] — [1]University of Heidelberg — [2]University of Augsburg — [3]IPF Dresden — [4]University of Potsdam

Odd-diffusive systems are characterized by transverse responses and exhibit unconventional behaviors in interacting systems. To address the dynamical interparticle rearrangements in a minimal system, we here exactly solve the problem of two hard disklike interacting odd-diffusing particles. We calculate the probability density function (PDF) of the interacting particles in the Fourier-Laplace domain and find that oddness rotates all modes except the zeroth, resembling a mutual rolling of interacting odd particles. We show that only the first Fourier mode of the PDF, the polarization, enters the calculation of the force autocorrelation function (FACF) for generic systems with central-force interactions. An analysis of the polarization as a function of time reveals that the relative rotation angle between interacting particles overshoots before relaxation, thereby rationalizing the recently observed oscillating FACF in odd-diffusive systems. — [Langer et al., Phys. Rev. Res. 6, 043036 (2024)]

DY 24.6 Wed 16:30 H43

Odd mobility in interacting particle systems — •Erik Kalz[1], Shashank Ravichandir[2], Johannes Birkenmeier[1], Ralf Metzler[1], and Abhinav Sharma[2,3] — [1]University of Potsdam — [2]IPF, Dresden — [3]University of Augsburg

Colloidal mobility characterises the response of an overdamped particle to an external drift. We present a many-body theory where the diffusion of particles is modelled in the presence of interactions with other colloids. A tracer particle therefore can respond to its own applied force as well as to the external drift of the host particles, an effect transferred via particle-particle interactions. We examine these direct and transferred mobilities in the context of odd systems and show that they display qualitatively different behaviours. Odd systems are characterized by a transverse — Hall-like response which occurs in addition to the ordinary, parallel response. We show that both components, the parallel and transverse are drastically altered by particle-particle interactions up to a complete reversal for each component. Our findings are validated by Brownian dynamics simulations.

Invited Talk DY 24.7 Wed 16:45 H43

Odd dynamics and universal flows of passive objects in a chiral active fluid — •Cory Hargus[1], Federico Ghimenti[1,2], Julien Tailleur[1,3], and Frédéric van Wijland[1] — [1]Laboratoire Matière et Systèmes Complexes (MSC), Université Paris Cité & CNRS (UMR 7057), 75013 Paris, France — [2]Department of Applied Physics, Stanford University, 348 Via Pueblo, Stanford, CA 94305, United

States of America — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, United States of America

A passive object submerged in a chiral active fluid is imbued with odd diffusivity, odd mobility, and rotational ratchet motion. We show how these different effects are interrelated, obtaining a Langevin equation for a sufficiently heavy object, and how they are determined by the symmetry properties of the object, as well as its size and mass. Finally, spontaneous flows of the chiral active fluid around the object are understood through a multipole expansion, and connected through odd diffusion to equations of state involving only bulk fluid properties.

DY 24.8 Wed 17:15 H43

Vortex formation and odd viscosity in a chiral active fluid — •Joscha Mecke[1,2], Yongxiang Gao[1], Gerhard Gompper[2], and Marisol Ripoll[2] — [1]Institute for Advanced Study, Shenzhen University, Shenzhen, PR China — [2]Institute of Advanced Simulation, Forschungszentrum Jülich, Germany

Materials consisting of active particles with an intrinsic rotation can be considered as chiral active matter. We study a colloidal chiral active system, consisting of magnetic microrotors of diameter 0.8 μm in an externally applied rotating magnetic field. The stabilised colloids synchronously rotate with the rotating field and solely interact via steric and hydrodynamic interactions, granting odd and active stresses already at low densities and large colloidal separations. We address the system by means of experiments as well as particle based hydrodynamics simulations (MPC) of the active colloidal suspension. The rotors' transverse, anti-symmetric, and non-reciprocal interactions lead to a pair-rotation about the centre of mass and subsequently to the formation of multiscale vortices. Energy is injected on the particle level and is transported to the largest scales in the system, unless it is dissipated at a hydrodynamic damping length, a process reminiscent of turbulence, even in the absence of dominant inertial contributions. The rich phenomenology of our system additionally includes odd diffusion and enhancement of effective diffusive transport by the introduction of obstruction, directed transport by virtue of symmetry breaking at confining walls, and correlations between vorticity and density which allow for a measurement of the system's odd viscosity.

DY 24.9 Wed 17:30 H43

Chirotactic response of microswimmers in 3D chiral active fluids with odd viscosity — •Yuto Hosaka[1], Michalis Chatzittofi[1], Ramin Golestanian[1,2], and Andrej Vilfan[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [3]Jožef Stefan Institute, 1000 Ljubljana, Slovenia

Odd viscosity is a property of chiral active fluids with broken time-reversal and parity symmetries. We show that the flow of such a fluid around a rotating axisymmetric body is exactly solvable [1]. Using this solution and the generalized Lorentz reciprocal theorem [2], we determine the orientational dynamics of microswimmers with an arbitrary surface slip velocity. Swimmers with a force-dipole moment exhibit precession around the axis of the odd viscosity. In addition, pushers show *bimodal chirotaxis*, i.e., alignment parallel or antiparallel to the axis, while pullers orbit in a plane perpendicular to it. A chiral swimmer that itself has a broken parity symmetry can exhibit *unimodal chirotaxis* and always align in the same direction. Since the chirotactic response of microswimmers is prohibited in 2D fluids, our theoretical results highlight the critical role of three-dimensionality in transport phenomena in chiral active fluids.

[1] Y. Hosaka, M. Chatzittofi, R. Golestanian, and A. Vilfan, Phys. Rev. Research **6**, L032044 (2024).

[2] Y. Hosaka, R. Golestanian, and A. Vilfan, Phys. Rev. Lett. **131**, 178303 (2023).

DY 24.10 Wed 17:45 H43

Chirality and symmetry breaking in Dictyostelium Discoideum: Probing odd dynamics in cellular behavior — •Fereydoon Taheri — IMSEAM, Heidelberg University, Heidelberg, Germany

The interplay between chirality and symmetry breaking is a fundamental aspect of many biological systems, and Dictyostelium discoideum offers a unique model to explore these phenomena. This bacteria-guzzling amoeba that lives in soil, serves as a powerful model organism for studying fundamental cellular processes such as cell-cell signalling, collective movement, and self-organization in multicellular complexes. In this study, we present an in-depth investigation into the motility patterns of D. discoideum, with a focus on the inherent chirality observed during intercellular interactions. By analyzing the off-diagonal components of the diffusion tensor, we connect this chirality to asymmetries in the velocity correlation function. These off-diagonal terms capture the coupling between orthogonal velocity components, providing a quantitative measure of non-reciprocal motion and breaking of time-reversal symmetry. Our analysis reveals that these contributions are directly linked to chiral trajectories and it is not merely a byproduct of individual behavior but plays a functional role in mediating the efficiency and directionality of cell-cell communication influencing both individual and collective behaviors during aggregation and morphogenesis.

Invited Talk DY 24.11 Wed 18:00 H43

How to model frictional contacts in sheared and active colloids — •Friederike Schmid[1], Kay Hofmann[1], Kay-Robert Dormann[2], and Benno Liebchen[2] — [1]Johannes Gutenberg Universität Mainz — [2]Technische Universität Darmstadt

In simulations of colloidal matter, frictional contacts between particles are often neglected. For spherical colloids, such an approximation may have a significant impact on the results in certain situations (e.g., colloids under shear, chiral active matter), since frictional contacts induce a coupling between translational and orientational degrees of freedoms of particles which is otherwise absent. Models for implementing frictional contacts have been proposed in the granular matter community. Owing to the large size of granular particles, these models do not include thermal noise. On the colloidal scale, thermal fluctuations are important and should be incorporated in a thermodynamically consistent manner.

In the present talk, we show how to derive the correct fluctuation-dissipation relation for frictional contacts with arbitrary - linear or nonlinear - relation between the friction force and the relative velocity at the contact point, and how to implement the corresponding stochastic force terms. Among other this results in a new generalized class of dissipative particle dynamics (DPD) thermostats with rotation-translation coupling. Possible effects of frictional contact interactions are demonstrated using the example of Poiseuille flow and motility induced phase separation in active Langevin particles.

DY 25: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Wednesday 15:00–18:00 Location: H44

DY 25.1 Wed 15:00 H44

Separating bio-condensates with surfactant-like proteins — Jannik Kindermann and •Tyler Harmon — Leibniz Institute for Polymer Research, Dresden, Germany

Biocondensates are prevalent in cells as individual compartments that separate material and reactions in space. Many condensates share similar components and/or chemical interactions that drive their formation. This would suggest that the condensate:condensate interface would have a very low surface tension compared to the condensate:solvent interfaces. Supported by in vitro results, this leads to condensate-inside-condensate or dumbbell-like architectures which minimize the condensate:solvent interfaces. However, in vitro, condensates are most often isolated in space from each other. This could play important roles such as limiting the direct flow of material from one condensate to another. The mechanism in cells that separates droplets in space is unknown.

We show using simulations and theory that proteins or other biopolymers that have surfactant like molecular architectures can separate condensates in space. We show how robust this mechanism can be with respect to condensate specificity and the expression levels of surfactant-like molecules in cells.

DY 25.2 Wed 15:15 H44

Phase separation in membranes and compartments with binding reactions — •Riccardo Rossetto, Gerrit Wellecke, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization

Biological cells exhibit a hierarchical spatial organization, where various compartments and membranes harbor condensates that form by phase separation. Cells can control the emergence of these condensates by affecting the physical interactions of the involved biomolecules, thus also tuning the binding affinity to the compartments. We describe this situation with a thermodynamically-consistent kinetic model considering passive and active binding reactions to elucidate their role in controlling the occurrence and timescales of phase separation in compartments. On the one hand, binding reactions can lead to the emergence of new equilibrium phenomena, such as re-entrant phase transitions and multistability. On the other hand, they can also affect the kinetics of phase separation. As a particular example, we consider protein droplets in cellular membranes when proteins can also unbind to the cellular bulk. For fast bulk diffusion, this leads to effective nonlocal transport, which fundamentally affects droplet dynamics. For instance, the seminal Lifshitz-Slyozov coarsening can be abolished. Furthermore, active binding reactions can both accelerate or fully suppress coarsening, leading to protein patterns on the membrane. The general conclusions from our model unveil fundamental mechanisms of phase separa-

tion in membranes and compartments, and will help us explain more biological observations in the future.

DY 25.3 Wed 15:30 H44

Reconciling conflicting selection pressures in the plant collaborative non-self recognition self-incompatibility system — Amit Jangid[1], Keren Erez[1], Ohad-Noy Feldheim[2], and •Tamar Friedlander[1] — [1]Faculty of Agriculture, food and environment, The Hebrew University of Jerusalem, Rehovot, Israel — [2]Einstein Institute for Mathematics, The Hebrew University of Jerusalem, Jerusalem, Israel

Complex biological systems should often reconcile conflicting selection pressures. Specifically, in systems relying on molecular recognition, molecules should recognize particular partners, but avoid others. Here we study how such selection pressures shape the evolution of the self-incompatibility system in plants. This system inhibits self-fertilization using specific molecular recognition between proteins, expressed in the plant female and male reproductive organs. We study the impact of these opposing selection pressures on the amino acid frequencies in these proteins' recognition domain. We construct a theoretical framework enabling promiscuous recognition between proteins and multiple partners each, as found empirically, and employ stochastic simulations. We find asymmetric responses to selection affecting mostly the female, but not the male protein composition. Using large deviations theory, we well-approximate the simulated frequencies and find agreement with genomic data. Our work offers a general theoretical framework to study the impact of multiple selection pressures, applicable to additional biological systems.

DY 25.4 Wed 15:45 H44

Learning the Equilibrium Free Energy from Non-Equilibrium Steady States with Denoising Diffusion Models — •Daniel Nagel and Tristan Bereau — Institute for Theoretical Physics, Heidelberg University, Germany

Estimating accurate free energy profiles is crucial for predicting the behavior of complex molecular systems. While biased molecular dynamics simulations enhance the sampling of rare events, extracting reliable free energy landscapes from these simulations remains challenging. On the other hand, stochastic thermodynamics, i.e. the concept of entropy production, provides valuable insights into the dynamics of complex systems in non-equilibrium states. However, its computational complexity, due to dependence on time-dependent probability distributions, limits its application to smaller systems.

This work presents a novel approach that combines stochastic thermodynamics with the established machine learning technique of denoising diffusion models to efficiently estimate free energy profiles from biased non-equilibrium steady states. By linking the diffusion and simulation times, we show that the training objective, known as the score, can be decomposed into a non-trivial conservative contribution from the equilibrium potential and a trivial non-conservative part determined by external driving forces. To showcase the effectiveness of our approach and its ability to learn equilibrium free energy profiles, we apply it to a driven toy model and a Martini force field molecular dynamics simulation of a small molecule biased through a lipid bilayer.

DY 25.5 Wed 16:00 H44

Multiple Pareto-optimal solutions of the dissipation-adaptation trade-off — •Jorge Tabanera-Bravo and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen

Adaptation refers to the ability to recover and maintain "normal" function upon perturbations of internal or external conditions and is essential for sustaining life. Biological adaptation mechanisms are dissipative, i.e. they require a supply of energy such as the coupling to the hydrolysis of ATP. Via evolution the underlying biochemical machinery of living organisms evolved into highly optimized states. However, in the case of adaptation processes two quantities are optimized simultaneously, the adaptation speed or accuracy and the thermodynamic cost. In such cases one typically faces a trade-off, where improving one quantity implies worsening the other. The solution is no longer unique but rather a Pareto set—the set of all physically attainable protocols along which no quantity can be improved without worsening another. We investigate Pareto fronts in adaptation-dissipation trade-offs for a cellular thermostat and a minimal ATP-driven receptor-ligand reaction network. We find convex sections of Pareto fronts to be interrupted by concave regions, implying the existence of distinct optimization mechanisms. We discuss the implications of such "compromise-optimal" solutions and argue that they may endow biological systems with a superior flexibility to evolve, resist, and adapt to different nvironments.

15 min. break

Invited Talk DY 25.6 Wed 16:30 H44

Centrosome positioning in cell migration and immune response — •Heiko Rieger — Department of Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Leukocytes are the key players of the immune system in eliminating pathogen-infected or tumorigenic cells. During these processes centrosome positioning plays a crucial role for establishing cell polarization and directed migration, targeted secretion of vesicles for T cell activation and cellular cytotoxicity as well as the maintenance of cell integrity. Here, we give an overview over microtubule organization and dynamics during immune processes and present models for centrosome repositioning during the formation of the immunological synapse and during cell migration. We focus particularly on actin-myosin crosstalk, which is involved in regulating the polarity and morphology of migrating cells and encompasses mechanical interactions, mediated by crosslinkers and molecular motors, as well as cytoskeletal regulators. Based on recent experimental results we develop a computational whole-cell model involving dynamical microtubules that interact not only mechanically but also via signaling with an active cell boundary. A rich self-organized dynamical behavior emerges, comprising varying positions of the microtubule organizing center relative to the nucleus in the migration direction, varying migration characteristics and cell shapes, and complex migratory behavior in obstacle parks and microfluidic setups. Specific dependencies of these behaviors from parameters like the average microtubule length or the cell-boundary stiffness are predicted and compared with experimental observations.

DY 25.7 Wed 17:00 H44

Modelling neuron growth dynamics and role of extra-cellular matrix — •Pritha Dolai, Federica Furlanetto, Sven Falk, Marisa Karow, and Vasily Zaburdaev — Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, Erlangen

Biological tissues are composed of cells embedded in extracellular matrix (ECM) and extracellular fluid. We study the role of cell-matrix interactions in the context of brain tissues and the mechanism of neuron growth through this matrix. We consider two modes for the neurite growth: linear growth by tip extension and growth by the traction force at the tip of the neurite with the ECM. In the second mechanism, growth happens solely due to the interaction of the growing appendages with the particles modeling the matrix. With an agent based model we recapitulate experimentally observed neuron growth patterns in healthy neurons and neurons with mutations corresponding to a disease state performed in organoid models. In experiments, neuron growth is quantified by the dynamics of the growing tips. Additionally we compare further growth characteristics such as track length and velocity of the tip, tortuosity, and angular correlation of growth direction. Our model provides mechanistic description of the neurite growth and can be useful in describing neuronal network formation during early development.

DY 25.8 Wed 17:15 H44

Cellular morphodynamics as quantifiers for functional states of resident tissue macrophages in vivo — •Miriam Schnitzerlein[1,2], Eric Greto[3,4], Anja Wegner[3,4], Anna Möller[3,4], Oliver Aust[3,4], Oumaima Ben Brahim[3,4], Stefan Uderhardt[3,4], and Vasily Zaburdaev[1,2] — [1]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — [4]Deutsches Zentrum für Immuntherapie, FAU

Resident tissue macrophages (RTMs) perform essential tasks such as clearing cellular debris to ensure tissue homeostasis. Such actions are accompanied by morphological changes in cell shape which reflect their functional states. Until now, RTMs were mostly studied *in vitro*, even though their dynamic behaviour *in vivo* is fundamentally different.

We employed a high-resolution, intravital imaging protocol to generate dynamic data of *in vivo* peritoneal RTMs of mice. Next we built a custom image processing pipeline to assess RTM morphodynamics via a set of human-interpretable cell shape and size features. Those features could quantitatively and also qualitatively differentiate between cells in different activation states. Furthermore, we showed that unperturbed RTMs exhibit a wide range of morphodynamical phenotypes, constituting a naive morphospace of behavioural motifs. Analysing cells challenged by chemical stimulations or due to aging gave us insights into how RTMs respond and adapt to inflammatory stimuli.

DY 25.9 Wed 17:30 H44

Slimming down through frustration — •Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France — PMMH, CNRS, ESPCI Paris, PSL University, Sorbonne Université, Université Paris-Cité, F-75005, Paris, France

In many disease, proteins aggregate into fibers. Why? One could think of molecular reasons, but here we try something more general. We propose that when particles with complex shapes aggregate, geometrical frustration builds up and fibers generically appear. Such a rule could be very useful in designing artificial self-assembling systems.

DY 25.10 Wed 17:45 H44

RNA fitness prediction with sparse physics based models - A way to explore the sequence space — •Christian Faber[1], Francesco Calvanese[2], Alexander Schug[1], and Martin Weigt[3] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Sorbonne-Université, Paris, France — [3]CNRS, Paris, France

The field of medicine uses macromolecules as a means of therapeutic intervention. Consequently, the functional attributes of these novel molecules are assuming greater significance. To complement the wet-lab experiments, we have devised a series of statistical physics based models that are capable of predicting the fitness of RNA molecules based on one- and two-point mutation scans. The experimental data were employed as training data to fit models of increasing complexity, commencing with an additive model and concluding with a model that accounts for global and local epistasis. The models were validated using fitness data from scans with higher order mutations of the wild-type. In contrast to conventional AI algorithms, the parameters of our models were designed for direct interpretation. In examining more distant sequences, we can distinguish the corresponding RNA family from random sequences with a high degree of accuracy. Moreover, the models facilitate interpretations of evolutionary processes and the significance of epistatic terms. Our model can be used to create a fitness landscape far beyond the experimental sequence space, thus identifying promising RNA molecules. Furthermore, the extension to the entire sequence space can be used as a blueprint for other molecules, providing a novel avenue for questions in biomolecular design.

DY 26: Networks, From Topology to Dynamics (joint session SOE/BP/DY)

Time: Wednesday 15:00–17:30 Location: H45

See SOE 8 for details of this session.

DY 27: Poster: Nonlinear Dynamics, Pattern Formation, Granular Matter

Time: Wednesday 15:00–18:00 Location: P4

DY 27.1 Wed 15:00 P4

Statistical field theory of linear spatio-temporally extended systems with multiplicative noise — •Frederik Gareis, David Aderbauer, and Michael Wilczek — Theoretische Physik I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Linear systems with multiplicative stochastic noise commonly exhibit non-Gaussian behavior in both space and time. We consider a classic example from statistical hydrodynamics, the Kraichnan model for a passive scalar convected in a stochastic velocity field. Describing such systems via a characteristic functional elegantly encodes the full statistics of the fields. However, the analysis of the resulting functional differential equations remains challenging due to the mathematical intricacy of treating second-order functional derivatives. Here, we show that a broad variety of such problems permit a solution of the functional differential equations in the form of a superposition of Gaussian functionals, even if the noise is correlated in space and time. While the linear terms, excluding the multiplicative noise, are compatible with Gaussian solutions, averaging over the multiplicative advection term introduces non-Gaussian statistics. Our approach provides a starting point for various systematic approximations such as a perturbation theory in terms of small multiplicative noise strength. On a conceptual level, it allows us to gain insights into the emergence of non-Gaussianity and intermittency, which could be relevant beyond statistical hydrodynamics.

DY 27.2 Wed 15:00 P4

Identifying Change Points in Local Air Temperature Time Series — •Fatemeh Aghaei A., Ewan Thomas Phillips, and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Global air temperature reconstructions consistently reveal a warming trend beginning around 1975, with signs of earlier increases since the early 20th century. However, regional temperature variations display complex, heterogeneous patterns that warrant deeper exploration. Understanding local climate change is critical for effective adaptation in health, agriculture, water management, and infrastructure sectors. By analyzing change points in regional warming trends, this study aims to identify periods of intensified climate change, suggesting potential historical tipping events.

In this paper, we analyze 2-meter mean daily temperature data from the ERA5 reanalysis project to track warming trends across a 1x1 degree global grid. By removing seasonal cycles, we capture temperature anomalies that reveal significant regional warming variations, with standard deviations of 4-6K depending on location. Recognizing that local warming is rarely linear, we fit two linear slopes with a change point to each grid point to capture change in warming trends. This approach produces global maps indicating the timing and magnitude of trend changes, highlighting regions where local warming has intensified.

DY 27.3 Wed 15:00 P4

Causal inference in nonlinear Covid-19 time series — •Adrian Pelcaru and Dirk Brockmann — SynoSys/TU Dresden, Dresden, Germany

Covid-19 pandemic exemplifies a spatio-temporal dynamic system which can hardly be studied by controlled experiments with "laboratory settings". Advances of computational power and availability of large datasets, causal discovery frameworks enable one to gain insight into the dynamics and couplings between observables of the system. We employ an approach rooted in state space reconstruction called Convergent Cross-Mapping (CCM) and investigate time-lagged interactions between multiple observables (temperature, interventions, human mobility, reproduction rate) of Covid-19 in 114 countries and 38 regions in Germany. Central, is the interrelationship between human mobility and reproduction rate. We find evidence for time lagged feedback couplings between human mobility and reproduction rate and identify other drivers of the reproduction rate acting either directly or indirectly through human mobility. Furthermore, we detect latitudinal dependence of coupling strengths and clear segregation of coupling strengths between historic east and west Germany. Finally, we measure dynamic tipping points of strong unidirectional forcing between human mobility and reproduction rate leading to distinct periods with characteristic dynamics. While many causal discovery frameworks and previous studies related to Covid-19 a priori reject potential feedback mechanisms between observables of a system, this study, to our knowledge, shows their existence for the first time.

DY 27.4 Wed 15:00 P4

Numerical Differentiation by Integrated Series Expansion (NDBISE) in the Context of Ordinary Differential Equation Estimation Problems — •Oliver Strebel — Angelstr. 17, D-75392 Deckenpfronn

Parameter or model estimation of ordinary differential equations (ODE) involves nowadays frequently the numerical calculation of derivatives from noisy data. This article presents a novel differentiation method (NDBISE) for such calculations. The method is benchmarked against 57 differential equations and compared to other numerical differentiation methods. The hyperparameters of all these methods are optimized in order to get a reasonable comparison. The resilience against larger noise or fewer data points per time interval is examined. It turns out that the novel method is overall superior to the other methods.

The derivative for the 42 real world data points of the Hudson bay lynx hare data (years 1900-1920) is also calculated. The results match the derivative of a curve fit to the data points astonishingly close. Using a Savitsky-Golay filter the method can be leveraged to calculate second and third order derivatives, so that the results are close to the theoretically expected outcome.

Preprint: https://doi.org/10.21203/rs.3.rs-5465961/v1

DY 27.5 Wed 15:00 P4

Origin of Frequency Clusters in Globally Coupled Phase Oscillators — •Yannick Schöhs, Nicolas Thomé, and Katharina Krischer — Technische Universität München

Frequency clusters arise in a wide range of physical, technological, and biological systems, making them a topic of significant interest both for their practical implications and for advancing the fundamental understanding of collective dynamics. Despite their importance, their origin remains relatively unexplored. In this study, we investigate the origin of frequency clusters using a model of globally coupled phase oscillators with adaptive coupling strength. By numerically solving the differential equations for a network of 100 oscillators, the formation of up to four distinct frequency clusters was confirmed. Additionally, we conducted a bifurcation analysis on a system of four oscillators. The reduced system size allowed for an analytical bifurcation analysis of the fixed points, while the bifurcation analysis of the limit cycles was performed numerically. The results reveal that the frequency clusters originate from a homoclinic bifurcation and lose their stability through a transcritical bifurcation.

DY 27.6 Wed 15:00 P4

Optimal Control of Fractional Bistable System — •Finn Biesterfeldt[1], Andreas Rauh[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany — [2]Department für Informatik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this work, a classic bistable system in continuous time and space and described by an ordinary integer-order differential equation is generalized to fractional order using the principles of Fractional Calculus. This results in an intrinsic mem-

ory effect and the time evolution depends on the full history of its prior configurations. In numerical simulations we observe that depending on the initial conditions, the system drives towards one of two possible fixed points of the integer order system. Initializing the system with a non-constant history leads to a complex time evolution that is highly dependent on the fractional order. In this study, the non-constant history can be interpreted as an external influence or control input that drives the system from one fixed point to the other. Influenced by the fractional order, the system may converge back to the initial fixed point. The optimal control strategy for transitioning the system from one to the other fixed point is computed numerically, revealing a dependence on the fractional order of the system.

DY 27.7 Wed 15:00 P4

Phase separation with long-range interactions — •Filipe Thewes, Yicheng Qiang, Oliver Paulin, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

It is well known that long-range interactions affect phase separation. For instance, such interactions can suppress droplet coarsening, leading to microscopic pattern with selected length scales. This effect is widely exploited by nature – from structure formation in living cells to food engineering by humans. Although the details of the transition from macroscopic phase separation to microscopic pattern formation are understood for particular systems, the general conditions for the existence of such transition remain unclear.

We propose a general field theoretical model that combines Flory's theory of phase separation and a broad class of long-range interactions. We then show that the particular details of these interactions are not relevant to the transition from macro phase separation to micro pattern formation and the most important parameter is the length-scale associated with the long-range interactions. We uncover the possibility of both first-order and second-order transitions as this length-scale crosses a threshold value, and we show how two macro phases can coexist with patterned phases. Extending these results to multi-component mixtures reveals even richer physics with multiple coexisting patterns. Our results open the possibility of systematic control of droplet sizes via different pathways, and depending on the nature of the phase transition, allow for an intricate design of pattern formation.

DY 27.8 Wed 15:00 P4

Rapid Control of Soliton Dynamics in Dual-Comb Lasers via Intra-Cavity Modulation — Julia Lang[1], •Simeon Schmitt[1], Luca Nimmesgern[1], Sarah Hutter[2], Alfred Leitenstorfer[2], and Georg Herink[1] — [1]Universität Bayreuth, Germany — [2]Universität Konstanz, Germany

We present a novel approach for controlling the timing of solitons in ultrafast mode-locked lasers, enabling the programmable synthesis of ultrashort soliton pulse patterns. The approach utilizes intra-cavity acousto-optic modulation in a single, harmonically mode-locked Er:fiber laser. By employing single-pulse modulation, we induce precise timing shifts between the two temporally separated, interlaced soliton combs. Through external splitting and recombination, we obtain temporally overlaying ultrashort soliton pulse-sequences that can be rapidly tuned above kHz scanning rates. We present real-time spectral interferometry data based on the dispersive Fourier transformation and corresponding simulations that resolve the underlying intersoliton motion due to ultrafast nonlinearities and laser gain dynamics. [1]

[1] J. A. Lang, S. R. Hutter, A. Leitenstorfer, and G. Herink. 'Controlling Intracavity Dual-Comb Soliton Motion in a Single-Fiber Laser'. Science Advances 10 (2024)

DY 27.9 Wed 15:00 P4

Driven BHD - onset of chaos and extendet KNH-Theorem — •Nico Fink, Viviane Bauer, and James Anglin — Physics Department and Research Center OSCAR, RPTU Kaiserslautern-Landau

When we investigate physical systems the method of description changes in dependence of scale: mechanics for individual particles but statistical methods for many. Indeed the latter should derive from mechanics, but how exactly do they relate? In other words: how does an increse in degrees od freedom influences the behaviour of a system and what kind of effects appear? In a Bose-Hubbard-dimer as a modelsystem it has been shown, that the existence of an instable fixpoint - and thereby a separatrix - can give rise to irreversibility. This is realised by adiabatically varying the potentialdifference of the sites, causing the ensemble to split into two sub-ensembles when crossing the separatrix. If the consicered meanfield Bose-Hubbard-Dimer is extendet by periodic driving a chaotic band emerges in the neighbourhood of the separatrix. We investigate the onset of chaos and the characteristic behaviour of the system in general and under the change of potential as described above.

DY 27.10 Wed 15:00 P4

QH plateau and CMB- CR near nontrivial zeros of the zeta function — •Otto Ziep — 13089 Berlin, Am Wasserturm 19a

Chaotic one-dimensional period-doublings as iterated hyperelliptic-elliptic curves are used to derive n-dim Kepler- and Coulomb singularities. Millikan experiment, quantum Hall (QH) effect, atmospheric clouds and universe clouds are self-similar of mass ratio 10^20 in a fractal zeta universe (FZU) of ripped spacetime [1]. The cosmic microwave background (CMB) and cosmic rays (CR) are explained as bifurcating ripped spacetime tensile forces below and above first Sharkovsky cycles from the tree root up to third branch. At QH CMB emissions 1...1000 GHz are predicted by the iterated binary tree cloud which are possibly already detected [2]. An interaction-independent universal vacuum density allows to predict large area correlated CR in QH-experiments which would generate local nuclear disintegration stars, enhanced damage of layers and enhanced air ionization [1]. A 10^20 self-similarity between conductivity plateau and atmospheric cloud as a superfluid having two cycles of entropy and temperature allows us to conclude that CMB and CR correlations in atmospheric layer influence global temperature and climate.

[1] The poster is based on trilogy Nucleosynthesis in Thin Layers, Fractal zeta universe and cosmic-ray-charge-cloud superfluid, The sensitive balance by O. Ziep www.epubli.de in 03/24,11/24, 01/25

[2]R. Bisognin und others, Microwave photons emitted by fractionally charged quasiparticles Nat, Commun, 2019.

DY 27.11 Wed 15:00 P4

Detection and Analysis of Topological Defgnetic Systems via Enhanced Topological Data Analysisects in Ma — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Insitute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany — [2]Faculty of Physics & Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Duisburg, Germany

Complex data structures, marked by multi-dimensional correlations and noise, pose significant challenges in various fields like genetics and complex dynamical quantum systems. Topological Data Analysis (TDA) [1], rooted in Persistent Homology can address this, e.g. by effective characterizing phase transitions in dynamical systems [2], enhancing large genome data analysis [3] and preprocessing data for machine learning [1]. By introducing series of graph structures into data point clouds intrinsic topological information can be extracted. Focusing on magnetic systems with topological defects, localized perturbations in the ordering field, we propose using TDA to enhance their detection and analysis. By combing conventional persistence diagram analysis with geometrical, topological, and graph-based measures applied directly to the representative clustering, our approach can provide an additional insight into the topological landscape and multi-scale nature of topological defects in magnetic systems.

[1] F. Hensel et al., Frontiers in AI, vol. 4 (2021)
[2] E. Cheng et al., IOP, vol.57 [30] (2024)
[3] S. Yara et al, Journal of Biomedical Informatics, vol. 130 (2022)

DY 27.12 Wed 15:00 P4

Force enhancement in-between suszeptible dipolar hard spheres - measurement vs computation — Andree Smolla[1], Alexandros G. Sourais[2], Sofia S. Kantorovich[3], Andreas Boudouvis[2], and •Reinhard Richter[1] — [1]Experimentalphysik 5, Universität Bayreuth, 95447 Bayreuth, Germany — [2]School of Chemical Engineering, National Technical University of Athens, Zografu Campus, 15780 Athens, Greece — [3]Computational Physics, University of Vienna, 1090 Vienna, Austria

We measure the force acting in-between two magnetized steel spheres used previously in ferrogranular model experiments [1]. When reducing the mutual distance r of the spheres the force r exceeds considerably the scaling $\sim r^{-4}$ known from dipolar hard spheres (DHS). To elucidate this deviation we measure the magnetization curves $M(H)$ of both steel spheres by means of a vibrating sample magnetometer. Their magnetization curves show a remanent magnetization plus a contribution which depends on an outer magnetic field, i.e. we have suszeptible dipolar hard spheres (SDHS). Taking into account $M(H)$ we solve the governing equations with the finite element method using FEniCS and COMSOL [2], showing a peak of the magnetization in the contact zone. The estimated force captures the enhanced force measured before.

[1] M. Biersack, A. Lakkis, R. Richter, O. Bilous, P. A. Sánchez, S. S. Kantorovich *Phys. Rev. E*, 108 (2023) 054905.

[2] Alexandros G. Sourais, Solution of magnetostatics problems with the Finite Element method using FEniCS computational platform, Master Thesis, National Technical University of Athens (2021).

DY 27.13 Wed 15:00 P4

Athermal jamming as a Manna class transition with a deterministic protocol — •Thomas Axmann, Mishael Derla, and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Athermal jamming can be understood as the transition point of an overlap reducing dynamical protocol of soft particles, where the absorbing (non-overlapping) states become inaccessible during configuration space sampling when increasing the density above the transition. The properties of this transition appear to be of $d + 1$ conserved directed percolation (Manna) universality, largely independent of the details of the dynamics implemented. To demonstrate this, we present a fully deterministic protocol that remains in the Manna class. The study was conducted numerically, but we further endeavor to illuminate the situation an-

alytically, by exploring possibilities for relating athermal jamming to directed percolation in time. We aim to determine the transition density for systems with Random Organization and Jamming and conditions to be in the Manna class.

(Note: Thomas Axmann and Mishael Derla contributed equally and will present the poster together)

DY 27.14 Wed 15:00 P4

Self-assembly of Eiffel Towers out of a ferrogranular gas — •Matthias Biersack, Ali Lakkis, and Reinhard Richter — University of Bayreuth, Experimental Physics 5, Universitätsstr. 30, 97440 Bayreuth, Germany

We are exploring in experiments a shaken granular mixture of glass and magnetized steel beads, filled in a horizontal vessel [1]. For strong shaking amplitude ($\Gamma > 3g$) we observe a ferrogranular gas. By means of a Helmholtz-pair of coils we apply a homogeneous magnetic field oriented normal to the vessel. Then we observe the self-assembly of ferrogranular crests resembling miniatur Eiffel Towers. Our findings are compared with the normal field instability emerging in a ferrofluid [2].

[1] M. Biersack, A. Lakkis, R. Richter, O. Bilous, P. A. Sánchez, S. S. Kantorovich *Phys. Rev. E*, 108 (2023) 054905.

[2] M. Cowley, R. E. Rosensweig *J. Fluid Mech.* 30 (1967) 671.

DY 28: Poster: Machine Learning, Data Science

Time: Wednesday 15:00–18:00 Location: P4

DY 28.1 Wed 15:00 P4

Thermal Neural Quantum States — •Atiye Abedinnia and Annabelle Bohrdt — Institute of theoretical physics, University of Regensburg

Finite-temperature effects play an important role in the design and optimization of quantum devices, as decoherence and noise often originate from thermal fluctuations. At finite temperatures, quantum systems are described by a statistical ensemble of states rather than a single pure state. Simulating such thermal states requires constructing the thermal density matrix, which suffers from significant computational challenges due to the exponential growth of the Hilbert space with system size. So far, purification methods(thermofield) in the context of MPS and Minimally Entangled Typical Thermal States (METTS) approach have been developed in the context of tensor networks. In this work, we propose using neural quantum states (NQS), leveraging the expressivity and scalability of transformer-based architectures to address the challenges of thermal equilibrium density matrix representation.

DY 28.2 Wed 15:00 P4

Neural Networks for Phase Recognition on Lattice Systems — •Shashank Kallappara and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

The Ising model undergoes a phase transition in dimensions d > 1, with its magnetisation as the order parameter. Fully connected neural networks have been shown to learn the translational invariance of the Ising model when learning its phases. This requires only a single hidden layer; analytic solutions for the same exist for highly compact networks that are constructed to obey the translational invariance automatically. Here, we show this learning of the invariance in single-layer networks of different widths and compare the networks performance in classifying the phases. We also consider a highly compact network to study the gradient descent dynamics during training over its loss landscape; we suggest a few changes to this that greatly improve its performance while preserving interpretability. Another problem we consider is percolation on a square two-dimensional lattice. Here, we leverage convolutional neural networks to detect the phase transition by training on different properties of the systems and evaluate its effectiveness.

DY 28.3 Wed 15:00 P4

optimization of the algorithm of operation of a series-parallel combined power plant — •Malika Allakulyyeva — Moscow, Russia

Over the past 15 years, work on the creation of a combined power plant (CEP) of a car has become an independent direction of modern electromechanics, characterized by its scientific problems, the specifics of performing applied research, and the expanding field of practical use of developments. This article presents the results of experimental studies of series-parallel power plants on the educational laboratory stand of the CO3221-6X model *Cars with power plants and electric vehicles* and proposes an alternative algorithm for the operation of a combined power plant.

DY 28.4 Wed 15:00 P4

Stability of Machine-Learned Interatomic Potentials in Molecular Dynamics Simulations for Complex Organic Crystals — •Martin Tritthart, Florian Linder, Lukas Legenstein, Florian Unterkofler, Martin Klotz, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, NAWI Graz, AUSTRIA

Understanding thermal conductivity and mechanical stability is crucial for several applications of organic semiconductors (OSCs) and metal-organic frameworks (MOFs). Molecular dynamics (MD) simulations are commonly used to deduce these properties, and in recent years, machine Learned interatomic potentials (MLIPs) have been employed to enhance accuracy compared to classical force fields. MLIPs are orders of magnitude faster than ab initio methods and can achieve close to DFT accuracy. Their accuracy,however, heavily depends on the quality of the training data. Incorrect predictions of forces and energies for atomic configurations outside the training dataset can accumulate in the MD trajectory, potentially even leading to disintegration of the (molecular) building blocks. This, however, limits long-time simulations, which are necessary to investigate thermal transport properties. To mitigate these issues and to realize a robust MLIP, reliable uncertainty estimates are needed especially for atomic configurations outside the region of the phase space sampled during training. Structures characterized by high uncertainties can then be calculated by ab initio methods and incorporated into the training dataset. This approach is tested in my contribution for prototypical MOF and OSC materials.

DY 28.5 Wed 15:00 P4

Estimating parameters for a simple tipping model from complex Earth system model output — •Jonathan Krönke[1,2], Jonathan F. Donges[1], Johan Rockström[1], Nils Bochow[3], and Nico Wunderling[1,2] — [1]Earth Resilience Science Unit, Potsdam-Insitute for Climate Impact Research, Potsdam, Germany — [2]Center for Critical Computational Studies, Goethe University Frankfurt, Frankfurt am Main, Germany — [3]Department of Mathematics and Statistics, UiT - The Arctic University of Norway, Tromsø, Norway

The existence of large-scale tipping points - thresholds where small changes can trigger drastic, often irreversible shifts in the climate system - has been a major concern of climate science in the past two decades. The ability to evaluate tipping risks using computationally manageable models is crucial to assess the resilience of the climate system and also to identify safe global warming trajectories for tipping elements. Here, we present an approach to estimate parameters of a simple tipping model based on complex Earth system model output. We validate our results by reproducing simulations that have not been used in the training process and apply the model to major earth system tipping elements such as the Greenland Ice Sheet. A simple model that captures essential behaviour of complex earth system models provides an important step towards a tipping point emulator for extensive tipping risk analyses.

DY 28.6 Wed 15:00 P4

Advanced Framework for State of Health Estimation Using Equivalent Circuit Models and Machine Learning — •Limei Jin[1,2], Franz Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IET-1, Forschungszentrum Jülich

Traditional Electrochemical Impedance Spectroscopy (EIS) techniques for characterizing a battery's behavior face several limitations, including time-consuming data collection, assumptions of system linearity, and difficulties in accurately assessing State of Charge (SoC) and State of Health (SoH). To address these challenges, we developed a robust framework for estimating SoH within a low-dimensional latent space using an autoencoder applied to raw time-domain battery data. This methodology combines synthetic training data from equivalent circuit models with machine learning techniques, specifically utilizing Chebyshev-based parameter space expansion to vary models on the SoC and SoH scale. Thereby, our framework effectively captures dynamic aging patterns while ensuring efficient data generation with minimal experimental input. Additionally, we introduced a stochastic pulse load profile to the models, which overcomes limitations of conventional frequency-based EIS measurements to better reflect real-world battery usage. This approach was initially validated on coin cell batteries in the lab, requiring only three standard spectroscopy experiments to train the framework. It will be extended to larger batteries, such as LFP batteries commonly used in automotive applications, offering scalable solutions for real-time monitoring and enhanced longevity.

DY 28.7 Wed 15:00 P4

Parameter estimation and Bayesian comparison of Langevin models describing cell motility — •Yusuke Kato[1,2], Jan Albrecht[1], Hiroshi Kori[2], Robert Grossmann[1], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Department of Complexity Science and Engineering, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan

In nature, motile bacteria and eukaryotic cells exhibit spontaneous movement. This cell motility plays an essential role in both maintaining homeostasis (such as the migration of immune cells to a wound site) and the pathogenesis of certain diseases (like the aggregation of cancer cells to other organs in metastasis). Various SDE-based Langevin models have been proposed to describe cell motility.

In this study, we adopt a Bayesian approach using the likelihood approximation technique introduced in Ref. [arxiv:2411.08692] to estimate parameters of tentative first- and second-order models. In order to compare the different models, we develop a framework that ranks them using Bayesian model comparison. We test and benchmark the approach using synthetic data and subsequently apply it to time-series data of ameboid cells in order to find the best model for their ameboid motility.

DY 29: Poster: Quantum Dynamics and Many-body Systems

Time: Wednesday 15:00–18:00 Location: P4

DY 29.1 Wed 15:00 P4

Prethermalization in Open Quantum Systems — •Saptarshi Saha[1] and Rangeet Bhattacharyya[2] — [1]Institute of Theoretical Physics, Technical University of Berlin Hardenbergstr. 36, Sekr. EW 7-1, 10623 Berlin, Germany. — [2]Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur-741246, West Bengal, India

A nearly-integrable isolated quantum many-body system reaches a quasi-stationary prethermal state before a late thermalization. Here, we revisit a particular example in the settings of an open quantum system (OQS). We consider a collection of non-interacting atoms coupled to a spatially correlated bosonic bath characterized by a bath correlation length. Our result implies that the integrability of the system depends on such a correlation length. If this length is much larger than the distance between the atoms, such a system behaves as a nearly-integrable OQS. We study the properties of the emerging prethermal state for this case, i.e. the state's lifetime, the extensive number of existing quasi-conserved quantities, the emergence of the generalized Gibbs state, and the scaling of von Neumann entropy, etc. We find that for the prethermal state, the maximum growth of entropy is logarithmic with the number of atoms, whereas such growth is linear for the final steady state, which is the Gibbs state in this case.

DY 29.2 Wed 15:00 P4

Quantum Fluctuations Approach to Many-Body Systems for Weak and Strong Coupling — •Erik Schroedter, Jan-Philip Joost, Tim Kalsberger, and Michael Bonitz — CAU, Kiel, Germany

The theoretical description of correlated quantum many-body systems out of equilibrium is a significant challenge across many areas, including condensed matter, ultracold atoms, and dense plasmas. Standard approaches used for their description include the formalisms of reduced density matrices (RDM) and nonequilibrium Green functions (NEGF). However, all approaches suited for the description of nonequilibrium systems are limited in their applicability due to their accuracy or numerical scaling. Here, we present an alternative approach based on fluctuations of field operator products and their correlation functions[1,2]. It is closely related to NEGF and RDM theory and offers an alternative approach to the GW and T-matrix approximations while exhibiting interesting complementary features, such as the capability to simulate many-body effects using stochastic methods[3]. This significantly reduces numerical complexity while preserving accuracy and allows for the description of both weakly and strongly coupled systems. Additionally, this improves numerical stability and allows for direct access to spectral two-particle quantities, such as the density response function or dynamic structure factor.

[1] E. Schroedter, et al., Cond. Matt. Phys. 25, 23401 (2022)
[2] E. Schroedter, and M. Bonitz, CTPP 202400015 (2024)
[3] E. Schroedter, et al., Phys. Rev. B 108, 205109 (2023)

DY 29.3 Wed 15:00 P4

Dynamics of topological defects in non-equilibrium magnon condensates — •Alexander Wowchik and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, 50937 Cologne, Germany

It has been demonstrated in the past that thin Yttrium Iron Garnet (YIG) films exhibit condensation of magnons in two degenerate minima of the band structure when driven with microwave radiation in the presence of an external magnetic field.

This creates a non-equilibrium many-body system at room temperature, which provides a framework to study the dynamics of self-propelling units that violate the conservation of energy, analogous to models of active matter.

We examine the behaviour of a single topological vortex defect in the magnon condensate after explicitly breaking the spatial inversion symmetry that restricts the dynamics of the ideal system. This is motivated by an asymmetric configuration in the typical experimental setup.

The study is performed by solving the driven-dissipative Gross-Pitaevskii equation for the emergent condensate degrees of freedom. It is derived from the semi-classical limit of an effective U(1) x O(2) symmetric Keldysh field theory.

The results are compared to micromagnetic simulations of the underlying ferromagnetic spin-Hamiltonian.

DY 29.4 Wed 15:00 P4

Wiedemann-Franz law violation domain for graphene and nonrelativistic systems — •Thandar Zaw Win, Cho Win Aung, Gaurav Khandal, and Sabyasachi Ghosh — Department of Physics, Indian Institute of Technology Bhilai, Kutelabhata, Durg 491002, India

Systematic and comparative research on Lorenz ratios for graphene and nonrelativistic systems has been studied to identify their Wiedemann-Franz law violation domain. Fermi energy and tem- perature are the main governing parameters for deciding the values of the Lorenz ratio, which is basically thermal conductivity divided by electrical conductivity times temperature times Lorenz number. Metals as three-dimensional nonrelativistic electron gas locate at higher Fermi energy by temperature domain, where Lorenz ratio remains one. Hence, they obey the Wiedemann-Franz law. By creating higher doping in a two-dimensional graphene system, one can again reach a higher Fermi energy by temperature domain and get a constant Lorenz ratio. For both graphene and nonrelativistic systems, the Lorenz ratio goes below one if we go lower Fermi energy by temperature domain, which is possible for the graphene system by decreasing the doping concentration. Experimentally observed greater than one Lorenz ratio in this lower Fermi energy by temperature domain or Dirac fluid domain indicates that non-fluid expressions of Lorenz ratio should be replaced by fluid-type expressions. We have noticed a divergent trend of Lorenz ratio in the Dirac fluid domain using its fluid-type expression, and it matches with the trend of experimental data.

DY 29.5 Wed 15:00 P4

Anisotropic Dicke model in the presence of periodic and quasiperiodic drive — •Pragna Das[1], Devendra Singh Bhakuni[2], Lea F. Santos[3], and Auditya Sharma[4] — [1]Department of Theoretical Physics, J. Stefan Institute, SI-1000 Ljubljana, Slovenia — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy — [3]Department of Physics, University of Connecticut, Storrs, Connecticut 06269, USA — [4]Indian Institute of Science Education and Research, Bhopal 462066, India

We analyze the anisotropic Dicke model in the presence of a periodic drive and under a quasiperiodic drive. We show that under a quasiperiodic Fibonacci (Thue-Morse) drive, the system features a prethermal plateau that increases as an exponential (stretched exponential) with the driving frequency before heating to an infinite-temperature state. In contrast, when the model is periodically driven, the dynamics reaches a plateau that is not followed by heating. In either case, the plateau value depends on the energy of the initial state and on the parameters of the undriven Hamiltonian. Surprisingly, this value does not always approach the infinitetemperature state monotonically as the frequency of the periodic drive decreases. We also show how the drive modifies the quantum critical point and discuss open questions associated with the analysis of level statistics at intermediate frequencies.

DY 29.6 Wed 15:00 P4

Enhancing quantum metric using periodic driving — •Dhruv Tiwari, Roderich Moessner, and Johannes S. Hofmann — Max Planck Institute for Physics of Complex Systems, Nöthnitzer Str., 01187, Dresden

The advent of periodically driven systems has revolutionized modern condensed matter physics by offering two transformative opportunities. First, they allow the realization of nonequilibrium analogs of well-established equilibrium phases under highly tunable conditions. Second, they facilitate the emergence of novel phases with no equilibrium counterparts. In this work, we focus on the former, leveraging the tunable parameters of periodically driven systems to enhance the quantum metric in flat-band systems. The quantum metric, a fundamental geometric property of the band structure, plays a critical role in the formation of superconductivity in flat-band systems with attaractive density interactions. Here, we present preliminary results demonstrating how the interplay between periodic driving and electron correlations can amplify the quantum metric, leading to enhanced physical properties compared to the equilibrium case. These findings pave the way for designing engineered quantum states and exploring the interplay of nonequilibrium dynamics and strong correlations in flat-band systems.

DY 29.7 Wed 15:00 P4

Phase-space correlations of resonances in chaotic scattering systems — •Florian Lorenz and Roland Ketzmerick — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

Chaotic eigenfunctions in closed quantum systems show strong phase-space correlations along classical trajectories [1]. These correlations extend across the whole system size and persist in the semiclassical limit [1]. We here expand this analysis to open quantum maps and scattering systems, in particular the kicked rotor and a dielectric cavity. To this end, we generalize a time-dependent correlator suggested in [1] to the case of an open system using left- and right resonance states. For quantum maps we find similar results as for closed systems. For the dielectric cavity the correlations propagate as wave fronts through the system.

[1] H. Schanz, Phase-Space Correlations of Chaotic Eigenstates, Phys. Rev. Lett. **94**, 134101 (2005).

DY 29.8 Wed 15:00 P4

Generalizing Quantum Question Equalities: Measurement Order Effects in Cognitive Decision-Making — •Michael Schnabel — Vanderbilt University, Nashville, TN (USA)

The quantum question (QQ) equality, formulated by Wang and Busemeyer [1] provides a non-parametric prediction for the pairwise probabilities of binary questions represented by two non-commutative observables A and B and their associated projection operators P_A and P_B. The QQ equality has played a significant role in the development of the quantum cognition research program as it enabled testing whether the order effects observed in a representative dataset of questionnaires could be represented as quantum interference within a quantum probability framework, providing compelling evidence [2]. Here, I formulate QQ equalities that extend beyond pairwise comparisons and binary outcomes, accommodating situations with $N \geq 3$ questions under the assumption that measurements are represented by idempotent projection operators. These results may be applicable to low-dimensional discrete quantum systems, such as qubits and qtrits, and potentially provide a generalizable framework for understanding order effects in cognitive decision-making across various domains of questionnaire design and experimental psychology.

[1] Wang and Busemeyer. *Top.Cogn.Sci.,* 5(4), (2013). [2] Wang, Solloway, Shiffrin, and Busemeyer.*PNAS,* 111(26), (2014).

DY 29.9 Wed 15:00 P4

Subordination approach for derivation of generalized quantum models in non-relativistic and relativistic cases — •Irina Petreska[1], Trifce Sandev[1,2,3], and Alexander Iomin[4,5] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [3]Korea University, Seoul, Korea — [4]Solid State Institute, Technion, Haifa, Israel — [5]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The generalized Schrödinger equation and the generalized Klein-Gordon equation are derived by applying the subordination approach to conventional quantum mechanics. The special cases of the fractional Schrödinger equation and the fractional Klein-Gordon equation are adequately introduced. Additionally, the subordination approach is also applied to derive the special case of the generalized Dirac equation for spin 1/2 particles and the directions for future research are discussed. It is evident that according to the subordination approach, the time fractional derivatives in quantum mechanics, including the relativistic one, can be related to the Lévy stable processes in time.

[1] T. Sandev, I. Petreska, A. Iomin, From standard to generalized Schrödinger and Klein-Gordon equations: Subordination approach, *submitted* (2024).

DY 30: Quantum-Critical Phenomena (joint session TT/DY)

Time: Thursday 9:30–12:45 Location: H31

See TT 41 for details of this session.

DY 31: Focus Session: Nonequilibrium Collective Behavior in Open Classical and Quantum Systems

Nonequilibrium classical and quantum systems coupled to thermal or (driven) non-equilibrium environments have recently been shown to exhibit rich collective phenomena and phase transitions without equilibrium counterparts. From the classical side, intriguing examples are flocking and phase separation in active matter, but also patterns and bifurcations in driven-diffusive systems and spontaneous parity-time symmetry breaking in systems involving nonreciprocal couplings. From the quantum side much interest has been devoted, e.g., to ordering and phase transitions in non-equilibrium steady states, the formation of time crystals, superradiance, as well as phase transitions or critical behavior in time. The symposium and the accompanying focus session is devoted to connections between the quantum and the classical realms, as they have been explored recently both in theory and experiment.

Organized by Sabine Klapp (TU Berlin) and André Eckhardt (TU Berlin)

Time: Thursday 9:30–12:45 Location: H37

DY 31.1 Thu 9:30 H37

Ultra-critical Fermi Surfaces, Quantum Oscillations, and Bosonic Metals — •Likun Shi and Inti Sodemann Villadiego — Institut für Theoretische Physik, Leipzig, Germany

Periodically driven quantum systems exhibit rich non-equilibrium phenomena that transcend equilibrium paradigms. We demonstrate the emergence of novel Fermi surface physics in particle-number-conserved fermionic and bosonic systems coupled to heat baths. In the fermionic case, we uncover "ultra-critical" Floquet non-Fermi liquid states characterized by persistent non-analyticities in momentum space occupation that remarkably retain their sharpness at finite temperature - a phenomenon without equilibrium analogues. These non-equilibrium Fermi surfaces manifest in quantum oscillation signatures and display power-law correlations immune to the finite-temperature bath. Extending beyond fermions, we discover analogous Fermi surface physics in bosonic systems, pointing to universal features in driven quantum systems that transcend particle statistics. Our findings open new avenues for realization of exotic non-equilibrium phases in driven quantum materials.

DY 31.2 Thu 9:45 H37

Giant Dynamical Paramagnetism in the driven pseudogap phase of YBa2Cu3O6+x — •Marios Michael[1], Duilio De Santis[2], Eugene Demler[3], and Patrick Lee[4] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany — [2]Physics and Chemistry Dept., Interdisciplinary Theoretical Physics Group, Palermo University, 90128 Palermo, Italy — [3]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — [4]Department of Physics, MIT, 77 Massachusetts Avenue, 02139 Cambridge, MA, USA

In this talk, I will discuss theory aimed at understanding recent experimental data on driven YBa2Cu3O6+x published recently in Nature: Fava, S., De Vecchi, G., Jotzu, G. et al. Magnetic field expulsion in optically driven YBa2Cu3O6+x Nature 632,75-80 (2024). Experiments on optically pumped YBa2Cu3O6+x in the pseudogap phase far above Tc have shown evidence of dynamical Meissner effect. In our effort to understand the new experimental signatures, we have uncovered a universal instability triggered in Josephson junctions under a magnetic field that are strongly driven with an AC field. The instability leads to the generation of giant paramagnetic currents at the edges of Josephson junctions. For strong enough drive such instabilities ultimately lead to a soliton ratchet after driving. I will focus on why this instability of a generic Josephson junction is applicable to the pseudogap YBa2Cu3O6+x far above Tc and how it matches the experimental observations.

DY 31.3 Thu 10:00 H37

entropy production in ultrafast quantum stochastic dynamics — •Yulong Qiao and Matthias Geilhufe — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Thanks to advancements in femto- and atto-second laser technologies, thermodynamics has entered the ultrafast era. Ultrafast dynamics provides a unique way to probe the transient properties of materials. In [1], ultrafast stochastic

thermodynamics was developed based on X-ray scattering experiments [2], and has been successfully applied to the study of entropy production in laser-excited phonons. However, how to develop a unifying theory for both classical and quantum systems remains an open challenge [3].

In the quantum realm, fluctuations arising from the uncertainty principle do not depend on temperature, meaning they are inevitable even in a vacuum. As a result, in the quantum analogues of the Langevin equations, classical stochastic forces are replaced by quantum noise operators. In this talk, I will discuss how to handle the quantum nosies in the frame of open quantum systems. I will also present the impact of quantum effects on the entropy production in the ultrafast processes.

[1] L. Caprini, H. Löwen, and R. M. Geilhufe, Nat. Commun. 15, 94 (2024).
[2] M. Kozina. et al., Nat. Phys. 15, 387 (2019).
[3] G.T. Landi and M. Paternostro, Rev. Mod. Phys. 93, 035008 (2021).

DY 31.4 Thu 10:15 H37

Cooling dynamics of the 2D Kitaev honeycomb model coupled to phonons — •Arkadeep Mitra, Francesco Piazza, and Markus Heyl — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The ground state of the Kitaev spin-1/2 model on a 2D honeycomb lattice hosts a quantum spin liquid (QSL) phase where excitations fractionalize into Majorana fermions. At high temperatures, however, it has recently been observed to enter a disorder-free localized phase, so that any experimental cooling of a Kitaev material has to cross this localized and associated phase transition. Motivated from this, we study theoretically the cooling dynamics upon coupling the Kitaev model to phonons. We envisage that signatures obtained from this dynamics could act as probes for QSL.

DY 31.5 Thu 10:30 H37

Hydrodynamic description of emergent long-range coherence in active quantum flocks — •Byjesh N Radhakrishnan[1,2], Thomas L. Schmidt[1], and Markus Heyl[2] — [1]Department of Physics and Material science, University of Luxembourg — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

The quantum analog of classical active matter flocking has recently been reported in [arXiv:2308.01603]. The reported model introduces the concept of active quantum matter in a system of hard-core bosons in a one-dimensional lattice. The results provide both analytical and large-scale numerical evidence that these systems can give rise to quantum flocks due to the interplay of spin-flipping and alignment interactions. One of the key findings is that these flocks, unlike classical ones, exhibit distinct quantum properties by developing strong quantum coherence over long distances. Our work focuses mainly on developing a hydrodynamics description to study the origin and properties of this long-range quantum coherence. We systematically explore the relationship between long-range coherence and system parameters like alignment strength and quantum amplitude and compare our analytical results with large-scale numerical simulations.

Invited Talk DY 31.6 Thu 10:45 H37

Strong coupling and coherence in quantum thermodynamics — •Janet Anders[1,2], Federico Cerisola[2], James Cresser[2], and et al[2] — [1]Universität Potsdam, Germany — [2]Exeter University, UK

The interaction of nanoscale and quantum systems with their environment can be relatively strong, and alter the equilibrium state. For open quantum systems, explicit expressions of these so-called mean force (MF) equilibrium states have been missing. In this talk I will report on useful analytic expressions of these states, valid for a general quantum system in contact with a bosonic bath [1]. The results are illustrated with the well-known spin-boson model, for which we provide the first classification of coupling regimes, from weak to ultrastrong, and for both the quantum and classical setting [2].

In the second part of the talk, I will briefly comment on quantum signatures that arise in thermodynamic processes due to the presence of coherences. For example, the work distribution of time-varying quantum systems violates the corresponding classical fluctuation-dissipation relation for slowly driven processes [3]. A geometric framework is proposed to find optimal trade-offs between dissipation and fluctuations. Coherences also give rise to quantum irreversibility. We unravel how this irreversibility manifests itself in energetic exchanges that differ from those in the classical regime [4].

[1] PRL 127, 250601 (2021)
[2] NJP 26, 053032 (2024)
[3] PRL 123, 230603 (2019)
[4] Comm. Phys. 3, 1 (2020)

15 min. break

DY 31.7 Thu 11:30 H37

Ultrafast Dynamics Across the Phase Transition of the Charge Density Wave in $K_{0.3}MoO_3$ — •Rafael T. Winkler[1], Larissa Boie[1], Yunpei Deng[2], Matteo Savoini[1], Serhane Zerdane[2], Abhishek Nag[2], Sabina Gurung[1], Davide Soranzio[1], Tim Suter[1], Vladimir Ovuka[1], Janine Zemp[1], Elsa Abreu[1], Simone Biasco[1], Roman Mankowsky[2], Edwin J Divall[2], Alexander R. Oggenfuss[2], Mathias Sander[2], Christopher Arrell[2], Danylo Babich[2], Henrik T. Lemke[2], Paul Beaud[2], Urs Staub[2], Jure Demsar[3], and Steven L. Johnson[1,2] — [1]Institute for Quantum Electronics, Physics Department, ETH Zurich, Zurich, Switzerland — [2]SwissFEL, Paul Scherrer Institute, Villigen, Switzerland. — [3]Faculty - Institute of Physics, Johannes Gutenberg-University Mainz

Blue Bronze ($K_{0.3}MoO_3$) is a quasi 1D material exhibiting a charge density wave (CDW) with a periodic lattice distortion (PLD). In a time resolved x-ray experiment, we study the dynamics of the PLD by pumping $K_{0.3}MoO_3$ with short laser pulses and probing it using x-ray diffraction. We construct reciprocal space maps (RSM) of superlattice reflections at different delays. The RSMs indicate a transient inversion of the phase of the CDW. We attribute the suppression of the diffracted x-ray intensity after this phase inversion to a fast decoherence of the CDW driven by local pinning of the phase of the CDW in the material. These observations were confirmed by numerical simulations of the time dependent Ginzburg-Landau equations, extended by including defects which favor a particular phase of the CDW in combination with a temperature dependent coherence factor.

DY 31.8 Thu 11:45 H37

Optimal dynamical regimes for reservoir computing with soft matter — •Mario U. Gaimann and Miriam Klopotek — Stuttgart Center for Simulation Science (SimTech), Cluster of Excellence EXC 2075, University of Stuttgart, Germany

Reservoir computing with physical systems is a promising approach for next-generation and *in materio* computing. Recently, active matter systems for reservoir computing were introduced by Lymburn *et al.* (*Chaos* 31(3), 033121, 2021). However, the optimal properties of active matter systems for reservoir computing remain poorly understood. Here we show that viscoelastic, overdamped dynamics yield high predictive performances. This is remarkable since it was previously believed that optimal swarm dynamics are found at a gas-to-liquid phase transition. We relate predictive performance to correlations of agent velocities and their fluctuations. The optimal overdamped swarms show rich phenomenology: interface formation and breaking, local shear thinning, and self-healing. We show that the overdamped regime is optimal across a range of different chaotic attractors. Notably the optimal dynamics are already uncovered by studying reservoir computing with a single particle. Our results demonstrate the importance of tuning basic dynamical properties in physical reservoir substrates to generate optimal correlative effects. Reservoir computing with viscoelastic soft matter inspires novel mechanisms for computing in matter and novel computing devices based on these principles.

DY 31.9 Thu 12:00 H37

Universality in time-crystalline matter — •Carl Philipp Zelle, Romain Daviet, Achim Rosch, and Sebastian Diehl — University of Cologne

Dynamical phases of matter in which time translation symmetry is broken spontaneously are fascinating examples of phases that can only occur far from equilibrium. In this talk, we show that paradigmatic O(N) models display time-crystalline order once driven suitably out of equilibrium.

We employ dynamic RG techniques to determine the universal phenomena at the ensuing transitions as well as within the time-crystalline phase: The transition between an ordered phase and the time-crystal occurs through a critical exceptional point which we show cause a fluctuation-induced first order transition. The transition between a symmetric and a time-crystalline phase defines a new, genuinely nonthermal universality class. We show, that the Goldstone-modes within the dynamical phases are a realisation of the KPZ universality class and offer new generalisations of KPZ to larger symmetry groups.

Surprisingly, these phenomena can be realized by rather simple driving protocols, i.e. weakly irradiating a ferrimagnetic spin system. Furthermore, we connect our results to recent advances in nonreciprocal active matter.

1) Zelle, Daviet, Rosch, Diehl; Phys. Rev. X 14, 021052 (2024)
2) Daviet, Zelle, Rosch, Diehl; Phys. Rev. Lett. 132, 167102 (2024)
3) Zelle, Daviet, Asadollahi, Diehl; in preparation

DY 31.10 Thu 12:15 H37

Thermalizing Lindbladians for many-body systems — •Nico Albert[1], Shovan Dutta[2], and Masudul Haque[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]Raman Research Institute, Bangalore, India

Thermalization is closely associated with the effect of a bath. For quantum systems, the most prominent type of bath is a Markovian bath, whose dynamics are governed by a Lindblad master equation. Therefore, it is important to understand Lindbladians that lead to a thermal (Gibbs) steady state. We will present some properties of thermalizing Lindbladians for many-body systems.

DY 31.11 Thu 12:30 H37

Signatures of Quantum Chaos and fermionization in the incoherent transport of bosonic carriers in the Bose-Hubbard chain — Pavel Muraev, Dmitri Maksimov, and •Andrey Kolovsky — Krasnoyarsk, Russia

We analyse the stationary current of Bose particles across the Bose-Hubbard chain connected to a battery, focusing on the effect of inter-particle interactions. It is shown that the current magnitude drastically decreases as the strength of inter-particle interactions exceeds the critical value which marks the transition to quantum chaos in the Bose-Hubbard Hamiltonian. We found that this transition is well reflected in the non-equilibrium many-body density matrix of the system. Namely, the level-spacing distribution for eigenvalues of the density matrix changes from Poisson to Wigner-Dyson distributions. With the further increase of the interaction strength, the Wigner-Dyson spectrum statistics changes back to the Poisson statistics which now marks fermionization of the Bose particles. With respect to the stationary current, this leads to the counter-intuitive dependence of the current magnitude on the particle number.

DY 32: Nonlinear Stochastic Systems

Time: Thursday 9:30–11:15 Location: H43

Invited Talk DY 32.1 Thu 9:30 H43

Fluctuation-Response Relations for Non-equilibrium Systems — •Benjamin Lindner — Institut für Physik, Humboldt-Universität Berlin

The fluctuations and the response of stochastic systems are related by fluctuation-dissipation theorems or, equivalently, fluctuation-response relations (FRRs). Originally introduced for systems in thermodynamic equilibrium, generalizations of such relations for non-equilibrium situations have been discussed since the 1970's and are particularly appealing for biological systems. FRRs may be used to e.g. (i) prove that a system is outside of equilibrium, (ii) prove that it does not follow Markovian dynamics, (iii) extract statistics of intrinsic noise sources. In my talk I report several FRRs in systems far from equilibrium. I discuss a nonlinear FRR for systems that can be perturbed by a step stimulus, which can be used as an efficient test of Markovianity. I present a universal description for stochastic oscillators, that results in a simple FRR in terms of a new complex-valued transform of the original oscillator variables. Last but not least, I derive a new class of FRRs for spiking neurons that relate the pronounced fluctuations of spontaneous neural firing to their average response to sensory stimuli, i.e. to the processing of sensory information that is the raison d'etre of neural systems.

Refs.: B. Lindner 129, 198101 Phys. Rev. Lett. (2022); A. Perez-Cervera et al. PNAS 120, e2303222120 (2023); K. Engbring et al. Phys. Rev. X 13, 021034(2023); J. Stubenrauch & B. Lindner Phys. Rev. X 14, 041047 (2024)

DY 32.2 Thu 10:00 H43

Oscillations and self-generated noise in a nonreciprocal single-species XY-model — •Thomas Suchanek[1] and Sarah Loos[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]DAMTP, University of Cambridge, Cambridge, United Kingdom

We study the low temperature dynamics of an XY-model with random nonreciprocal couplings. Upon increasing average nonreciprocity, we observe a transition from a state of coherent oscillations to a chaotic stationary state. For a randomly selected degree of freedom, we derive an effective description of the dynamics in terms of a stochastic differential equation. This allows us to analyze the properties of the stochastic motion as well as the response of the system to perturbations.

DY 32.3 Thu 10:15 H43

Cross-correlation-response relations for systems driven by shot noise — •Jakob Stubenrauch and Benjamin Lindner — BCCN Berlin and Physics Department HU Berlin, Germany

In the analysis of stochastic dynamics, the Furutsu-Novikov [1,2] theorem (FNT), linking the input-output cross-correlation of a system driven by Gaussian noise to the response function of the system, has proven important in various applications.

In several situations, such as photon-detectors or neurons, it is inaccurate to model the input process as Gaussian noise; in the two examples the input is instead a sequence of pulses at random times (shot noise). Here, we present recently discovered analogues of the FNT for systems driven by shot noise [3]. Specifically, we show that the input-output cross-correlation of any system driven by Poissonian shot noise is linearly related to the linear response of the system to modulations of the intensity of input shots. We further present extensions for colored shot noise and for shot noise with random amplitudes.

To illustrate the wide applicability of our general result, we further present a fluctuation-response relation of a leaky integrate-and-fire neuron: Building on previous work [4], we show how the spontaneous output fluctuations of a spike-driven neuron are related to its susceptibility. Lastly, as teasers, we present applications to single-photon-detection, remote control in neural networks, and synaptic plasticity.

[1] Furutsu, J. Res. Natl. Bur. Stand. (1963) [2] Novikov, J. Exp. Theor. Phys. (1965) [3] Stubenrauch and Lindner, Phys. Rev. X (2024), [4] Lindner, Phys. Rev. Lett. (2022)

DY 32.4 Thu 10:30 H43

A Framework for Sparse Kinetic Monte-Carlo Models — •Bat-Amgalan Bat-Erdene, Roya Ebrahimi Viand, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

The long-time dynamics of many problems in condensed matter physics are controlled by the interplay of rare events, e.g. chemical kinetics or crystal growth. Such problems are typically formulated as discrete-state Markov jump processes and can be simulated by kinetic Monte Carlo (kMC) methods. We are developing a software framework for implementing efficient kMC simulation models for arbitrary such processes. The key ingredients are i) a code generator for an optimized C++ skeleton where the user specifies the problem via a Python interface, and ii) the possible formulation as a sparse kMC model. Prototypical examples for sparsity appear in spatially extended models, where in each step the state changes only locally and interactions are only short ranged. This can then be exploited to achieve near-constant computational complexity per kMC time step. We evaluate the framework's efficiency on a dynamical Ising and a CO oxidation model on regular lattices. We find that our framework achieves a similar performance as specialized state-of-the-art kMC software for lattice kMC. Moreover, our framework offers a much larger flexibility, which we demonstrate on an implementation of Coupled Finite Differences for parameter sensitivity.

DY 32.5 Thu 10:45 H43

Dynamic instability in dissipative self-assembly: common principles in single and multi-filament polymers — •Seeralan Sarvaharman and Aljaž Godec — Max Planck Insitute for Multidisciplinary Sciences, Göttingen, Germany

Dissipative self-assembly underpins the formation of complex biological structures by breaking time-reversal symmetry. Microtubules, essential cytoskeletal polymers, exemplify this through "dynamic instability", where the growth and shrinkage of the polymer are governed by the instantaneous composition of the constituent filaments. The microtubule length, the observable most commonly used to quantify this behaviour, obscures the many-body physics involved. As such, the principles underpinning this instability have remained elusive.

Here, we address this challenge by modelling the dynamics using a three-state Potts framework with thermodynamically consistent driving, capturing the stochastic interactions within and between filaments. By employing a pair approximation and local equilibrium reasoning, we derive a chemical master equation that describes the system's probabilistic evolution in terms of the length and composition. To uncover the macroscopic dynamics, we apply WKB analysis and use Filippov theory to analyse the resultant piecewise continuous ODEs that describe the evolution of the most probable paths. This analysis allows us to construct a dynamical phase diagram, revealing distinct regimes of behaviour, including dissipative limit cycles that underlie the observed macroscopic fluctuations in microtubule length.

DY 32.6 Thu 11:00 H43

The effect of noise on the breather solutions of the discrete nonlinear schrödinger equation — •Mahdieh Ebrahimi[1], Barbara Drossel[1], and Wolfram Just[2] — [1]Institute of Condensed Matter Physics, Technical University of Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany — [2]Institute of Mathematics, University of Rostock, D-18057 Rostock Germany

The Discrete Nonlinear Schrödinger Equation (DNSE) finds applications across diverse scientific fields, including physics, chemistry, and biology. This dynamical equation is characterized by localized solutions known as breathers. Gaining insights into the processes governing discrete systems is crucial for understanding phenomena such as excitations in crystal lattices and molecular chains, light propagation in waveguide arrays, and the dynamics of Bose-condensate droplets. In this study, we treat the DNSE as an effective macroscopic equation for a quantum many-particle system and investigate the impact of two types of noise (additive and multiplicative noise) on its Hamiltonian equations of motion using symplectic integration. Our findings reveal that the system's normalization increases linearly with time under additive noise, leading to unbounded energy. Conversely, multiplicative noise preserves normalization but causes the system to heat up, ultimately destabilizing the breather in the presence of noise. Our results vividly illustrate the relevance of conserved quantities for the stochastic dynamics in Hamiltonian systems.

DY 33: Machine Learning in Dynamics and Statistical Physics I

Time: Thursday 9:30–13:00 Location: H47

DY 33.1 Thu 9:30 H47

Learning Mechanisms of Neural Scaling Laws — •Konstantin Nikolaou[1], Samuel Tovey[1], Sven Krippendorf[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Cavendish Laboratory and DAMTP University of Cambridge, United Kingdom, CB3 0WA

Recent works have identified neural scaling laws, which describe the trade-off between neural network performance and computation cost. Understanding the underlying mechanisms leading to scaling behavior might be one of the most important questions in current machine-learning research.

We compare the behavior of neural networks for data and model scaling by analyzing the learning dynamics through the lens of the neural tangent kernel. We find similar performance scaling in both regimes but uncover fundamentally distinct internal model mechanisms underlying the scaling. Additionally, we investigate scaling towards the infinite-width limit of neural networks and identify a transition, we coin the Feature-Kernel Transition, separating two regimes: Below, a model refines features to resolve a task, while above the transition the refinement declines and the initial state becomes the dominant factor. We argue that the transition marks the trade-off between model size and maximum feature learning.

DY 33.2 Thu 9:45 H47

Finite integration time drives optimal dynamic range into subcritical regime — Sahel Azizpour[1,2], Viola Priesemann[3,4], •Johannes Zierenberg[3,4], and Anna Levina[1,2] — [1]Eberhard Karls University of Tübingen, Germany — [2]Max Planck Institute for Biological Cybernetics, Tübingen, Germany — [3]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany — [4]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Sensitivity to small changes in the environment is crucial for many real-world tasks, enabling living and artificial systems to make correct behavioral decisions. It has been shown that such sensitivity is maximized when a system operates near the critical point of a second-order phase transition. However, proximity to criticality introduces large fluctuations and diverging timescales. Hence, it would require impractically long integration periods to leverage the maximal sensitivity. Here, we analytically and computationally demonstrate how the optimal tuning of a recurrent neural network is determined given a finite integration time. Rather than maximizing the theoretically available sensitivity, we find networks to attain different sensitivity depending on the time available. Consequently, the optimal dynamic regime shifts from critical to subcritical when integration times are finite, highlighting the necessity of incorporating finite-time considerations into studies of information processing.

DY 33.3 Thu 10:00 H47

Self-Organizing Global Computation from Local Objective Functions Based on Partial Information Decomposition — Andreas C. Schneider[1,2], •Valentin Neuhaus[2,1], David A. Ehrlich[3], Abdullah Makkeh[3], Alexander S. Ecker[4,2], Viola Priesemann[2,1], and Michael Wibral[3] — [1]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self Organisation, Göttingen, German — [3]Campus Institute for Dynamics of Biological Networks, University of Göttingen — [4]Institute of Computer Science and Campus Institute Data Science, University of Göttingen

In modern deep neural networks, individual neuron learning dynamics are often obscure due to global optimization. In contrast, biological systems use self-organized, local learning to achieve robustness and efficiency with limited global information. We propose a method for achieving self-organization in artificial neurons by defining local learning goals based on information theory. These goals leverage Partial Information Decomposition (PID), which breaks down information from sources into unique, redundant, and synergistic contributions. Our framework enables neurons to locally determine how input classes contribute to the output, expressed as a weighted sum of PID terms derived from intuition or numerical optimization. This approach enhances task-relevant local information processing and neuron-level interpretability while maintaining strong performance, providing a principled foundation for local learning strategies.

DY 33.4 Thu 10:15 H47

Explaining Near-Zero Hessian Eigenvalues Through Approximate Symmetries in Neural Networks — •Marcel Kühn and Bernd Rosenow — Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany

The Hessian matrix, representing the second derivative of the loss function, offers crucial insights into the loss landscape of neural networks and significantly influences optimization algorithms, model design, and generalization in deep learning. A common characteristic of the Hessian eigenspectrum is the presence of a few large eigenvalues alongside a bulk of near-zero eigenvalues. We propose that this bulk structure arises from approximate symmetries inherent in network architectures – an often overlooked aspect. First, we demonstrate that in deep, fully connected linear networks, exact continuous symmetries that leave the loss invariant lead to zero eigenvalues in the Hessian. These zero eigenvalues and their corresponding eigenvectors can be attributed to symmetries such as rotations between weight layers. Extending this concept, we suggest that in networks with nonlinear activation functions, approximate symmetries introduce a large number of small but finite eigenvalues, viewed as perturbations of the linear case. We illustrate this phenomenon in a two-layer ReLU student-teacher setup and in a multi-layer network trained on CIFAR-10, showing that eigenvectors with small eigenvalues predominantly align with symmetry directions. Finally, we apply our symmetry-based analysis to convolutional networks, demonstrating the generality of our approach in understanding the Hessian eigenspectrum across different architectures.

DY 33.5 Thu 10:30 H47

Efficient mapping of phase diagrams with conditional Boltzmann Generators — •Maximilian Schebek[1], Michele Invernizzi[2], Frank Noé[1,2,3,4], and Jutta Rogal[1,5] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin, 14195 Berlin — [3]Department of Chemistry, Rice University, Houston, 77005, Texas, USA — [4]AI4Science, Microsoft Research, 10178 Berlin — [5]Department of Chemistry, New York University, New York, NY 10003, USA

The accurate prediction of phase diagrams is of central importance for both fundamental and applied material sciences. However, the computational prediction of the relative stability between phases based on their free energy is a daunting task, as traditional free energy estimators require a large amount of uncorrelated equilibrium samples over a grid of thermodynamic states. In this work, we develop deep generative machine learning models based on the Boltzmann Generator approach for entire phase diagrams, employing normalizing flows conditioned on the thermodynamic states that they map to. By training a single model to transform the equilibrium distribution sampled at only one reference thermodynamic state to a wide range of target temperatures and pressures, we can efficiently generate equilibrium samples across the entire phase diagram. We demonstrate our approach by predicting the solid-liquid coexistence line for a Lennard-Jones system in excellent agreement with state-of-the-art free energy methods while significantly reducing the number of energy evaluations needed.

DY 33.6 Thu 10:45 H47

Sampling rare events with neural networks: Machine learning the density of states — •Moritz Riedel[1], Johannes Zierenberg[2], and Martin Weigel[1] — [1]Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

Neural networks can be trained to generate samples from the Boltzmann distribution of many-particle systems. If suitable architectures such as normalizing flows or variational autoregressive networks are chosen, exact generation weights are known and hence present biases can be corrected for. Still, such networks typically struggle to learn and reproduce configurations from the full range of configuration space since effects such as mode collapse occur. For the simulation of rare events and suppressed states accessible in generalized frameworks such as the multicanonical ensemble such broad exploration is crucial. Here, we show how a combination of variational autoregressive network and autoencoder allows for a systematic exploration of configuration space in spin models, during which the network is able to learn the density of states. We demonstrate the efficacy of the approach in the Potts system in the strong first-order regime.

DY 33.7 Thu 11:00 H47

stable diffusion for microstructure: from microstructural properties to 2D-to-3D reconstruction — •Yixuan Zhang[1], Teng Long[2], Mian Dai[1], and Hongbin Zhang[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Shandong University, Jinan, China

We propose a novel framework that combines Stable Diffusion and ControlNet to generate microstructures tailored to specific properties, such as coercivity. By leveraging latent alignment techniques, our method enables direct reconstruction of 3D microstructures from 2D inputs, ensuring geometric and property consistency across dimensions. This approach not only facilitates accurate 2D-to-3D reconstruction but also opens possibilities for studying and predicting microstructural transformations during various manufacturing processes. By integrating generative AI with material design, this work provides a robust foundation for property-driven microstructure generation, offering a potential pathway to optimize materials for targeted applications.

15 min. break

DY 33.8 Thu 11:30 H47

Machine learning for prediction of dynamical clustering in granular gases — •Sai Preetham Sata[1], Dmitry Puzyrev[2,1], and Ralf Stannarius[3,2] — [1]AMS, Otto von Guericke University, Germany — [2]MTRM and MARS, Otto von Guericke University, Germany — [3]Department of Engineering, Brandenburg University of Applied Sciences, Germany

Granular gases are sparse ensembles of free-moving macroscopic particles that interact via inelastic collisions. One peculiar property of granular gas is dynamical clustering, i.e. spontaneous increase of local number density. To quantify this effect, microgravity experiments and simulations were performed [1-3] and two gas-cluster transition criteria were established:Kolmogorov-Smirnov test, and caging effect criterion [2]. We perform simulations based on the VIP-GRAN experiment [3] and test these criteria for various combinations of system parameters, revealing their advantages and drawbacks. In addition, we investigate additional criteria that can help to understand the dynamical properties of gas-cluster transition. Based on the simulation data, machine learning can be used to detect dynamical clusters and predict the state of the system for a given set of system parameters. This study is funded by the German Aerospace Center (DLR) within projects VICKI (50WM2252) and EVA II (50WK2348). References: [1] É. Falcon et al., Phys. Rev. Lett., 83:440, 1999. [2] E. Opsomer et al., Europhys. Lett., 99:40001, 2012. [3] S. Aumaître et al., Rev. Sci. Instr., 89:075103, 2018.

DY 33.9 Thu 11:45 H47

Automated construction of complex reaction networks — •Weiqi Wang[1], Xiangyue Liu[1], and Jesús Pérez Ríos[2] — [1]Fritz-Haber-Institut, Berlin — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794, USA

Kinetic models are essential for understanding chemical reaction mechanisms and estimating reaction rates. Typically, kinetic models are constructed based on transition state theory, using stable and intermediate species with zero-Kelvin energy calculations. However, they often fail to account for temperature effects and anharmonic influences, limiting their accuracy for real-world reactions.

This talk will discuss our method for automatically constructing reaction networks at finite temperatures using *ab initio* molecular dynamics simulations. Based on extensive sampling of configurational space, temperature-dependent free energies, and transition probabilities can be derived, enabling the construction of reaction networks to analyze temperature effects.

DY 33.10 Thu 12:00 H47

Data-Driven Sparse Identification with Adaptive Function Bases — •Gianmarco Ducci, Maryke Kouyate, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Interpretable data-driven methods have proven viable for deriving kinetic equations directly from experimental data. However, such numerical methods are inherently susceptible to noise, which affects the sparsity in the resulting models. In order to promote such a sparsity condition, finding the optimal set of basis functions is a necessary prerequisite, but yet a challenging task to determine in advance.

We here present our in-house developed `ddmo` (Data-Driven Model Optimizer) software, which allows precise control over the space of candidate constituent terms. Such a complete framework comprises two main novel features. The first feature permits to include parametric functions in the library. The second feature is an adaptive library sizing routine that progressively adds or removes elements based on the learning from the dataset. We show a practical application of our algorithm tailored at identifying Langmuir-Hinshelwood mechanisms from experimental data.

DY 33.11 Thu 12:15 H47

Kalman filter enhanced adversarial Bayesian optimization for active sampling in inelastic neutron scattering — Yixuan Zhang[1], •Nihad Abuawwad[2], Samir Lounis[2], and Hongbin Zhang[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Peter Grünberg Institute (PGI), Jülich, Germany

Spin waves, or magnons, are fundamental excitations in magnetic materials that provide insights into their dynamic properties and interactions. Magnons are the building blocks of magnonics, which offer promising perspectives for data storage, quantum computing, and communication technologies. These excitations are typically measured through inelastic neutron or x-ray scattering techniques, which involve heavy and time-consuming measurements, data processing, and analysis based on various theoretical models. Here, we introduce a machine learning algorithm that integrates adaptive noise reduction and active learning sampling, which enables the restoration from minimal inelastic neutron scattering point data of spin wave information and the accurate extraction of magnetic parameters, including hidden interactions. Our findings, benchmarked against the magnon spectra of CrSBr, significantly enhance the efficiency and accuracy in addressing complex and noisy experimental measurements. This advancement offers a powerful machine learning tool for research in magnonics and spintronics, which can also be extended to other characterization techniques at large facilities.

DY 33.12 Thu 12:30 H47

Accelerating the Training and Improving the Reliability of Machine-Learned Interatomic Potentials for Strongly Anharmonic Materials through Active Learning — •Kisung Kang, Thomas A. R. Purcell, Christian Carbogno, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max Planck Society

Machine-learned interatomic potentials (MLIP) can efficiently implement molecular dynamics (MD) simulations with large spatial and long time scales. However, immature training for rare dynamical events, such as defect creation, may happen due to their absence or insufficiency in training data or their fade-out during regularization, leading to the critical deterioration of MLIP predictions regarding dynamical properties like transport phenomena. To improve the MLIP's reliability and accelerate the whole training process, we adopt a sequential active learning ($\mathscr{AL}$) scheme via MD employing MLIP (MLIP-MD) and uncertainty estimates [1]. In each iterative step, MLIP-MD serves as an efficient exploration tool for configurational space to generate training data, while uncertainty estimates identify unfamiliar data to be sampled for subsequential MLIP models. The representative examples of CuI and $AgGaSe_2$ among 112 materials display erroneous MLIP predictions of missing and fictitious rare events. We demonstrate how $\mathscr{AL}$ addresses these issues, specifically correcting unfamiliar regions for the MLIP potential energy surface. At last, the over(under)estimation of their phonon lifetimes is rectified after the $\mathscr{AL}$ steps.

[1] K. Kang, T. A. R. Purcell, *et al.*, arXiv:2409.11808 (2024).

DY 33.13 Thu 12:45 H47

Molecular Dynamics of Endohedral CaX@C60 Fullerenes: Reproducing Correlated Movement Features Using Machine Learning Applications — •Mihaela Cosinschi[1,3], Amanda Teodora Preda[1,3], Calin Andrei Pantis Simut[1,3], Nicolae Filipoiu[1,3], Ioan Ghitiu[4], Mihnea Alexandru Dulea[3], Andrei Manolescu[5], and George Alexandru Nemnes[1,2,3] — [1]University of Bucharest, Faculty of Physics, Magurele, Romania — [2]Research Institute of the University of Bucharest, Bucharest, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineering, Magurele, Romania — [4]National Institute for Laser, Plasma and Radiation Physics, Magurele, Romania — [5]Department of Engineering, School of Technology, Reykjavik University, Reykjavik, Iceland

Fullerenes are allotropes of carbon with remarkable properties due to their high degree of symmetry, cage-like structures and ability to support addition of internal or external atoms. In the present work, we have conducted a molecular dynamics (MD) study on the C60 fullerene containing one to four encapsulated calcium atoms. All-atomistic ab initio DFT methods were employed to perform calculations through the Orca MD Module, albeit at a high computational cost. Results proved that the internal atoms adopt minimal-energy configurations and exhibit coupled motion, maintaining constant characteristics after a period of equilibration. Furthermore, we have built an artificial neural network (ANN) that can pick up the dynamics patterns and recreate trajectories to reasonable accuracy, allowing for MD calculations in significantly shorter times, even under small perturbations.

DY 34: Nonlinear Dynamics, Synchronization, and Chaos

Time: Thursday 11:30–13:00 Location: H43

DY 34.1 Thu 11:30 H43

Hierarchical Clustering in Mean-Field Coupled Stuart-Landau Oscillators — •Nicolas Thomé and Katharina Krischer — Technische Universität München

Coupled oscillator networks are fundamental in many physics, chemistry, and biology fields, representing a captivating subject of study in nonlinear science. A persistent challenge is understanding the transition from a coherent synchronous solution to a completely incoherent one. This work explores this transition using globally coupled Stuart-Landau oscillators under mean-field interactions. We show that a cascade of codimension-2 points, coined Type-II cluster singularities, organizes the transition from two- to three-cluster solutions. These Type-II cluster singularities naturally induce a hierarchal structure to the clustering behavior and pave the way for the formation of chimera and incoherent solutions. Based on numerical bifurcation and Floquet multiplier analyses, our findings offer new insights into intermediate synchronization states and their role in complex oscillator systems.

DY 34.2 Thu 11:45 H43

Synchronization in the Fully Disordered Kuramoto Model of Coupled Oscillators — •Axel Prüser, Sebastian Rosmej, and Andreas Engel — Carl von Ossietzky University Oldenburg, Institut für Physik, D26111 Oldenburg, Germany

We investigate the dynamics of phase oscillators in fully disordered Kuramoto networks with defined degree of asymmetry. Both disordered couplings and disordered phases are considered. Employing the dynamical cavity method, the mean-field dynamics is reduced to a self-consistent stochastic single-oscillator problem which we analyze perturbatively and by numerical simulations. We elucidate the influence of the disorder characteristics on the correlation and response function of the system, together with their impact on the distribution of the order parameter. The mechanism of the so-called volcano transition and its relation to the existence of an oscillator glass phase is clarified.

DY 34.3 Thu 12:00 H43

Training of neuromorphic systems based on coupled phase oscillators via equilibrium propagation: effects of network architecture — •Qingshan Wang[1], Clara Wanjura[1], and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstrasse 2, Erlangen, Germany — [2]Department of Physics, University of Erlangen-Nuremberg, 91058 Erlangen, Germany

The increasing scale and resource demands of machine learning applications have driven research into developing more efficient learning machines that align more closely with the fundamental laws of physics. A key question in this field is whether both inference and training can exploit physical dynamics to achieve greater parallelism and acceleration. Equilibrium propagation, a learning mechanism for energy-based models, has shown promising results in physical systems with energy functions more complex than Hopfield-like models.

In this study, we focus on equilibrium propagation training of coupled phase oscillator systems. We investigate the influence of different experimentally feasible network architectures on the training performance. We analyze lattice structures, convolutional networks, and autoencoders, examining the effects of network size and other hyperparameters. Our findings lay the ground work for future experimental implementations of energy-based neuromorphic systems for machine learning, encompassing systems such as coupled laser arrays, CMOS oscillators, Josephson junction arrays, coupled mechanical oscillators, and magnetic systems

DY 34.4 Thu 12:15 H43

Stability of Grid-Following Inverters Under Forced Oscillations and Sequential Load Switching — •Benedikt Grüger and Florian Steinke — Technical University of Darmstadt, Darmstadt, Germany

The growing integration of renewable energy sources has led to a proliferation of inverter technologies in modern distribution grids. This shift introduces new dynamic stability challenges, particularly during periodic fluctuations in demand or generation caused by equipment malfunctions or cyber-physical attacks. Our work investigates the dynamic stability of grid-following inverters subjected to periodic grid voltage fluctuations. While forced oscillations in high-voltage grids have been widely studied, related research at the low-voltage level has primarily focused on bifurcations in inverter dynamics (e.g., Ma et al., 2020) or the impact of current limits (Zhang et al. 2024). However, the behavior of inverter-dominated distribution grids under forced oscillations remains largely unexplored. Our study employs a dynamic grid model that includes control mechanisms operating on time scales comparable to load switching, such as direct voltage control and phase-locked loop. This approach results in a fourth-order differential-algebraic system, akin to that proposed by Ma et al. (2023). We show that periodic grid voltage fluctuations can destabilize controllers, leading to inverter failures. By varying internal controller time scales, we identify different stability regimes and destabilizing effects are characterized. In sum, these findings highlight dynamic vulnerabilities in inverters and point out cyber-physical risks in inverter-dominated grids.

DY 34.5 Thu 12:30 H43

Shrimp structure as a test bed for ordinal pattern measures — Yong Zou[1], Norbert Marwan[2,3], Xiujing Han[4], •Reik V. Donner[2,5], and Jürgen Kurths[2] — [1]East China Normal University, Shanghai, China — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]University of Potsdam, Germany — [4]Jiangsu University, Zhenjiang, China — [5]Magdeburg-Stendal University of Applied Sciences, Magdeburg, Germany

Identifying complex periodic windows surrounded by chaos in the two or higher dimensional parameter space of certain dynamical systems is a challenging task for time series analysis. This holds particularly true for the case of shrimp structures, where different bifurcations occur when crossing different domain boundaries. Here we propose to use ordinal pattern transition networks (OPTN) to characterize shrimp structures. Our results demonstrate that among different ordinal characteristics, the OPTN out-link transition entropy exhibits better classification accuracy between chaotic and periodic time series than other existing measures like permutation entropy. This improved performance results from the fact that the transition behavior between ordinal patterns encodes additional dynamical information that is not captured by traditional ordinal measures that are solely based on pattern occurrence frequencies. Ultimately, the new OPTN based entropy measure also outperforms previously used measures based on recurrences in phase space.

DY 34.6 Thu 12:45 H43

Designing Robust Edge Oscillations with Topological Protection in Nonlinear Coupled Systems — •Sayantan Nag Chowdhury and Hildegard Meyer-Ortmanns — School of Science, Constructor University, 28759 Bremen, Germany

Topological protection, a powerful concept in physics, ensures robust states across quantum and classical systems. While topological insulators exemplify its applications in quantum systems with electric currents protected along the edges, an example from classical physics is provided by topoelectrical circuits with stable signal transduction. However, the role of topological protection in the context of classical oscillatory systems has been much less explored. Our study applies tools from band theory of condensed matter physics to systems with nonlinear dynamics to achieve robust edge oscillations. This means that oscillations are restricted to the edge of a two-dimensional grid, while those in the bulk settle into near-steady-state dynamics. This pattern is resilient to parameter mismatches, structural defects, and blockages. By calculating the Zak phase as topological characteristic for this phenomenon, we explain edge-localized oscillations through bulk-boundary correspondence. We further analyze the collective behavior by examining the limiting case of weak coupling strength in our directed network, which alternates between strong and weak values. We validate our findings for different prototypical oscillator models with possible applications in biochemical systems. Our findings establish a robust design for controlling the state of oscillation of units that are attached to a spatial grid.

DY 35: Fluctuations, Noise and Other Transport Topics (joint session TT/DY)

Time: Thursday 15:00–18:30 Location: H31

See TT 47 for details of this session.

DY 36: Microswimmers and Microfluidics (joint session DY/BP/CPP)

Time: Thursday 15:00–17:45 Location: H37

Invited Talk DY 36.1 Thu 15:00 H37

Light-Driven Manipulation of Passive and Active Microparticles — •Svetlana Santer — Institute of Physics and Astronomy, University of Potsdam, Germany

Chemical gradient near a solid/liquid can result in lateral long-range fluid transport termed diffusioosmotic (DO) flow. For instance, when photosensitive surfactant is irradiated with light converting the majority of the molecules in one of the possible isomers, emerging concentration gradient of isomers generates an osmotic pressure gradient tangent to the wall actuating the surrounding liquid to flow. [1-3] In my talk I will show how one can manipulate microparticles and even induce their self-propulsion by light urtilizing light driven diffusioosmotic (LDDO) phenomenon. Depending on the applied wave length one can either disperse/remove or gather particles. We will discuss how to establish light-driven hydrodynamics as a useful and versatile tool for investigating collective motion of self-propelled particles and aggregation

[1] Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S. Scientific Reports, 6 (2016) 36443. [2] Santer, S. J. Phys. D: Applied Physics, 51 (2017) 013002. [3] Arya, P.; Umlandt, M.; Jelken, J.; Feldmann, D.; Lomadze, N.; Asmolov , E. S.; Vinogradova, O. I.; Santer, S. A. The European Physical Journal E, 44(50) (2021), 1-10.

DY 36.2 Thu 15:30 H37

Regulated polarization of active particles in local osmotic flow fields — •Lisa Rohde, Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Regulation in living systems is a fundamental principle for achieving robust functionality and maintaining specific non-equilibrium states. The control of certain properties and functionalities of systems on the microscale presents particular challenge since thermal fluctuations and environmental perturbations dominate. While synthetic active matter has demonstrated remarkable self-organization capabilities, examples of autonomous regulation processes at the single-particle level remain scarce. Here, we show experimentally that the interplay of two non-equilibrium processes leads to a regulated polarization state of active particles in local osmotic flow fields. Based on thermophoretic repulsive and attractive forces that are generated by a single heat source at the boundary, the active particles encircle the heat source at a stable distance depending on the heat source temperature. The balance of these temperature-induced processes causes a polarization of the active particles that is independent of the heat source temperature. The individual control of heat source and active particles in the experiment allows detailed investigation of the self-regulated polarization effect in which we find hydrodynamic interactions to dominate. As the effects rely on osmotic flows and phoretic interactions, we expect that the observed phenomena can be generalized to other active systems and flow fields.

DY 36.3 Thu 15:45 H37

Active particle steering in three dimensions — •Gordei Anchutkin and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Leipzig, Germany

Synthetic active particles serve as a model system that mimic the self-propulsion of living matter to explore fundamental aspects of non-equilibrium physics. Various collective phenomena of active agents have been studied, but mostly in the presence of hydrodynamic and physicochemical boundary effects. While theoretical works predict different collective dynamics in 3D, experimental investigations remain limited due the lack of experimental control over active swimmers in three dimensions.

Here we introduce three-dimensional control to the study of synthetic active matter. We demonstrate simultaneous control of thermophoretic microswimmers in 3D using single-particle tracking through digital holography and dark-field pattern tracking, with real-time wavefront shaping for steering. With the help of these experiments, we explore the interplay of thermophoretic propulsion, gravity, and optical forces for the active particles. By creating a three-dimensional active ensemble, we reveal how bulk interactions and boundary effects shape the collective behavior of active particles.

DY 36.4 Thu 16:00 H37

***Trypanosoma brucei* in microchannels: the role of constrictions** — •Zihan Tan, Julian I. U. Peters, and Holger Stark — Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Trypanosoma brucei (*T. brucei*), a single-celled parasite and natural microswimmer, is responsible for the fatal sleeping sickness in infected mammals, including humans. Understanding how *T. brucei* interacts with fluid environments and navigates through confinements is crucial for elucidating its movement through blood vessels and tissues, and across the blood-brain barrier.

Using a hybrid multiparticle collision dynamics (MPCD)–molecular dynamics (MD) approach, we investigate the locomotion of an in-silico *T. brucei* in three types of fluid environments: bulk fluid, straight cylindrical microchannels, and microchannels with constrictions. We observe that the helical swimming trajectory of the in-silico *T. brucei* becomes rectified in straight cylindrical channels compared to bulk fluid. The swimming speed for different channel widths is governed by the diameter of the helical trajectory. The speed first slightly increases as the channel narrows and then decreases when the helix diameter is compressed. An optimal swimming speed is achieved when the channel width is approximately twice the bulk helix diameter. Furthermore, *T. brucei* notably slows down when entering the narrow constriction in a microchannel and strongly speeds up upon exiting due to a release of deformation energy of the straightened cell body.

DY 36.5 Thu 16:15 H37

Helical motion of microorganisms can be more persistent than straight motion — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[2], Freddy Frischknecht[2], and Ulrich S. Schwarz[1] — [1]BioQuant & Institute for Theoretical Physics, Heidelberg University — [2]Center for Integrative Infectious Disease Research, Heidelberg University

The movement of microorganisms has been extensively modeled by stochastic active particle models. In three dimensions, both swimming microorganisms, like sperm cells and some bacteria, and gliding microorganisms, like malaria sporozoites in the skin, often exhibit helical trajectories. If the internal driving force is the primary source of noise in the system, it induces random, yet time-correlated variations in the torque. To investigate this effect, we introduce a three-dimensional active rotational Ornstein-Uhlenbeck particle model. We find that the presence of a rotational component and the resulting helical path can mitigate the effect of intrinsic noise in the drive, allowing for larger long-time mean square displacements than straight movement at the same speed. The model not only provides qualitative insights into the constraints faced by microbes that may have led to the evolutionary selection of certain motility patterns, but also presents an analytical, quantitative tool for extracting information from these movements. We present and analyze corresponding data for malaria parasites gliding through hydrogels.

15 min. break

DY 36.6 Thu 16:45 H37

Corrugated channels can filter ciliated microorganisms based on the metachronal wavelength — •Gonçalo Antunes and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Many microorganisms (e.g. Paramecium) move by a carpet of cyclically beating cilia that cover their surface. These cilia often beat in an organized fashion, such that the beating phases form a traveling wave, referred to as a metachronal wave. In this study, we investigate the swimming of such microorganisms in corrugated microchannels. We model the motion of the cilia via a time-varying effective slip velocity applied on the microorganism's surface, which we approximate as an infinite slab. By employing the lubrication approximation, we show analytically that the swimming speed of ciliated microorganisms placed inside a corrugated channel is sensitive to the corrugation height, provided that the wavelength of the corrugation matches that of the metachronal wave. Indeed, the direction of motion itself may invert with respect to swimming in bulk fluid, with the channel acting as a virtual barrier which blocks microorganisms under specific conditions for corrugation and slip-velocity modulations, but allow others to pass through. We also show that the interplay between the corrugation and the slip velocity profile allows for the swimming of microorganisms with zero time-averaged slip velocity, which thus cannot swim in bulk fluid. Finally, we complement our theory with preliminary results from hydrodynamic simulations for radially-symmetric microorganisms of finite length in radially-symmetric corrugated channels.

DY 36.7 Thu 17:00 H37

Motion of a single particle partially exposed in a simple shear flow — •Dominik Geyer[1,2], Aouane Othmane[1], and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), FZ Jülich — [2]Department of Physcis, FAU Erlangen-Nürnberg

Sand immersed in the water can be imagined as a wet granular matter. Besides sedimentation, friction, and surface roughness are two relevant physical phonemes within this system. Many body systems in a turbulent regime have been studied using discrete elements methods for a long time, but a single particle in the Stokes flow regime is particularly interesting for biological systems and microfluidic devices.

A layer of quadratic-arranged spheres models the rough surface. The question arises of how to describe the motion of a single traveling particle over this substrate.

We choose a combined numerical and analytical approach. The Stokes equation is solved analytically for the sphere near a rough wall. Lattice Boltzmann simulations with momentum-exchange particle coupling are performed for different wall roughness and friction coefficients.

Although, the Stokes equation assumes that the particle Reynolds number is zero. Surprisingly, the numerical results match our theoretical description until a particle Reynolds number of two. In this regime, friction between the moving particle and the substrate significantly influences the angular velocity but has a minor influence on the traveling velocity in the flow direction.

DY 36.8 Thu 17:15 H37

Rational Design of Smart Microfluidics in Responsive Channels — •Arwin Marbini — Albert-Ludwigs Universität Freiburg

Responsive microfluidics offers exciting potential for self-regulating biomimetic systems. This study explores bifurcating microchannel networks with pressure-sensitive resistances, combining experiments with simulations based on the Hagen-Poiseuille equation and a linear model. These methods extract critical, experimentally inaccessible parameters under steady-state and dynamic conditions. Our findings enable the design of adaptable microfluidic networks, unlocking precise flow control for future applications in biology, soft robotics, and advanced material systems.

DY 36.9 Thu 17:30 H37

Blue Water: A passive, reusable microfiltration device for water purification — •Tim R. Baumann, Ioannis Gkekas, Martina Viefhues, and Dario Anselmetti — Experimental Biophysics, Bielefeld University

Water is the most vital resource for life on Earth. Due to pollution of freshwater and oceans, this valuable resource has become globally endangered. The effects

of microplastic pollution are widely discussed in scientific, political, and socioeconomic contexts. Despite regulations on single-use plastics and microplastic output, efforts should also focus on reintegrating microplastics to achieve a sustainable circular economy. Furthermore, microplastic-sized particles can migrate through organic tissue and can therefore be classified as contaminants of emerging concern. However, filtering plastics of this size is a challenging task.

Thus, this work examines and extends the findings of Divi et al. regarding the suspension feeding mechanisms of various ray species. We studied the filtration performance and efficiency for different geometric ratios of channel widths in simulations and laboratory environments. First, we have the main inner channel connected to the pressure inlet. From this, two rows of tilted lamellae structures branch off laterally to the outer secondary channels.

By applying sufficiently high pressure ($> 6 \cdot 10^5\ Pa$) to the inlet and achieving flow and particle velocities of $> 35\ \frac{m}{s}$, we can purify 82 % of half of the initial fluid. To prevent rupturing of our microfluidic chip under this pressure, we further investigated using glass fiber reinforced PDMS and lowering the operating pressure.

DY 37: Brownian Motion and Anomalous Diffusion

Time: Thursday 15:00–17:15 Location: H43

DY 37.1 Thu 15:00 H43

A universal class of exactly solvable diffusions — •Costantino Di Bello[1], Edgar Roldan[2], and Ralf Metzler[1] — [1]Potsdam University, Institute of Physics and Astronomy, Potsdam-Golm, Germany — [2]ICTP, Quantitative Life Sciences section, Trieste, Italy

We consider a general one-dimensional overdamped diffusion model described by the Ito stochastic differential equation (SDE) $dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t$, where W_t is the standard Wiener process. We obtain a specific condition that μ and σ must fulfill in order to be possible to solve the SDE via mapping the generic process, using a suitable space-time transformation, into the simpler Wiener process. By taking advantage of this transformation, we obtain the propagator in the case of open, reflecting, and absorbing boundary conditions for a large class of diffusion processes. With the same technique, we were also able to derive the first passage time (FPT) statistics of a large class of models. Moreover, as many physical observables in stochastic thermodynamics are described by an SDE of the same form, our result can provide the analytical expression of the probability distribution of many observables like work, entropy et similia. We stress the fact that our results are valid for many non-autonomous, non-linear and non-homogeneous processes.

DY 37.2 Thu 15:15 H43

Thermodynamic bounds on generalized transport: From single-molecule to bulk observables — •Cai Dieball and Aljaž Godec — Mathematical biophysics group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

We prove that the transport of any scalar observable in d-dimensional nonequilibrium systems is bounded from above by the total entropy production scaled by the amount the observation "stretches" microscopic coordinates. The result, a time-integrated generalized speed limit, reflects the thermodynamic cost of transport of observables, and places underdamped and overdamped stochastic dynamics as well as deterministic motion on equal footing. Our work fills an important gap in thermodynamic inference, since microscopic dynamics is, at least for short times, underdamped. Requiring only averages but not sample-to-sample fluctuations, the proven transport bound is practical and applicable not only to single-molecule but also bulk experiments where only averages are observed, which we demonstrate by examples.

[1] Phys. Rev. Lett. 133, 067101 (2024)

DY 37.3 Thu 15:30 H43

Foundation of classical dynamical density functional theory: uniqueness of time-dependent density–potential mappings — Michael Andreas Klatt[2,3,1], •Christian Bair[1], Hartmut Löwen[1], and René Wittmann[1,4] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität, Düsseldorf, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Ulm, Germany — [3]DLR, Institut für Materialphysik im Weltraum, Köln, Germany — [4]Institut für Sicherheit und Qualität bei Fleisch, Max Rubner-Institut, Kulmbach, Germany

When can we uniquely map a classical density profile to an external potential? In equilibrium, without time dependence, the one-body density is known to uniquely specify the external potential that is applied to the many-body system. This mapping from a density to the potential is the cornerstone of classical density functional theory (DFT). Here, we consider non-equilibrium, time-dependent many-body systems that evolve from a given initial condition. We derive explicit conditions, for example, no flux at the boundary, that ensure that the mapping from the density to a time-dependent external potential is unique. We thus prove the underlying assertion of dynamical density functional theory (DDFT) - without resorting to the so-called adiabatic approximation often used in applications. By ascertaining uniqueness for all n-body densities, we ensure that the proof - and the physical conclusions drawn from it - hold for general superadiabatic dynamics of interacting systems.

DY 37.4 Thu 15:45 H43

Phase locking and fractional Shapiro steps in collective dynamics of microparticles — •Seemant Mishra[1], Artem Ryabov[2], and Philipp Maass[1] — [1]Institut für Physik, Universität Osnabrück, Germany — [2]Charles University, Faculty of Mathematics and Physics, Czech Republic

Nonlinear systems under time-periodic driving often exhibit phase locking, where synchronization between the system's dynamics and driving leads to robust stationary states. In this work, we show that phase-locked dynamics in a driven system of hardcore-interacting microparticles arises from running solitary cluster waves. Such cluster waves were recently predicted to occur in overdamped Brownian motion [1,2] and shortly after confirmed in experiments [3]. Particle currents are related to soliton velocities due to a unit displacement law saying that the total average shift of all particle positions per soliton period equals one wavelength of the periodic potential. The collective particle dynamics synchronize with the driving for certain particle diameters only. Based on an effective potential for solitary wave propagation, we derive dynamical phase diagrams of integer and fractional synchronization modes.

[1] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[2] A. P. Antonov, A. Ryabov, P. Maass, Chaos, Solitons & Fractals 132, 115079 (2024).
[3] E. Cereceda-López, A. P. Antonov, A. Ryabov, P. Maass, and P. Tierno Nat. Commun. 14, 6448 (2023).

DY 37.5 Thu 16:00 H43

Modeling charge attachment induced ion transport in glasses — •Quinn Emilia Fischer and Philipp Maass — Department of Physics, Universität Osnabrück, Germany

In charge attachment induced ion transport (CAIT), material foreign mobile ions can replace native mobile ions near the surface of a glass below the glass transition temperature. Insight into the ion dynamics during CAIT experiments is provided by measurements of near-surface concentration profiles.

We discuss the modeling of concentration profiles by coupling the Poisson equation to kinetic equations of linear irreversible thermodynamics. Solving the kinetic equations requires knowledge on the dependance of both the Onsager coefficients and chemical potentials of the mobile ions on the ion concentrations.

We show how chemical potentials can be derived for a model, where mobile ions occupy sites in a disordered energy landscape, and how Fermi energies are generalized to a system of multiple ion types. We further explain the determination of Onsager coefficients by modeling thermally activated hopping motion in the energy landscape and the relation between the coefficients and ion mobilities.

The dependence of both the Onsager coefficients and the chemical potentials on mobile ion concentration is sensitive to the form of the energy landscape. It is argued that this sensitivity needs to be taken into account in a consistent theoretical modeling of CAIT experiments, which requires solutions of the coupled Poisson and kinetic equations to reproduce measured concentration profiles.

DY 37.6 Thu 16:15 H43

Local and Diffusive Dynamics of Interlayer Lithium ions in Synthetic Fluoro-Hectorites: ^{2}H and ^{7}Li NMR-Study — •Jepsinraj Kakkuzhiyulla Parambath and Michael Vogel — TU Darmstadt, Institut for Condensed Matter Physics, Hochschulstr. 6, 64289, Darmstadt, Germany

Investigating ion transport is a crucial part of developing robust devices for energy storage and sensors. Fluoro-Hectorite, a clay mineral of the Smectite group serves as a model material for this investigation, specifically Lithium Hectorite with the structural formula of $Li_{0.5}[Mg_{2.5}Li_{0.5}]Si_4O_{10}F_2$ and a layered structure. Due to the swelling properties of the Hectorites, the interlayer spacing and thus the degree of confinement can be varied with water content. The charge transports results from interlayer lithium ions, which are dissolved in water. The Hectorite confinements provide mechanical stability and guide the charge carriers over long distances, leading to fast ion transport [Hiebl et al., Chem. Mater. 2020, 32, 7445]. We use ^{2}H and ^{7}Li NMR to study the dynamics of the interlayer water molecules and lithium ions. Spin lattice relaxometry studies of local dynamics, including field cycling and static field gradient(SFG) measurements of diffusive dynamics show a strong dependence on the interlayer spacing.

DY 37.7 Thu 16:30 H43

Random Walks of Intermittently Self-Propelled Particles — Agniva Datta[1], Carsten Beta[1,2], and •Robert Grossmann[1] — [1]University of Potsdam, Potsdam, Germany — [2]Kanazawa University, Kanazawa, Japan

We present a dynamical model of intermittently self-propelled particles: active particles that recurrently switch between two modes of motion, namely an active run-state and a turn state, in which self-propulsion is absent. The durations of these motility modes are drawn from arbitrary waiting-time distributions. We derive the expressions for exact forms of transport characteristics like mean-square displacements and diffusion coefficients to describe such processes. Furthermore, the conditions for the emergence of sub- and superdiffusion in the long-time limit are presented. We give examples of some important processes that occur as limiting cases of our system, including run-and-tumble motion of bacteria, Lévy walks, hop-and-trap dynamics, intermittent diffusion and continuous time random walks. We eventually apply this modeling framework to describe bacterial swimming in polysaccharide matrices.

DY 37.8 Thu 16:45 H43

First-passage time for generalized telegrapher's processes under stochastic resetting — •Trifce Sandev — Macedonian Academy of Sciences and Arts, Skopje, Macedonia — Ss. Cyril and Methodius University in Skopje, Macedonia — Korea University, Seoul, Korea

We consider different generalizations of the telegrapher's process. One possible generalization is the so-called subordinated telegrapher's process, which can be obtained from the standard telegrapher's process subordinated by Lévy noise. Another possible generalization is a heterogeneous telegrapher's process which is a stochastic process with a multiplicative dichotomic noise and a position-dependent velocity. For both cases we analyze the non-equilibrium stationary states approached in the long time limit, as well as the survival probability, the first-passage time density and the mean first-passage time in the presence of Poissonian stochastic resetting of the particle to the initial position.

[1] T. Sandev, A Iomin, *Phys. Rev. E* **110**, 024101 (2024)
[2] K. Górska, F. J. Sevilla, G. Chacón-Acosta, T. Sandev, *Entropy* **26**, 665 (2024)
[3] P. Jolakoski, P. Trajanovski, A. Iomin, L. Kocarev, T. Sandev, sibmitted (2024)

DY 37.9 Thu 17:00 H43

Diffusion and Homogeneous Linewidth – Phthalocyanine on Solid Rare-Gas Clusters — •Philipp Elsässer, Arne Morlok, Ulrich Bangert, Li Yilin, Felix Riedel, Lukas Bruder, Frank Stienkemeier, and Tanja Schilling — Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Doped clusters are an important tool in the spectroscopy of organic molecules and the study of basic properties of confined quantum systems. It is crucial in these structures to understand the characteristics of the configurations between dopant and cluster. The binding sites may vary over time due to diffusion. Because of this, the diffusion behavior is valuable to characterize doped clusters.

We have studied the diffusion of free-base phthalocyanine (H_2Pc) on solid, icosahedral, rare-gas clusters of argon and neon by molecular dynamics simulations. We observe on both systems that the spacial motion of H_2Pc is confined on a single face of the icosahedron. The rotational movement of the molecule shows a cluster-size dependent anomalous-diffusive behavior on a picosecond timescale. This overall anomalous diffusion is in agreement with the homogeneous line width broadening observed in action-based two-dimensional electronic spectroscopy experiments.

DY 38: Focus Session: Innovations in Research Software Engineering (joint session BP/DY)

Research software engineering (RSE) is an emerging field in science, with practitioners spanning a continuous spectrum from "researchers who code" to "software engineers developing for science". In Germany, a growing movement supported by deRSE e.V. is gaining recognition, and more institutions are acknowledging the increasing demand across various disciplines. This focus session will provide a platform to highlight recent advances in applications, tooling, and software in the fields of biophysics, dynamics, and statistical physics, as well as developments in the recognition and proliferation of RSE as a profession within our field and academia in general.

Organized by Simon Christ and Sophia Rudorf (Hannover).

Time: Thursday 15:00–18:00 Location: H44

Invited Talk DY 38.1 Thu 15:00 H44

Community-driven software and data training for computational biology — •Toby Hodges — The Carpentries, Oakland, CA, USA

The Carpentries is a global community teaching essential software and data skills for research. Certified Instructors teach hundreds of workshops to thousands of learners all over the world every year, introducing them to essential skills for computational research such as programming, version control, and data organisation. In recent years, the community has also begun to develop and deliver lessons that build on these foundations, teaching more intermediate and advanced Research Software Engineering skills such as HPC, parallel programming, and containerised computing. This talk will explore how open source, collaborative training efforts can build capacity for computational research, discuss what makes this model work and some lessons learned along the way, and finish with a look at what the community plans to do next.

DY 38.2 Thu 15:30 H44

Python-based interface to micromagnetic simulation software: Ubermag — •Hans Fangohr[1,2,3], Martin Lang[1,2], Samuel J.R. Holt[1,2], Swapneel Amit Pathak[1,2], Kauser Zulfiqar[1,2,4], and Marijan Beg[5] — [1]MPSD, Hamburg, Germany — [2]CFEL, Hamburg, Germany — [3]Univ. Southampton, UK — [4]Univ. Hamburg, Germany — [5]Imperial College London, UK

We describe the Python-based user environment "Ubermag" to help scientists use well-established (micromagnetic) simulation packages.

Within Ubermag [1], researchers can express the physics problem they want to simulate in a scientist-friendly but machine readable problem definition based on Python syntax [2]. Ubermag translates this problem into the configuration files needed for micromagnetic simulation packages such as OOMMF or mumax3. On completion of the simulation, the computed data is presented back to the user at the Python level. Ubermag is often used in Jupyter Notebooks, and supports rich media to provide figures and equations within the notebook.

We report on the motivation for Ubermag, the design and implementation process, and our experiences made both from the perspective of science users and from the research software engineers. We touch on a range of topics, including interface design, domain specific languages, testing, packaging, Jupyter, and reproducibility.

This work was supported by EPSRC UK Skyrmion Grant EP/N032128/1, and the European research projects OpenDreamKit (676541) and MaMMoS (101135546).

[1] DOI 10.1109/tmag.2021.3078896; [2] DOI 10.1063/1.4977225

DY 38.3 Thu 15:45 H44

OCTOPOS.jl: A Julia-based tool for synonymous codon optimization — Simon Christ[1], Jan-Hendrik Trösemeier[2], and •Sophia Rudorf[1] — [1]Institute of Cell Biology and Biophysics, Leibniz University Hannover, Germany — [2]independent researcher

OCTOPOS.jl is a research software designed to optimize synonymous mRNA sequences for improved heterologous gene expression in various host organisms. Combining a detailed mechanistic model of in-vivo protein synthesis with machine learning, OCTOPOS.jl predicts protein expression based on codon choice. Originally developed as a Java desktop application, the software has been reimplemented in the Julia programming language to enhance performance, modularity, and scalability. The new implementation serves as the foundation for a graphical user interface and a web application, accessible at https://octopos.cell.uni-hannover.de/. These updates improve accessibility and usability, broadening its appeal to both computational and experimental biologists. OCTOPOS.jl supports organism-specific genetic sequence engineering and detailed analysis of translation dynamics, thus providing a valuable resource for the synthetic biology and biotechnology communities.

DY 38.4 Thu 16:00 H44

Invert pattern forming systems with BayesFlow to bridge the gap from simulation to experimental observation — •Hans Olischläger — Interdisciplinary Center for Scientific Computing (IWR) — Heidelberg University

The description of experimental systems by complex spatial models, be it with (stochastic) partial differential equations, agent-based simulation or otherwise, is often the condensation of all the central scientific hypotheses regarding a particular object of study.

I argue, that making progress in this kind of modelling is currently hindered by the lack of a tool that enables solving the following inverse problem: Given an observation, determine all the model configurations that are able to produce

it. In other words, what is the posterior probability of all model configurations given some (set of) experimental data.

Instead of just preaching that in theory a Bayesian treatment would be nice, I will then continue to present such a tool: amortized Bayesian inference (as implemented in the software package BayesFlow). I will give examples on the classical Gierer-Meinhardt pattern forming PDE and a biophysical model, the Min system, which is used by E. coli to control cell division.

I will also take a step back to give a broader picture of the newly available statistical methods that support complex spatial modelling and their limitations. The aim is to provide some guidance on what you can and cannot infer from your state-of-the-art scientific simulator given observations, and how to do it.

DY 38.5 Thu 16:15 H44

FAIR Data Management for Soft Matter Simulations using NOMAD — •Bernadette Mohr[1], Esma Boydas[1], Nathan Daelman[1], José M. Pizarro[1], Tristan Bereau[3], Claudia Draxl[1], Luca M. Ghiringhelli[4], Martin Girard[2], Denis Usvyat[6], Roser Valentí[7], Silvana Botti[5], and Joseph F. Rudzinski[1,2] — [1]CSMB, HU Berlin — [2]MPIP Mainz — [3]ITP, Heidelberg Uni. — [4]Dept. of Mater. Sci. and Eng., FAU Erlangen — [5]RC-FEMS and Faculty of Physics, RUB Bochum — [6]Inst. für Chem., HU Berlin — [7]ITP, GU FfM

NOMAD [nomad-lab.eu][1, 2] is an open-source, community-driven data infrastructure designed to facilitate FAIR data management in materials science. Currently, it supports over 60 computational codes and encompasses DFT, classical MD, and many-body methods. This contribution will focus on recent developments, following modern software practices, to enhance NOMAD's applicability to soft matter and biological systems, including support for coarse-grained representations and advanced workflows such as free energy calculations. Combined with a schema for representing force fields, molecular topologies, and hierarchical system structures, NOMAD tracks data provenance and streamlines data analysis and the creation of AI-ready datasets. The NOMAD framework meets the classical simulation community's needs for improved data management standards and provides a foundation for building a cohesive, interconnected scientific data ecosystem. [1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

DY 38.6 Thu 16:30 H44

Estimation of kinetic rates by constrained optimization — •Federico Marotta[1], Maria Zimmermann-Kogadeeva[1], Peer Bork[1], Julia Mahamid[1], and Sophia Rudorf[2] — [1]European Molecular Biology Laboratory — [2]Leibniz Universität Hannover

Biological systems often rely on molecular motors to perform useful work. The kinetics of the reactions in a motor's cycle can be easily investigated *in vitro* or in model organisms, but it is difficult to generalize them to a different system. We present a method to estimate the transition kinetics in an uncharacterized system, where minimal data are available, by leveraging a reference system where the kinetics have been elucidated. The motor's activity is represented as a continuous-time Markov chain, characterized by an infinitesimal generator matrix Q whose entries are functions of the transition rates of the cycle (the vector ω) and possibly of the concentrations of external molecules. In the uncharacterized system, the available data induce a constraint on the admissible rates. By employing an extremum principle, we estimate the rates ω_{unc} that minimize the kinetic distance with respect to the reference rates ω_{ref} while respecting such constraint. As an application of this strategy, we describe a model of the translation elongation cycle, where reference data are available for *E. coli in vitro*, and estimate the rates either *in vivo* or in a different organism, under constraints on the total elongation time or the steady-state occupancies, respectively.

DY 38.7 Thu 16:45 H44

Software provisioning for HPC and RSE — •Martin Lang[1,2], Henning Glawe[1,2], Jehferson Mello[1,2], and Hans Fangohr[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Free-Electron Laser Science, Hamburg, Germany — [3]University of Southampton, Southampton, UK

All research software relies on existing libraries for various functionalities such as low-level math operations, FFTs, IO, or other domain-specific operations. Installing these dependencies, potentially based on different compilers or in multiple versions, with all inter-dependencies fulfilled is notoriously difficult.

In the first part of this talk we introduce the open-source package manager Spack, which has a strong focus on HPC and research software. Spack can install software in multiple versions and variants, and supports optimised compilation for the underlying hardware, including compiling on exotic hardware. It comes with a large, community-provided collection of commonly used packages. Spack's packaging files make it easy to specify required dependencies, provide optional features of a software, and ensure compatibility with other libraries.

In the second part we present the concrete setup at our institute. We use Spack to provide the software stack on the local HPC, including pre-compiled packages and toolchains (sets of compilers and libraries) for users to compile their own software. We report on requirements and challenges, and how we address these with Spack. We also touch on scripting the Spack-based installation process including the option to recreate the HPC software environment on a scientist's laptop.

DY 38.8 Thu 17:00 H44

Small scale Research Software Engineering — •Simon Christ — Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Computational Biology

While we are in dire need of research software organizations on a faculty level or larger, small scale software engineering, that is one research software engineer in a group or institute, is something that can be achieved in a short time frame and is probably the most common form today. A field report from Computational Biology where research software engineers are involved in modeling, developing solutions, teaching and maintenance.

DY 38.9 Thu 17:15 H44

Estimation of pKa values in membrane bound proteins — •Jesse Jones[1], Nereu Montserrat i Busquets[1,2], Ana Gamiz Hernandez[3], Ville Kaila[3], and Maria Andrea Mroginski[1] — [1]Technische Universität Berlin, Berlin — [2]Freie Universität Berlin, Berlin — [3]Stockholm Universität, Stockholm

Many key bioenergetic processes involving electron and proton reactions take place in membrane bound protein complexes, generating a proton motive force. Yet the ionizable groups which facilitate these reactions are often buried in hydrophobic pockets in the membrane. These processes are mainly described through pK_a values, which continue to be poorly understood and difficult to obtain despite structural, biochemical and computational advances. Hence, estimating pK_a values of these residues without the need for weeks of work in a laboratory, is important to describe the dynamics of the system, providing information on possible proton pathways. In this work we preview Karlsberg3, a software which uses a Poisson Boltzmann Equation solver (APBS) for proteins and calculates pKa values. Karlsberg3 is, in contrast to its predecessor Karlsberg2+, parallelized, running in modern software environments, and able to take membranes into consideration.

DY 38.10 Thu 17:30 H44

The teachingRSE project - Towards a professionalization of RSE education. — •Florian Goth[1] and Simon Christ[2] — [1]Universität Würzburg, Institut für theoretische Physik und Astrophysik, Am Hubland, 97074 Würzburg — [2]Leibniz Universität Hannover, Institut für Zellbiologie und Biophysik, Herrenhäuser Str. 2 30419 Hannover

At the deRSE23, the second conference for research software engineering(RSE) in Germany, a group of people came together for a small workshop to discuss how to deal with questions revolving around RSE education. Overwhelmed by the immense resonance to that workshop we took home a tremendous amount of feedback that made obvious that a short blog post will not suffice to adequately represent it. Now it is two years later, and the project produced its first output, the second position paper https://arxiv.org/abs/2311.11457 of de-RSE e.V. and it has sprawled out into a multitude of follow-up projects. In this talk, I will give an overview over the original ideas that we tried to convey in the position paper, and go into more detail on how domain sciences like physics need to change in light of this new specialization.

DY 38.11 Thu 17:45 H44

Python-Based Analysis Pipeline for the Quantification of Mechanics in Neural Organoids — •Michael Frischmann[1,2], Elijah R. Shelton[1], Achim T. Brinkop[1,2], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Institute of Biophysics, Ulm University, Ulm, Germany — [3]SyNergy & GSN, Munich, Germany

Neuronal tissues form under the influence of mechanical forces guiding cellular movements. In the mammalian retina, neuronal translocations occur over hours. However, mechanical probing at those timescales in situ have posed experimental challenges. We employed magnetic ferrofluid droplets in mouse stem cell-derived retinal organoids to probe tissue mechanics from seconds to hours. To quantify tissue strain we have developed a Python-based analysis pipeline featuring an accessible graphical user interface (GUI). This pipeline automates strain quantification, image segmentation, and fitting procedures, enabling high-fidelity creep compliance measurements over extended durations. Our measurements reveal power-law scaling of dynamic compliance as well as tensile loss and storage modulus, consistent with soft glassy rheology just above the glass transition. These results demonstrate that neuronal tissues remodel in a scale-free manner while maintaining solid-like properties. This discovery provides a framework for understanding how mechanical signals may govern connectivity in the central nervous system. Integrating neural organoid models, mechanical probing, and computational methods, prepares us to investigate the interplay between biomechanics and neurodevelopment.

DY 39: Machine Learning in Dynamics and Statistical Physics II

Time: Thursday 15:00–16:30 Location: H47

DY 39.1 Thu 15:00 H47

Fast and energy-efficient reservoir computing using a resonant-tunneling diode — •Osamah Sufyan[1], Antonio Hurtado[2], and Kathy Lüdge[1] — [1]Technische Universität Ilmenau, Institut für Physik, Weimarer Straße 25, 98693 Ilmenau, Germany — [2]University of Strathclyde, Institute of Photonics, Glasgow, United Kingdom

Resonant-tunneling diodes (RTDs) have garnered significant attention as platforms for neuromorphic computing, owing to their fast operation and intricate nonlinear dynamics. Among the most hardware-friendly and energy-efficient paradigms in this domain is reservoir computing (RC), where the nonlinear dynamics of a physical system are leveraged to perform complex computational tasks.

In this work, we explore the use of a single RTD as a reservoir, employing time-multiplexing techniques for chaotic time-series prediction achieving similar performance to previous RC approaches [1]. Our findings highlight the relationship between the RTD's distinct dynamical regimes and the reservoir's performance in predicting future values of the Mackey-Glass and Lorenz system time series. Additionally, we investigate the RTD as an excitable system, demonstrating its potential for spiking neural network applications. We examine various data encoding and decoding strategies for spike-based operations, further underscoring the versatility of RTDs in neuromorphic computing.

[1] L. Jaurigue and K. Lüdge, *Neuromorph. Comput. Eng.*, **4**, 014001 (2024).

DY 39.2 Thu 15:15 H47

Tailored minimal reservoir computing: Connecting nonlinearities in the input data with nonlinearities in the reservoir — Davide Prosperino[1], Haochun Ma[1], Vincent Gross[2], and •Christoph Räth[3,2] — [1]Allianz Global Investors (AGI) — [2]Ludwig-Maximilians-Universität (LMU) — [3]Deutsches Zentrum für Luft- und Raumfahrt (DLR)

The traditional setup of reservoir computing (RC) for predicting time series uses random matrices to define the underlying network and the input layer. Here, we show that a few modifications, which eliminate randomness and minimize computational resources and data requirements, lead to significant and robust improvements in short- and long-term predictive performance. We introduce block-diagonal reservoirs, which implies that a reservoir can be composed of multiple smaller reservoirs. Further, the non-linear activation function at the nodes can be dispensed with if the non-linear step in the analysis chain is shifted to the output layer. The input weights are determined according to well-defined rules. Any random initialization has thus been eliminated. By varying the remaining four hyperparameters, it is now possible to systematically investigate the transition from a linear, disjunct mapping of the input data to the output data to a combined nonlinear one. It is further demonstrated that there is a connection between the nonlinearities in the input data and the nonlinearities in the reservoir such that the best prediction results are obtained when both nonlinearities match. It becomes thus possible to define an optimally tailored setup for minimal RC for data sets with given nonlinearities.

DY 39.3 Thu 15:30 H47

Physical Reservoir Computing with Ferroelectric Oxides — •Atreya Majumdar[1], Yan Meng Chong[2], Dennis Meier[2], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Physical reservoir computing has shown remarkable potential in magnetic systems by utilizing their complex, non-linear, and history-dependent intrinsic dynamics for machine learning tasks [1]. More recently, ferroelectric materials - the electrical analogs of magnetic systems - have garnered attention. These materials not only meet all the essential criteria for reservoir computing but also bring unique advantages [2]. Here, we introduce the ferroelectric semiconductor ErMnO3 as a novel physical reservoir. By utilizing the material's non-linear and history-dependent photocurrent response, we demonstrate its capability to recognize varying input light pulse intensities. This study highlights the potential of ferroelectric materials in physical reservoir computing, paving the way for energy-efficient and scalable computing architectures.

[1] O. Lee, et al., Perspective on unconventional computing using magnetic skyrmions. Appl. Phys. Lett. 122, 260501 (2023).

[2] K. Everschor-Sitte, A. Majumdar, et al., Topological magnetic and ferroelectric systems for reservoir computing. Nat. Rev. Phys. 6, 455 (2024).

DY 39.4 Thu 15:45 H47

Describing heat transport in crystalline polymers in real and reciprocal space — Lukas Reicht[1], Lukas Legenstein[1], Sandro Wieser[2], and •Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria

Heat transport modelling either relies on describing the propagation of phonons employing the Boltzmann transport equation or on simulating the real-space dynamics of atoms using (non)-equilibrium molecular dynamics techniques. Due to the structural complexity of crystalline polymers both approaches call for a highly accurate but at the same time numerically extremely efficient strategy for describing inter-atomic interactions. This is achieved via machine-learned potentials, where we combine an efficient active-learning strategy with moment-tensor potentials.[1,2] Additionally, real-space and reciprocal space approaches make fundamentally different approximations regarding anharmonicities and phonon occupations. Here, we show that for polymers of intermediate complexity, like crystalline polythiophene, real- and reciprocal space approaches yield consistent values of the thermal conductivities at least when using an accurate machine-learned potential. Interestingly, for the seemingly much simpler crystalline polyethylene such an agreement is only obtained when higher-order phonon scattering is considered. This can be traced back to a selection rule arising from the comparably simple phonon band structure of polyethylene. [1] npj Comput Mater 10, 18 (2024); [2] Molecules 29, 3724 (2024)

DY 39.5 Thu 16:00 H47

Reinforcement learning for autonomous navigation of active particles in complex flow fields — •Diptabrata Paul and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany

Sensing and feedback on environmental stimuli are integral to regulating diverse functions in living systems, ranging from sub-cellular processes to evolution of navigation strategies such as chemotaxis and phototaxis. Unlike living systems, noisy artificial microswimmers have limited ability to adapt to various stationary and dynamic environmental perturbations to yield optimized behaviour for a given task. Consequently, reacting to such environmental cues becomes indispensable for achieving effective navigation and control in complex and noisy settings. In this context, we explore incorporation of machine learning algorithm for autonomous decision making for navigation of an active microswimmer within noisy environments. While naive navigation policies yield inefficient and ineffective solutions under changing conditions, employing actor-critic reinforcement learning (RL) framework trained in experiments leads us to quasi-optimal policies that are capable of navigating, even in presence of complex flow fields. Our study exhibits that a model trained under noisy conditions successfully learns effective navigation policies and are robust with respect to environmental perturbations such as hydrodynamic flow fields as well as varying initial conditions. This work paves the way for development of online RL for modelling adaptive behaviour and navigation of active microswimmers in complex fluidic scenarios.

DY 39.6 Thu 16:15 H47

Predictability Analysis of Discrete Time-Series Data with a Hamiltonian-Based Filter-Projection Approach — •Henrik Kiefer and Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin, Deutschland

The generalized Langevin equation (GLE), derived by projection from a general many-body Hamiltonian, exactly describes the dynamics of an arbitrary coarse-grained variable in a complex environment. However, analysis and prediction of real-world data with the GLE is hampered by slow transient or seasonal data components and time-discretization effects. Machine-learning (ML) techniques work but are computer-resource demanding and difficult to interpret. We show that by convolution filtering, time-series data decompose into fast, transient and seasonal components that each obey Hamiltonian dynamics and, thus, can be separately analyzed by projection techniques. We introduce methods to extract all GLE parameters from highly discretized time-series data and to forecast future data including the environmental stochasticity. For daily-resolved weather data, our analysis reveals non-Markovian memory that decays over a few days. Our prediction accuracy is comparable to ML long short-term memory (LSTM) methods at a reduced computational cost compared to LSTM. For financial data, memory is very short-ranged and the dynamics effectively is Markovian, in agreement with the efficient-market hypothesis; consequently, models simpler than the GLE are sufficient. Our GLE framework is an efficient and interpretable method for the analysis and prediction of complex time-series data.

DY 40: Members' Assembly

Time: Thursday 18:00–19:00 Location: H43

All members of the Dynamics and Statistical Physics Division are invited to participate.

DY 41: Quantum Dynamics, Decoherence, and Quantum Information (joint session DY/TT)

Time: Friday 9:30–11:15 Location: H37

DY 41.1 Fri 9:30 H37

Entanglement phase transitions in unitary circuit games with free fermions — •Raúl Morral-Yepes[1,2], Marc Langer[1,2], Adam Smith[3,4], Barbara Kraus[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences — [2]Munich Center for Quantum Science and Technology (MCQST) — [3]School of Physics and Astronomy, University of Nottingham — [4]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems

In the recently introduced framework of unitary circuit games, two competing parties an entangler and a disentangler can induce an entanglement phase transition, distinct from measurement-induced transitions. In this work, we study such games within the context of matchgate dynamics, which correspond to free fermion systems. First, we investigate the entanglement properties of fermionic Gaussian states (FGS) and explore different methods for their disentangling. We propose a representation of FGS using a minimal matchgate circuit in a standard form, and introduce algorithms for updating this representation as unitary operations are applied. Within this framework, we define a natural disentangling procedure that reduces the number of gates in the circuit, thereby decreasing the system's entanglement. We then analyze the unitary game using this gate disentangler, observing a phase transition between a volume-law and area-law entanglement phase. The nature of this transition differs depending on whether we examine Rényi-0 or other entanglement entropies.

DY 41.2 Fri 9:45 H37

Measurement Induced Entanglement Transitions in Random Qudit Clifford Circuits — •Aamod Vinayak Atre, Raúl Morral Yepes, and Frank Pollmann — Department of Physics, Technical University of Munich

Random quantum circuits with local projective measurements uncover the universal dynamical properties of generic chaotic quantum many-body systems, as their unitary evolution is independent of the microscopic features of Hamiltonians. Entanglement measures characterize these universal dynamics into volume-law and area-law regimes, which exhibit bipartite entropy scaling proportional to the system volume and system boundary respectively. This continuous entanglement scaling transition, driven by the rate of measurement, has been extensively studied in spin-1/2 (qubit) systems of various spatial geometries. In this talk, we discuss the characterization the entanglement transitions in 1D random quantum circuits of spins (qudits) with arbitrary local Hilbert-space dimension d. This work employs the generalized stabilizer formalism, taking advantage of the Clifford group which forms a unitary 2-design on the space of unitaries. We find the nature of the entanglement transition, from volume-law to area-law regimes, to be preserved for $d > 2$. The critical measurement density increases, converging to $1/2$ in the limit $d \to \infty$. Lastly, we describe the stabilizer dynamics in the limit $d \to \infty$, by a dynamical classical model.

DY 41.3 Fri 10:00 H37

Entanglement phases, localization and ergodicity of monitored free fermions in 2D — •Karim Chahine and Michael Buchhold — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Monitored quantum systems, characterized by the interplay between unitary evolution and mid-circuit measurements, have recently emerged as a novel expression of quantum dynamics. Despite their inherently out-of-equilibrium nature, these systems can host robust quantum phases and display measurement-induced phase transitions (MIPT) in the entanglement entropy. Remarkably, they are also unique in providing a link between quantum dynamics in D dimensions and quantum statistical mechanics in $D+1$ dimensions. In this talk, I will present our recent work on a new arena with a rich phenomenology: continuously monitored, $U(1)$-symmetric free fermions in 2D. I will address the emerging MIPT and its similarities and differences with Anderson-type localization transitions. Some emphasis will be put on the low-measurement regime, where intriguing features in the entanglement structure and ergodic properties emerge, revealing a richer phenomenology than previously anticipated.

DY 41.4 Fri 10:15 H37

Spectral Properties and Magic generation of T-doped Random Clifford Circuits — •Dominik Szombathy — Budapest University of Technology and Economics

We investigate the spectral properties and magic generation of T-doped random Clifford circuits. There is a direct relation between the structure of Pauli string orbits and the eigenvalue spectrum of a Clifford circuit. Operatively, we sample the closed trajectories with brick-wall circuits and determine the distribution of the eigenvalues $\lambda = e^{i\Theta}$. The autocorrelation function of the phases of the eigenvalues displays peculiar properties: extreme degeneracies as well as some level-repulsion, and features reminiscent of a fractal pattern.

To investigate the stability of orbits and head towards universal quantum computation, we introduce $\pi/4$ phase shift gates (T-gates). We find that even a single T-gate completely changes the properties of the circuit. By increasing the number of T-gates (N_T), the correlation function rapidly approaches that of the random unitary circuits. Nevertheless, some statistically significant fraction of non-trivial orbits persists at low T-gate densities (N_T/N).

We observe a similar phenomenology in the magic generation as a function of T-gate density. In particular, we find universal scaling of the maximum and mean magic as a function of N_T/N . We also highlight the structure of magic generated by these circuits. Injecting a few T-gates the distribution is discrete but becomes continuous as N_T increases. At large densities N_T/N , most of the weight is found in a sharp peak well below the theoretical maximum.

DY 41.5 Fri 10:30 H37

Magic transition in measurement-only circuits — •Poetri Sonya Tarabunga[1,2] and Emanuele Tirrito[3,4] — [1]Technical University of Munich, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 München, Germany — [3]The Abdus Salam International Centre for Theoretical Physics (ICTP), 34151 Trieste, Italy — [4]Dipartimento di Fisica "E. Pancini", Università di Napoli "Federico II", 80126 Napoli, Italy

Magic quantifies the distance of a quantum state to the set of stabilizer states, and it serves as a necessary resource for potential quantum advantage over classical computing. In this work, we study magic in a measurement-only quantum circuit with competing types of Clifford and non-Clifford measurements, where magic is injected through the non-Clifford measurements. This circuit can be mapped to a classical model that can be simulated efficiently, and the magic can be characterized using any magic measure that is additive for tensor product of single-qubit states. Leveraging this observation, we study the magic transition in this circuit in both one- and two-dimensional lattices using large-scale numerical simulations. Our results demonstrate the presence of a magic transition between two different phases with extensive magic scaling, separated by a critical point in which the mutual magic exhibits scaling behavior analogous to entanglement. We further show that these two distinct phases can be distinguished by the topological magic. In a different regime, with a vanishing rate of non-Clifford measurements, we find that the magic saturates in both phases.

DY 41.6 Fri 10:45 H37

Developing a Framework for Predicting Useful Quantum Advantage in the Calculation of Molecular NMR Spectra — •Keith Fratus, Andisheh Khedri, Juha Leppäkangas, Michael Marthaler, and Jan Reiner — HQS Quantum Simulations GmbH, Karlsruhe, Germany

Demonstrating useful quantum advantage remains a primary goal of quantum computing efforts in the NISQ era. Key to such efforts is the ability to estimate the accuracy and performance of competing classical approximation methods when exact comparisons are not available. In this talk we report on our efforts to develop and understand the behaviour of various classical approximation methods which aim to solve a specific class of chemical simulation problems. In particular, we develop classical simulation methods designed to predict molecular NMR spectra, with the aim of being able to quantify the accuracy and computational requirements of performing these simulations, even for parameter regimes which we do not directly simulate. Using such methods, we work towards a framework for predicting in which parameter regimes, system sizes, and target accuracies one can expect the failure of classical methods for this class of systems, thus allowing for the possibility of quantum advantage.

DY 41.7 Fri 11:00 H37

Linear differential equation approach to the Loschmidt amplitude — •Michael Vogl — King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

The Loschmidt amplitude is a popular quantity that allows making predictions about the stability of quantum states under time evolution. We present an approach that allows us to find a linear differential equation that can be used to

compute the Loschmidt amplitude. This approach, while in essence perturbative, has the advantage that it converges at finite order. We demonstrate that the approach for generically chosen matrix Hamiltonians often offers advantages over Taylor and cumulant expansions even when we truncate at finite order. Even in low dimensional systems such as two band Hamiltonians (multi-Weyl semimetals and AB bilayer graphene) it can be used to obtain general formulas for the Loschmidt amplitude after a quench. Results readily generalize to find transmission amplitudes and specific contributions of the partition function, too. Our method can also be applied to many body spin and fermionic Hamiltonians. Here, while the approach still offers advantages, more care has to be taken than in a generic case. We also provide an estimate for a breakdown time of the approximation.

DY 42: Stochastic Thermodynamics

Time: Friday 9:30–11:15 Location: H43

DY 42.1 Fri 9:30 H43

Stochastic Thermodynamics of the Interacting Non-reciprocal Particles and Fields — •Atul Tanaji Mohite and Heiko Rieger — Saarland University, Saarbrücken, Germany

Non-reciprocal interactions that violate Newtons law 'actio=reactio' are ubiquitous in nature and are currently intensively investigated in active matter, chemical reaction networks, population dynamics and many other fields. An outstanding challenge is the thermodynamically consistent formulation of the underlying stochastic dynamics that obeys local detailed balance and allows for a rigorous analysis of the stochastic thermodynamics of non-reciprocally interacting particles. Here we present such a framework for a broad class of active systems and derive by systematic coarse-graining exact expressions for the macroscopic entropy production. Four independent contributions to the thermodynamic dissipation can be identified, among which the energy flux sustaining vorticity currents manifests the presence of non-reciprocal interactions. Then, Onsager's non-reciprocal relations, the fluctuation-response relation, the fluctuation relation and the thermodynamic uncertainty relations for non-reciprocal systems are derived. Finally, we demonstrate that our general framework is applicable to a plethora of active matter systems and chemical reaction networks and opens new paths to understand the stochastic thermodynamics of non-reciprocally interacting many-body systems.

DY 42.2 Fri 9:45 H43

Staying on Time: Precision and Cost of a Controlled Clock — •Till Welker and Patrick Pietzonka — School of Physics and Astronomy, University of Edinburgh, United Kingdom

The precision of an autonomous clock is associated with an entropic cost. In overdamped systems, the precision-cost tradeoff is bounded by the thermodynamic uncertainty relation (TUR). To avoid paying immense costs while staying accurate over an extended period, the clocks in our phones, radios, and computers adapt their dynamics according to a precise reference clock.

We study the minimal model of the two-state controlled clock with one state running slower and one state running faster than the reference clock. At a rate R, the controlled clock reads out the reference clock and adjusts its state accordingly. While the clock hand progresses, the offset reaches an analytically solvable steady state, and the clock's error remains bounded.

The combined cost of the controlled and reference clock obeys the TUR. However, the operator of the controlled clock only needs to pay a part of that cost, namely the driving of the controlled clock and the cost of state adjustment. We show that there is an R-dependent tradeoff between the controlled clock's cost and its total error, and we explore the Pareto front of optimal clocks.

DY 42.3 Fri 10:00 H43

Active Brownian information engine: Self-propulsion induced colossal performance — •Rafna Rafeek and Debasish Mondal — Department of Chemistry and Center for Molecular and Optical Sciences and Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India

Many biological systems operating in athermal (active) environments, can be modeled as an information engine, with the key aspect of utilizing information on the fluctuation to extort work from the noisy environment. In this study, we propose a feedback-driven information engine operating in a Gaussian-correlated active reservoir with characteristic strength (D_a) and correlation time (τ_a), which outperforms its thermal counterpart. We obtain the optimal functioning criteria for the enhanced performance of the active Brownian information engine (ABIE), reliant on the dispersion of the steady state, which is analogous to its passive analog. We notice that a weakly correlated active bath extracts colossal work due to the reduced relative loss of information in the relaxation process. In the limit of fractionally smaller correlation time ($t_a/t_r \rightarrow 0$, t_a is thermal relaxation time), the upper bound on colossal work extraction is $0.202(D+D_a)$. The excess amount of extracted work reduces and converges to its passive counterpart in the higher limit of correlation time ($t_a/t_r \rightarrow high$). Interestingly, when correlation time is equivalent to relaxation time ($t_a/t_r = 1$), half the upper bound of excess work is achieved irrespective of activity strength. This study provides a new insight into understanding and designing the information-energy exchange of biological submicrometer motors.

DY 42.4 Fri 10:15 H43

Entropy estimation for partially accessible Markov networks based on imperfect observations: Role of finite resolution and finite statistics — •Jonas H. Fritz, Benjamin Ertel, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Estimating entropy production from real observation data can be difficult due to finite resolution in both space and time and finite measurement statistics. We characterize the statistical error introduced by finite sample size and compare the performance of three different entropy estimators under these limitations for two different paradigmatic systems, a four-state Markov network and an augmented Michaelis-Menten reaction scheme. We consider the thermodynamic uncertainty relation, a waiting-time based estimator for resolved transitions and a waiting-time based estimator for blurred transitions in imperfect observation scenarios. For perfect measurement statistics and finite temporal resolution, the estimator based on resolved transitions performs best in all considered scenarios. The thermodynamic uncertainty relation gives a better estimate than the estimator based on blurred transitions at low driving affinities, whereas the latter performs better at high driving affinities. Furthermore, we find that a higher temporal and spatial resolution leads to slower convergence of measurement statistics, implying that for short measurement times, a lower resolution may be beneficial. Additionally, we identify a self-averaging effect for the waiting-time based entropy estimators that can reduce their variance for observations with finite statistics.

DY 42.5 Fri 10:30 H43

Stochastic Calculus Approach to Thermodynamic Bounds for Jump Processes — •Lars Stutzer, Cai Dieball, and Aljaž Godec — Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

Thermodynamic inequalities bound dissipation from below in terms of fluctuations of, and correlations between, observable currents and densities. They are at the heart of thermodynamic inference. By establishing a stochastic-calculus for functionals of Markov-jump dynamics, we allow for immediate extensions of results derived for overdamped diffusion to discrete state spaces, which expands the range of bounds available for jump processes. Moreover, we use the calculus to prove new bounds for jump-processes, including transient thermodynamic uncertainty relations, finite-time correlation bounds, and the recently established transport bounds. While it was expected for these results carry over to discrete spaces, the methodological advance establishes them as an inherent property of stochastic equations of motion. Our results put Langevin and Markov-jump dynamics on a common footing on the level of individual stochastic trajectories. We illustrate the results by means of biologically motivated examples.

DY 42.6 Fri 10:45 H43

Is learning in Neural Networks just very high dimensional parameter fitting? — •Ibrahim Talha Ersoy — Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland

Neural Networks (NNs) are known for their highly non-convex loss landscapes, shaped by the data and the error function. Unlike in convex optimization, the model navigates regions of changing curvature to find the global minimum. We anticipate qualitative changes in the model occurring at points where new error basins are explored. In information bottleneck settings, Tishby et al. (2015) suggested that transitions between distinct loss regions are associated with phase transitions, a concept proven in L2 setups by Ziyin et al. (2023), where they examined the onset of learning when varying the L2 regularizer strength. We extend the findings of Ziyin et al. (2023), interpreting them from an information geometric perspective and demonstrate further phase transitions when model changes. By distinguishing between the loss and error landscapes, we provide a rigorous argument that extends the scope of our results beyond the L2 setup. This approach enables a better understanding of the limitations of the free energy interpretation of the L2 loss function and provides a more accurate depiction. Finally, our results suggest a clear distinction between learning, characterised by phase transitions at points of model change, and fitting, where the model remains qualitatively fixed, lacking phase transitions.

DY 42.7 Fri 11:00 H43

Coherent effects in the semiclassical limit of quantum work — •Nicolás Torres-Domínguez[1], Carlos Viviescas[2], and JD Urbina[3] — [1]Chalmers tekniska högskola, Göteborg, Sweden — [2]Universidad Nacional de Colombia, Bogotá, Colombia — [3]Universität Regensburg, Institut für Theoretische Physik

Within the framework of quantum thermodynamics, the use of quasiprobabilities can provide a comprehensive approach to the work statistics of quantum systems. In this formulation the effects of coherences in the initial state of the system are accounted in a natural way for all protocols and are expected to be displayed in the quantum features of the chosen quasidistribution [1]; yet clear examples of this are scarce in the literature. In this work we consider the semiclassical limit of the quantum work distribution obtained using the Kirkwood-Dirac quasiprobability, highlighting the effects of initial coherences on the energetics of the system and on the quantum behavior of the quasidistribution. We illustrate our results in a study of the work distribution of a forced quantum harmonic oscillator [2] in the Weyl-Wigner representation in phase space.

[1] M. Lostaglio, A. Belenchia, A. Levy, S. Hernández-Gómez, N. Fabbri, and S. Gherardini, Quantum 7, 1128 (2023). [2] P. Talkner, P. S. Burada, and P. Hänggi, Phys. Rev. E 78, 011115 (2008).

DY 43: Active Matter IV (joint session BP/CPP/DY)

Time: Friday 9:30–13:00 Location: H44

Invited Talk DY 43.1 Fri 9:30 H44

Wave propagation in systems of active filaments — •Kirsty Y. Wan — Living Systems Institute, University of Exeter, UK

Active hair-like protrusions called cilia are found in many eukaryotes where they produce physiological flows for a variety of functions. Cilia assume a myriad of configurations both external to an organism for the purposes of feeding or swimming motility, but also internally where they mediate mucociliary clearance in vertebrate tissues. Single cilia can propagate large-amplitude non-decaying bending waves, even in the absence of a cell body. These waves assume a variety of stereotyped forms and frequencies, depending on the species. Multiple cilia also interact to produce different types of local and global coordination patterns, including robust metachronal waves. Do these dynamic states of coordination arise spontaneously, or do they require some form of internal control by the cell or animal? We propose new and emerging organisms to address these questions.

DY 43.2 Fri 10:00 H44

Metabolic activity controls the emergence of coherent flows in microbial suspensions — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to the spatio-temporal variations of environmental parameters within their habitat. In the absence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment may be deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we study the effect of motility and cell density of *C. reinhardtii* in a confined system, on the emergence of bioconvection [2]. This collective phenomenon can be reversibly switched by light and arises due to the natural tendency of the bottom-heavy cells to move against gravity. We show that the rate at which the system evolves, as well as the dominant wavelength of the instability can both be directly controlled by the number density of cells. Further, we provide insights on the internal flow fields and density profiles of single bioconvection plumes for different parameters.

[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).
[2] A.A. Fragkopoulos et al., *arXiv*:2407.09884 (2024)

DY 43.3 Fri 10:15 H44

Tumbling *E.coli* in bulk and close to surfaces — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian institute of science education and research (IISER), Tirupati, India

Escherichia coli (*E. coli*) swims by rotating multiple flagella which are connected to the cell body forming a thick bundle. To change direction, *E. coli* performs tumble events by reversing the rotation of one or more flagella. The involved filaments undergo a series of polymorphic transformations, altering both their helicity and handedness. This complex phenomenon involves the interplay of semiflexible filaments and hydrodynamic flow fields.

Here, we have developed a detailed numerical framework to simulate *E. coli*, capturing the full dynamics of flexible flagella, including their polymorphism and their hydrodynamic interactions. The filaments and the cell body are embedded in a viscous fluid, which we model using multi-particle collision dynamics. We analyzed a large number of tumble events, with fixed tumble time or taken from a gamma distribution, exploring the roles of hook and flagellar flexibility as well as flagellar polymorphism. We find that they strongly influence the distribution of tumble angles. Finally, we also show that close to a flat surface the mean tumble angle is strongly shifted to smaller values. This indicates that tumble events may not be recognized, which could give the impression of suppressed tumbling near surfaces.

DY 43.4 Fri 10:30 H44

***Trypanosoma brucei* (un)chained - effects of confinement on a parasitic microswimmer** — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth — [2]Laboratory of Molecular Parasitology, University of Bayreuth

Trypanosoma brucei is a parasitic unicellular microswimmer that causes the African sleeping sickness. An active spiral movement of the parasite, mediated by a microtubule-driven flagellum that wraps around the cell body, is mandatory to evade the host's immune system while exploring tissues and blood vessels. In addition, the nematic subpellicular micotubule array plays a pivotal role in the elasticity, propulsion, and navigation of the parasite. To study the features and mechanisms behind the cell's motion in such complex environments, we have mimicked spatial confinement in microfluidic devices with different geometries. Our data show that spatial constraints in narrow channels and channel networks can improve cell locomotion of wild-type trypanosomes, supposedly due to the interaction of the elastic cell body and nearby walls. The addition of microtubule-disrupting drugs or the use of mutant strains with altered post-translational modifications of microtubules resulted in significantly altered swimming velocities and marked changes in the intermittent switching between run and tumble phases. Shape analyses of individual cells suggest that microtubules in the sub-pellicular array, the corset that keeps trypanosomes in their native spindle-like shape, are most affected in these cases.

DY 43.5 Fri 10:45 H44

Micro-swimmer motility in presence of signaling factors — Agniva Datta, Robert Grossmann, and •Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

The navigation of bacteria through aqueous environments, driven by the rotation of helical flagella, has been a significant region of interest in the biophysics community for the last few decades. In this study, we focus on the motility of our model organism, Pseudomonas putida, which exhibits persistent mobile episodes (Active Brownian motion) interrupted by stochastic reorientation events (turns), driven by flagellar self-propulsion, thereby leading to a run-and-turn motility.

Key motility parameters including tumbling rates, run lengths, trajectory persistence (rotational diffusion coefficient), and the characteristics of the self-propulsion force*are hypothesized to depend on the density of quorum-sensing autoinducer molecules, produced by the bacteria themselves as signaling factors. To test this hypothesis, we expose swimming bacteria to aqueous environments with controlled autoinducer concentrations and analyze the resulting changes in motility patterns. Through a combination of experimental data and theoretical modeling, we aim to elucidate the principles of micro-swimmer motility in presence of signaling molecules.

DY 43.6 Fri 11:00 H44

Collective dynamics of active dumbbells near a circular obstacle — •Chandranshu Tiwari[1] and Sunil Singh[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India. — [2]Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

We present the collective dynamics of active dumbbells in the presence of a static circular obstacle using Brownian dynamics simulation. The active dumbbells aggregate on the surface of a circular obstacle beyond a critical radius, and the aggregate size increases with the activity and the curvature radius. The dense aggregate of active dumbbells displays persistent rotational motion with a certain angular speed, which linearly increases with activity. Furthermore, we show a strong polar ordering of the active dumbbells within the aggregate. The polar ordering exhibits long-range correlation, with the correlation length corresponding to the aggregate size. Additionally, we show that the residence time of an active dumbbell on the obstacle surface increases rapidly with area fraction due to many-body interactions that lead to a slowdown of the rotational diffusion. This article further considers the dynamical behavior of a tracer particle in the solu-

tion of active dumbbells. Interestingly, the speed of the passive tracer particle displays a crossover from monotonically decreasing to increasing with the size of the tracer particle upon increasing the dumbbells' speed. Furthermore, the effective diffusion of the tracer particle displays non-monotonic behavior with the area fraction; the initial increase in diffusivity is followed by a decrease for a larger area fraction.

DY 43.7 Fri 11:15 H44

Free growth under tension — •Chenyun Yao and Jens Elgeti — Forschungszentrum Jülich GmbH, Jülich, Germany

Ever since the ground breaking work of Trepat et al. in 2009, we know that cell colonies growing on a substrate can be under tensile mechanical stress. The origin of tension has so far been attributed to cellular motility forces being oriented outward of the colony. Works in the field mainly revolve around how this orientation of the forces can be explained, ranging from velocity alignment, self-sorting due to self-propulsion, to kenotaxis.

In this work, we demonstrate that tension in growing colonies can also be explained without cellular motility forces! Using a combination of well established tissue growth simulation technique and analytical modelling, we show how tension can arise as a consequence of simple mechanics of growing tissues. Combining these models with a minimalistic motility model shows how colonies can expand while under even larger tension. Furthermore, our results and analytical models provide novel analysis procedures to identify the underlying mechanics.

15 min. break

DY 43.8 Fri 11:45 H44

A route to active turbulence in circular activity spots — •Arghavan Partovifard and Holger Stark — Institute of Theoretical Physics, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623Berlin, Germany.

Active nematics exhibit distinctive behavior such as active turbulence and regular flow patterns under spatially varying activity [1]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investigate active nematics confined to a circular spot by switching off activity outside the spot. The open boundary allows topological defects to enter and leave the spot.

We calculate the total topological defect charge inside the spot using three approaches: counting all defects, measuring the rotation of the director field along the rim of the spot, and integrating the diffusive charge density. All methods agree that for spot radii just larger than the nematic coherence length, the system has a total topological charge of +1, where two +1/2 defects perform a regular swirling motion. As the radius increases, more defects enter and their motion becomes more and more chaotic. Ultimately, the charge per unit area saturates at the value characteristic of bulk active turbulence. For the range of radii where the total charge in the spot is +1, the nematic director exhibits shear-induced anchoring at an angle of 45° with respect to the tangent at the spot rim. With increasing radius, when more defects enter, the anchoring angle deviates from 45° but its distribution still peaks around this value.

[1] A. Partovifard *et. al.*, Soft Matter **20**, 1800 (2024)

DY 43.9 Fri 12:00 H44

Cognitive flocks: order-disorder transitions and threat evasion — •Priyanka Iyer[1], Cecilia Soroco[2], and Gerhard Gompper[1] — [1]Forschungszentrum Jülich — [2]University of British Columbia, Canada

Directed self-propulsion is ubiquitous in living organisms. From E.Coli dispersing in biofilms to migrating bird flocks, living organisms are constantly out-of equilibrium. By sensing their environment and adjusting their movement, organisms can exhibit emergent patterns and collective behaviors, such as self-organization in human crowds [1], bird flocks, and fish schools. The Inertial Spin Model (ISM) was introduced to explain the fast and robust propagation of information in bird flocks [2], when only alignment interactions are considered. However, more generally, agents exhibit a variety of interactions like local avoidance, cohesion and threat evasion. We show how such behaviors can be incorporated within the framework of the ISM. It is found that local avoidance introduces emergent noise in the system, triggering an order-disorder transition. Exploring the flock dynamics near this transition reveals a complex interplay between cohesion, alignment, and local avoidance, resulting in diverse behaviors such as pronounced shape and density fluctuations, and diffusive motion of the flock. Lastly, by applying the model to a stationary threat scenario, we analyze flock properties that govern threat information propagation in the flock.

[1] Iyer, P. et al. , Comm. Phys. 7.1 (2024): 379.
[2] Attanasi, A. et al. , Nat. Phys. 10, 691-696, (2014)

DY 43.10 Fri 12:15 H44

Myosin-independent amoeboid cell motility — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell motility is essential for many physiological and pathological processes, such as the immune system, embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode which allows them to move rapidly in a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. We introduce a model for an amoeboid cell where the cortex is described as a thin shell along the cell surface. The cell shape evolves due to polymerization of actin filaments and the forces acting on the cortex. We find analytically and numerically that the state of a resting, non-polarized cell can become unstable for sufficiently large actin polymerization velocities, resulting in the spontaneous onset of cell polarity, migration, and dynamical shape changes. Notably, this transition only relies on actin polymerization and does not necessitate molecular motors, such as myosin. These findings yield a deeper understanding of the fundamental mechanisms of cell movement and simultaneously provide a simple mechanism for cell motility in diverse configurations.

DY 43.11 Fri 12:30 H44

Active membrane deformations of a synthetic cell-mimicking system — Alfredo Sciortino[1], •Dmitry Fedosov[2], Gerhard Gompper[2], and Andreas Bausch[1] — [1]Physik Department, Technische Universität München, Garching bei München, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Biological cells are fascinating micromachines capable of adapting their shape due to the complex interaction between a deformable membrane and the dynamic activity of the cytoskeleton. We investigate the behavior of an active synthetic cell-mimicking system using simulations and experiments. In simulations, the model consists of a fluid vesicle with a few encapsulated growing filaments. In experiments, giant vesicles contain an active cytoskeletal network composed of microtubules, crosslinkers, and molecular motors. These active vesicles show strong shape fluctuations reminiscent of shape changes of biological cells. We analyze membrane fluctuations and show how the intricate coupling between soft confinement and internal active forces results in fluctuation spectra with distinct spatial and temporal scales, differing significantly from those of passive vesicles. Simulations demonstrate the universality of this behavior, quantifying the impact of correlated activity on the dynamics of membrane deformations. This model makes a step toward quantitative description of shape-morphing artificial and living systems.

DY 43.12 Fri 12:45 H44

Force Generation by Enhanced Diffusion in Enzyme-Loaded Vesicles — Eike Eberhard, •Ludwig Burger, Cesar Pastrana, Giovanni Giunta, and Ulrich Gerland — Physik komplexer Biosysteme, Technische Universität München, Deutschland

Recent experiments show that the diffusion coefficient of some metabolic enzymes increases with the concentration of their cognate substrate, a phenomenon known as enhanced diffusion. In the presence of substrate gradients, enhanced diffusion induces enzymatic drift, resulting in a non-homogeneous enzyme distribution. In this work, we study the behavior of enzyme-loaded vesicles exposed to external substrate gradients using a combination of computer simulations and analytical modeling. We observe that the spatially inhomogeneous enzyme profiles generated by enhanced diffusion result in a pressure gradient across the vesicle, which leads to macroscopically observable effects, such as deformation and self-propulsion of the vesicle. Our analytical model allows us to characterize dependence of the velocity of propulsion on experimentally tunable parameters. The effects predicted by our work provide an avenue for further validation of enhanced diffusion, and might be leveraged for the design of novel synthetic cargo transporters, such as targeted drug delivery systems.

DY 44: Droplets, Wetting, Complex Fluids, and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:45 Location: H47

Invited Talk DY 44.1 Fri 9:30 H47

From Cavitation in Soft Matter to Erosion on Hard Matter — •Claus-Dieter Ohl — Institute of Physics, Otto-von-Guericke University, Magdeburg, Germany

Cavitation is the technical term for the formation of empty spaces in a liquid. These unstable voids eventually implode and focus energy on small volumes. Shock wave emission, light emission, erosion, and even nuclear reactions are the consequence of this near singular energy focusing. Here, I will present recent

research related to cavitation not only in liquids but also in elastic solids and particularly at the interface of both materials. Singularities developing on the axis of symmetry in non-spherical collapses near boundaries are able to amplify shock waves through self focusing. We think that this mechanism is the primary cause for erosion. In contrast, the non-spherical collapse and shock wave focusing near a tissue allows for the penetration of the tissue with liquid jets at 1000m/s and above. The mechanism at play may be relevant in sports and battle zones, as they could lead to traumatic brain injuries.

DY 44.2 Fri 10:00 H47

Shape switching and tunable oscillations in adaptive droplets — •Tim Dullweber[1,2], Roman Belousov[1], Camilla Autorino[1,4], Nicoletta Petridou[1], and Anna Erzberger[1,3] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]University Heidelberg, Heidelberg, Germany — [3]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [4]Faculty of Biosciences, Heidelberg University, Heidelberg, Germany

Soft materials can undergo irreversible shape changes when driven out of equilibrium. When shape changes are triggered by processes at the surface, geometry-dependent feedback can arise. Motivated by the mechanochemical feedback observed in multicellular systems, we study incompressible droplets that adjust their interfacial tensions in response to shape-dependent signals. We derive a minimal set of equations governing the mesoscopic droplet states, controlled by just two dimensionless feedback parameters. We find that interacting droplets exhibit bistability, symmetry-breaking, excitability and tunable shape oscillations ranging from near-sinusoidal to relaxation-type. We apply our framework to model shape measurements in zebrafish embryos and identify a shape-switching mechanism promoting boundary formation. The underlying critical points reveal novel mechanisms for physical signal processing through shape adaptation in soft active materials, and suggest new modes of self-organization at the collective scale.

DY 44.3 Fri 10:15 H47

Impact of the history force on the motion of droplets in shaken liquids — •Frederik Gareis and Walter Zimmermann — Theoretical Physics, University of Bayreuth

The Basset-Boussinesq history (BBH) force acts on droplets and solid particles in flows, alongside stationary viscous friction, inertia, and gravitational forces. This force arises from vortex shedding around objects undergoing unsteady acceleration. In this study, we analytically calculate the BBH force for spherical, sedimenting heavy particles in horizontally shaken (periodically accelerated) fluids at low Reynolds numbers and identify the parameter ranges where BBH effects are significant. Our results reveal that BBH can increase particle displacement amplitude by over 60 percent, particularly in the transition region between the low-frequency viscous Stokes regime and the high-frequency inertia-dominated regime. Additionally, we derive a power law for the oscillatory displacement amplitude of a particle around its mean position in a horizontally shaken fluid, facilitating clear experimental identification of BBH effects.

DY 44.4 Fri 10:30 H47

Bubble Dynamics and Transport in Porous Structures: Insights from Mesoscale Simulations — •Qingguang Xie[1], Othmane Aouane[1], and Jens Harting[1,2] — [1]Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen-Nürnberg (IET-2), Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Bubble formation, detachment, and transport within porous structures are critical phenomena in various applications, including electrolyzers and chemical reactors. We numerically investigate the dynamics of bubble growth and detachment at a catalytic surface using the lattice Boltzmann method. The departure radius of a bubble, growing with either a pinned or moving contact line, shows good agreement with theoretical predictions. Beyond detachment, we examine the subsequent transport of bubbles through a porous transport layer, systematically evaluating transport efficiency by considering factors such as pressure gradients, reaction rates, and pore wettability. Our findings provide valuable insights for optimizing the design of porous structures, potentially resulting in enhanced performance in electrolyzers and other gas-evolving devices.

DY 44.5 Fri 10:45 H47

Displacements in thin fluid and elastic films — •Andreas M. Menzel — Otto von Guericke University Magdeburg, Germany

We address the displacements of comparatively small objects in flat thin fluid films under low-Reynolds-number conditions or in flat thin elastic sheets under linear elasticity.

It is well-known that the fundamental solution of the corresponding continuum equations for forced in-plane displacements diverges logarithmically in strictly two-dimensional systems, the so-called Stokes paradox. We provide an illustrative way of interpretation and demonstrate how the divergence cancels under pairwise interactions and confinement [1,2]. Interestingly, logarithmic spatial dependencies prevail under rectangular clamping of elastic membranes [3]. Moreover, the divergence is still present in free-standing sheets of finite thickness, unless they are stabilized, for instance, by substrates [4,5].

We are confident that our analytical results will prove useful in corresponding quantitative experimental evaluations.

[1] S. K. Richter, A. M. Menzel, Phys. Rev. E **105**, 014609 (2022).
[2] T. Lutz, S. K. Richter, A. M. Menzel, Phys. Rev. E **106**, 054609 (2022).
[3] A. R. Sprenger, H. Reinken, T. Richter, A. M. Menzel, EPL (Europhys. Lett.) **147**, 17002 (2024).
[4] T. Lutz, A. M. Menzel, A. Daddi-Moussa-Ider, Phys. Rev. E **109**, 054802 (2024).
[5] A. Daddi-Moussa-Ider, E. Tjhung, T. Richter, A. M. Menzel, J. Phys.: Condens. Matter **36**, 445101 (2024).

DY 44.6 Fri 11:00 H47

Magnetic dynamics in ferromagnetic liquid crystal emulsions — •Christoph Klopp[1], Hajnalka Nádasi[1], Darja Lisjak[2], and Alexey Eremin[1] — [1]Otto von Guericke University, Institute of Physics, 39106 Magdeburg, Germany — [2]Jozef Stefan Institute, Department for Materials Synthesis, 1000 Ljubljana, Slovenia

We explore magnetic liquid crystal (LC) emulsions for applications as manipulatable chemical sensors in giant cells of Characean algae. Such emulsions can be controlled by magnetic fields and provide targeted drug delivery or sensing [1]. The investigated emulsions consist of a ferromagnetic liquid crystal [2] dispersed in an aqueous solution. We investigate the dynamic magnetic response using AC-susceptometry [3] as a function of the carrier medium viscosity and the particle or droplet size distribution. The emulsions' magnetic spectra differ drastically from those in the bulk of the hybrid liquid crystal mixture. We demonstrate the influence of the liquid crystal director configuration at the water-droplet interface by analyzing the effect of different surfactants (mainly SDS and PVA) in the aqueous phase.

[1] F. von Rüling et al., Liquid Crystals, 2024, 51, 1546
[2] A. Mertelj, et al., Nature, 2013, 504, 237-241
[3] M. Küster et al., J. Magn. Magn. Mater., 2023, 588, 171368

This study was supported by DFG with projects ER 467/14-1 and NA1668/1-3.

15 min. break

DY 44.7 Fri 11:30 H47

Drying effects in soft colloidal monolayers — •Kai Luca Spanheimer[1], Matthias Karg[2], Nicolas Vogel[3], Liesbeth Janssen[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [3]Lehrstuhl für Partikelsynthese Friedrich-Alexander-Universität,91058 Erlangen, Germany — [4]Soft Matter and Biological Physics Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

Langmuir-Blodgett deposition is a staple of colloidal monolayer research. It is used in sample preparation for imaging techniques, that spatially resolve colloid patterns. Recent experimental observations have shown that drying can strongly rearrange micron sized microgel patterns after their deposition. The usual dictum that these drying effects do not play a role for colloidal deposition can thus not be held up as a general rule. While capillary effects are well known to be strong at microscopic length scales and play a significant role in drying processes they have been mostly neglected concerning Langmuir-Blodgett deposition. In order to better understand the mechanism of drying we propose a model based on capillary attraction as well as hard core and soft shell repulsion. This model reproduces colloid patterns observed at interfaces as well as ones that occur after drying in the corresponding parameter regimes. From here we are able to derive parameter ranges where drying can play a role in rearranging patterns of colloids and where it can't.

DY 44.8 Fri 11:45 H47

Interplay of Elasticity and Capillarity in Droplets on Flexible Sheets — •Salik Sultan and Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Droplets resting on flexible sheets deform into lens-like shapes, offering promising applications in areas like tunable liquid lenses. We have extended and employ our fully three-dimensional Boundary Element Method (BEM) simulation framework [1] to investigate dynamic wetting on thin flexible sheets. Our study focuses on the intricate interplay between the mechanical properties of the sheet and droplet behavior, particularly emphasizing contact angle and droplet shape. By varying the tension and mechanical properties of the sheet, our model demonstrates how we can control and tune the shape of the droplet. Additionally, by introducing stiffness gradients, we aim to explore the potential to steer droplets along the sheet via durotaxis. The versatility of our model suggests potential extensions to other soft material and droplet interactions, such as capillary origami. This work sheds light on the complex interactions between soft substrates and liquid interfaces, leading the way for advancements in material science and interfacial biology.

[1] J. Grawitter and H. Stark, Steering droplets on substrates with plane-wave wettability patterns and deformations, Soft Matter 20, 3161 (2024).

DY 44.9 Fri 12:00 H47

Cluster quasicrystals composed of ultrasoft particles vs. soft quasicrystals built of colloids with hard cores — Robert F.B. Weigel and •Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study and compare two different approaches for the stabilization of quasicrystals:

First, we consider a Phase Field Crystal model of complex patterns that self-assemble in systems consisting of ultrasoft colloids. Quasicrystals can be either stabilized by interactions with multiple length scales [1,2] or by preferred binding angles as in patchy colloids [3].

Second, we study a system with patchy colloids with a hard core with a Density Functional Theory. The hard-core is implemented by using a variant of the Fundamental Measure Theory [4] that probably is the best mean field approach to hard particles.

While the ultrasoft particles assemble in cluster quasicrystals where the particles can completely overlap, in case of hard cores we observe structures that are rather dominated by the tiles that occur on a local level. Our results explain the differences between quasicrystlas that occur in different systems.

[1] Lifshitz, Petrich, PRL 79, 1261 (1997).

[2] Achim et al., PRL 112, 255501 (2014).

[3] Weigel, Schmiedeberg, Modelling Simul. Mater. Sci. Eng. 30, 074003 (2022).

[4] Rosenfeld, PRL 63, 980 (1989).

DY 44.10 Fri 12:15 H47

Beyond rings and chains: exploring porous crystals and flexible networks with magnetic colloids — •Carina Karner — Technische Universität Wien

We report on the self-assembly of magnetic colloids engineered with two distinct magnetic patches positioned at their poles, an advancement from traditional Janus particles with a single magnetic dipole. While Janus particles are known to form a variety of superstructures including chains, rings, and close-packed arrangements [1], the two-patch design significantly expands the range of achievable structures. Our simulation study reveals the formation of porous networks with adjustable flexibility, variable pore sizes, and controllable crystalline order. Notably, we observe the formation of a porous Kagome lattice, reminiscent of the experimental Kagome lattice observed colloids with two hydrophobic patches, the well known Janus-triblock system [2]. This enhanced self-assembly behavior in two-patch magnetic particles opens up further possibilities for creating fully tunable, field-responsive ferrofluids. Such systems could useful for applications requiring externally modulated viscosity, such as adaptive damping systems in automotive and aerospace engineering. [1] Vega-Bellido, G. I., DeLaCruz-Araujo, R. A., Kretzschmar, I., & Córdova-Figueroa, U. M. (2019). Self-assembly of magnetic colloids with shifted dipoles. Soft Matter, 15(20), 4078-4086. [2] Chen, Q., Bae, S. C., & Granick, S. (2011). Directed self-assembly of a colloidal kagome lattice.Nature,469(7330), 381-384.

DY 44.11 Fri 12:30 H47

Effect of geometrical confinement on friction in soft solids — •Aashna Chawla and Deepak Kumar — Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India

Soft and biological materials come in a variety of shapes and geometries. When two soft surfaces with mismatched Gaussian curvatures are forced to fit together, beautiful patterns emerge at the interface due to geometry-induced stress. In this study, we explore the effect of geometrically incompatible confinement of a thin sheet on a soft hydrogel substrate on friction. We use a novel experimental setup to measure the friction between a thin flat elastic sheet placed on a low-friction hydrogel substrate. We show that the frictional force at the interface strongly depends on the geometry and is significantly larger for the geometrically incompatible configuration of a flat sheet on a spherical substrate compared to the other two geometrically compatible configurations: flat sheet on a flat substrate and flat sheet on a cylindrical substrate. Furthermore, for the incompatible configuration of the flat sheet on a spherical substrate, we observe that the frictional force increases monotonically with the sheet radius, with a transition in the behavior at an intermediate radius. We show that these effects arise from the coupling of the stress developed in the sheet due to its geometrically incompatible confinement with the curvature of the interface, resulting in an increased normal force, thereby increasing friction. The insights gained from this study could have significant implications for our understanding of friction in various biological, nanoscale, and other soft systems.

DY 45: Quantum Chaos (joint session DY/TT)

Time: Friday 11:30–13:00 Location: H37

DY 45.1 Fri 11:30 H37

Semiclassical foundation of universality in many-body quantum circuits — •Maximilian Kieler[1], Felix Fritzsch[2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

For single particle systems the fundamental equivalence of quantum chaotic systems and random matrix theory is well-understood by means of semiclassical periodic orbit theory. We propose an extension to spatially local many-body systems by incorporating the concept of symmetry-breaking. Using this we show that random matrix behavior arises generically in quantum chaotic many-body systems in the form of a symmetry breaking of local time-translation symmetries. This general framework is applied to quantum circuits where an explicit correspondence to the random matrix result for the spectral form factor can be shown.

DY 45.2 Fri 11:45 H37

Distribution of resonance poles of chaotic scattering systems — •Jan Robert Schmidt, Florian Lorenz, and Roland Ketzmerick — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

The distribution of resonance poles of chaotic scattering systems is investigated in the semiclassical limit at unprecedented small wavelengths. For the paradigmatic three-disk scattering system, we study the spectral gap towards the real axis, the fractal Weyl law, which counts the number of resonance poles, and the distribution of decay rates. These properties are compared to previous analytical results, e.g. from random matrix theory. In contrast to this system with full escape, systems with partial escape have significantly different properties. For the example of a dielectric cavity, we show that results from random matrix theory cannot explain the distribution of decay rates.

DY 45.3 Fri 12:00 H37

Solved after 60 years: Exact Derivation of the Ericson Transition in Quantum Chaotic Scattering — •Simon Köhnes and Thomas Guhr — University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Scattering experiments are the prime source of information on the quantum world. Scattering theory nowadays has numerous applications in various branches of physics and beyond, even including classical wave phenomena. We analyze chaotic scattering systems in the framework of Random Matrix Theory. The distribution of the scattering matrix elements is the key quantity. A strong sign of chaos in complex quantum systems is the Ericson regime of strongly overlapping resonances in which the cross sections exhibit random behavior. We apply the Supersymmetry Method. For the three Wigner-Dyson symmetry classes, we analytically calculate the transition to the Ericson regime, facilitating direct comparison with experimental results. In the course of doing so, we also gather new information on features of the underlying supersymmetric non-linear sigma model.

DY 45.4 Fri 12:15 H37

Chaotic Quantum Scattering: Exact Solutions for Systems with Spin — •Nils Gluth and Thomas Guhr — Universität Duisburg-Essen, Duisburg, Germany

Scattering experiments facilitate access to quantum systems. Scattering theory is needed to fully describe the involved experimental situations. Over the years, it became a powerful tool with applications to a large variety of different systems, such as for example compound nuclei, atoms, molecules, quantum graphs or even microwave networks and cavities. These systems are typically complex or in a broad sense chaotic, calling for statistical approaches, in particular Random Matrix Theory. Considerably extending our previous work, we calculate the distribution of scattering matrix elements and cross sections using Supersymmetry. We focus on the symplectic symmetry class which had not yet been solved, because a theoretical understanding is needed in view of recent experiments. We provide a comparison of our results with experimental data.

DY 45.5 Fri 12:30 H37

Phase-space representations and exceptional points of coupled polarized modes in cylindrical cavities — •Tom Rodemund[1], Shilong Li[2], Síle Nic Chormaic[3], and Martina Hentschel[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]College of Information Science and Electronic Engineering, Zhejiang University, Hangzhou, China — [3]Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

Optical microcavities are often assumed to be two-dimensional (2D). This allows a convenient phase-space representation in 2D, where Poincaré surface of section for particle dynamics and the Husimi function for their wave counterpart are prominent methods. Here we extend the concept of Husimi functions for open systems [1] to three-dimensional (3D) optical microcavities of arbitrary

shape. In particular we study deformed cylindrical cavities and illustrate their mode dynamics in terms of generalized Husimi functions.

The coupling between the two different polarizations (TE and TM) is a new feature in realistic 3D optical cavities that is not present in 2D. We find the interaction of polarized modes to be governed by a network of exceptional points that reflects the openness, or non-Hermiticity, of the system. The mode coupling is analyzed using the extended Husimi formalism that we find to be a comprehensive and useful way to represent the mode structure of 3D microcavities [2].

[1] Hentschel et al., Europhys. Lett. 62 636 (2003)

[2] Rodemund et al., to be submitted.

DY 45.6 Fri 12:45 H37

The classical Maldacena-Shenker-Standford bound — •Gerrit Caspari, Fabian Haneder, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Regensburg, Deutschland

The Maldacena-Shenker-Stanford (MSS) bound [1] is a condition on a system's quantum Lyapunov exponent, defined as half the growth rate of the regularised out-of-time-ordered correlator (OTOC), which states that said exponent is bounded by the system's temperature, with, e.g., black holes as characteristic systems saturating the bound.

From the perspective of classical chaos, this is surprising, since the classical Lyapunov exponent seems not to be bounded. We study chaotic quantum systems in a hyperbolic geometry with and without cusps and magnetic fields [2][3] via Selberg's Trace Formula (STF). Through this we derive bounds on the classical Lyapunov exponent from analyticity conditions in the trace formula and relate them to the MSS bound.

We report our progress in studying these bounds using the STF, which entails an investigation of the analyticity condition needed to prove the STF for the partition function of our systems and its relation to possible phase transitions.

[1] Maldacena, J., Shenker, S.H. & Stanford, J. High Energ. Phys. 2016, 106 (2016).

[2] Aurich, R., & Steiner, F. (1992)., Proceedings: Mathematical and Physical Sciences, 437(1901), 693-714

[3] Avron, J.E., Klein, M. & Pnueli, A., Phys. Rev. Lett. 69 (1992)

DY 46: Statistical Physics of Biological Systems II (joint session DY/BP)

Time: Friday 11:30–13:00 Location: H43

Invited Talk DY 46.1 Fri 11:30 H43

Equilibrium and non-equilibrium dynamics of biological systems with memory — •Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin

Biological systems are many-body systems. Thus, their dynamics, when described in terms of a low-dimensional reaction coordinate, is governed by the generalized Langevin equation (GLE), an integro-differential equation of motion which contains friction memory [1]. Two examples will be discussed:

Protein-folding kinetics is standardly described as Markovian (i.e., memoryless) diffusion in a one-dimensional free-energy landscape. By analysis of molecular-dynamics simulation trajectories of fast-folding proteins the friction is demonstrated to exhibit significant memory with a decay time of the same order as the folding and unfolding times [2,3,4]. Memory friction leads to anomalous and drastically modified protein kinetics: the folding and unfolding times are not dominated by free-energy barriers but rather by non-Markovian friction.

Active motion of organisms obviously is far from equilibrium. The parameters of an appropriate non-equilibrium GLE are extracted from trajectories. It is demonstrated that the motion of single-cellular algae is characterized by pronounced memory friction, which allows to classify and sort individual cells.

[1] Memory and Friction: From the Nanoscale to the Macroscale, BA Dalton, A Klimek, H Kiefer, F N Brünig, H Colinet, L Tepper, A Abbasi, RR Netz, https://arxiv.org/pdf/2410.22588

DY 46.2 Fri 12:00 H43

Mean transient drift of synaptic weights in feed-forward spiking neural networks with spike-timing-dependent plasticity — •Jakob Stubenrauch and Benjamin Lindner — BCCN Berlin and Physics Department HU Berlin, Germany

Spike-timing dependent plasticity (STDP) [1] is a phenomenological model for the dynamics of single synaptic weights. This concise microscopic (single-synapse) description allows for the derivation of macroscopic network theories, capturing for instance learning, forgetting, and representational drift.

For the development of such theories it is important to characterize the stochastic process of synaptic weights. Early attempts capture this process for Poissonian presynaptic spikes and conditionally Poissonian postsynaptic spikes [2]. However, since STDP depends on fine spike-timing differences below 20 ms [1], it is important to characterize the synaptic dynamics for neuron models that describe the fast response mechanistically.

Leveraging a recent theory [3] as well as established results for the leaky integrate-and-fire neuron [4,5], we analytically compute the drift and diffusion of feed-forward synapses in a setup where a layer of presynaptic Poisson processes feeds into a recurrent network of leaky integrate-and-fire neurons.

[1] Bi and Poo, J. Neurisci. (1998) [2] Kempter et al., Phys. Rev. E (1999) [3] Stubenrauch and Lindner, Phys. Rev. X (2024) [4] Brunel et al., Phys. Rev. Lett. (2001) [5] Lindner and Schimansky-Geier, Phys. Rev. Lett. (2001)

DY 46.3 Fri 12:15 H43

A Biophysical Model for Temperature-Sensitivity of Neurons — •Julian Voits[1], Wojciech Ambroziak[2,3], Jan Siemens[2,4], and Ulrich S. Schwarz[1,5] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]Department of Pharmacology, University of Heidelberg, Germany — [3]Department of Translational Disease Understanding, Grünenthal GmbH, Aachen, Germany — [4]Molecular Medicine Partnership Unit (MMPU), European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [5]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

Control of body temperature is essential for our well-being and especially important during periods of fever or heat acclimation, e.g. due to traveling or climate change. An essential element of body temperature control are temperature-sensitive neurons, particularly warm-sensitive ones in the preoptic area of the hypothalamus. Since the discovery of temperature-sensitive ion channels, it has become clear that the underlying molecular mechanisms are rather diverse. In this work, we introduce a mathematical model based on a reduced version of the Hodgkin-Huxley model that can predict the frequently observed linear dependence of spiking rates on temperature in warm-sensitive neurons. Additionally, we present data showing how neurons adapt to varying temperatures over time, along with evidence of hysteresis in many temperature-sensitive neurons.

DY 46.4 Fri 12:30 H43

Position-Dependent Non-Markovian Effects Improve Protein Folding Simulations — •Lucas Tepper, Cihan Ayaz, Benjamin Dalton, and Roland Nezt — Freie Universität Berlin

It's common to project a protein's full atomic resolution onto a one-dimensional reaction coordinate to capture key aspects of its folding process. As a direct consequence of this dimensionality reduction, non-Markovian memory effects emerge. Accounting for memory effects in the framework of the generalized Langevin equation (GLE) with linear friction has proven efficient, accurate and insightful. However, recent advances in deriving GLEs with non-linear, position-dependent friction kernels raise questions about their applicability to protein folding simulations. We derive a novel method to extract position-dependent friction kernels from time series data via conditional Volterra equations. When applied to two protein test systems, the position- and time-dependent friction is strongest for long memory times in the folded states, where atoms are tightly packed. Additionally, we propose a novel and numerically efficient GLE simulation setup, confirming the accuracy of the extracted kernels. Compared to linear friction GLE simulations, our results show that position-dependent non-Markovian effects are critical for accurately reproducing protein folding kinetics when using low-dimensional reaction coordinates.

DY 46.5 Fri 12:45 H43

Multicomponent mixtures exhibit a vast nucleation-and-growth regime — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Phase coexistence is crucial for understanding how cells regulate biomolecular condensates. Despite of the multicomponent and multiphase nature of such condensates, the direct study of coexisting phases is limited to only few components since the parameter space is high-dimensional. So far, no theory provides a direct and concrete estimation of the phase coexistence behavior of multicomponent mixtures. As a first-level description of multicomponent phase behavior, we derive scaling relations for the number of coexisting phases in typical multicomponent mixtures in equilibrium. The scaling relations reveal that the interactions required to have many coexisting phases only scales very weakly with the number of components, whereas the stability analysis of the homogeneous state suggests a much stronger scaling. This discrepancy implies that large parts of the phase diagram of multicomponent mixture are in the nucleation-and-growth regime, where the homogeneous state is locally stable while multiple coexisting phases are preferred energetically. This suggests that multicomponent mixtures can achieve versatility and controllability in phase behavior with moderate interactions, which might be utilized by cells to create or destroy biomolecular condensates.

DY 47: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H2

Invited Talk DY 47.1 Fri 13:15 H2

Active control of forces, movement and shape: from biological to non-living systems — •Ulrich S. Schwarz — Heidelberg University, Heidelberg, Germany

Animal cells are highly dynamic and continuously generate force, for example for division, migration and mechanosensing. Their main force generators are myosin II molecular motors, whose activity is precisely controlled by biochemical circuitry. We first discuss how this system can be hijacked by optogenetics, thus that cellular force generation can be controlled in time and space using light. Next, we use active gel theory combined with van der Waals theory for myosin II molecules to demonstrate that cell contractility is sufficient to explain cell migration and that optogenetics can be used to initiate and revert migration. For two myosin II species, we predict the possibility of oscillations. We then move up in scale and analyze force generation in intestinal organoids, which are epithelia with the topology of a sphere. Combining experimental data, image processing and the bubbly vertex model, we show how apico-basal asymmetries can lead to cell extrusion and budding. We finally discuss how force generation and shape changes can be achieved in non-living systems, in particular for nematic elastomers, in which the direction of contraction is imprinted during polymerization and actuation is achieved by temperature control.

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Overview of Invited Talks and Sessions

(Lecture halls H13, H14, H15, and H17; Poster P1 and P3)

Invited and Prize Talks

HL 3.1	Mon	9:30–10:00	H17	**Alexandria Database - Improving machine-learning models in materials science through large datasets** — •Jonathan Schmidt, Tiago Cerqueira, Aldo Romero, Silvana Botti, Miguel Marques
HL 3.2	Mon	10:00–10:30	H17	**Generative Models on the Rise - Which one shall I pick for my Inverse Design Problem?** — •Hanna Türk, Elisabetta Landini, Christian Kunkel, Patricia König, Christoph Scheurer, Karsten Reuter, Johannes Margraf
HL 3.3	Mon	10:30–11:00	H17	**Machine-learning accelerated prediction of two-dimensional conventional superconductors** — Thalis H. B. da Silva, Théo Cavignac, Tiago F. T. Cerqueira, •Haichen Wang, Miguel A. L. Marques
HL 3.4	Mon	11:15–11:45	H17	**Machine Learning for Design, Understanding, and Discovery of (Semiconducting) Materials** — •Pascal Friederich
HL 3.5	Mon	11:45–12:15	H17	**OptiMate: Artificial intelligence for optical spectra** — •Malte Grunert, Max Grossmann
HL 18.1	Tue	9:30–10:00	H17	**Ultrafast Nano-Spectroscopy of Photo-Induced Dynamics in Low-Dimensional Materials** — •Takashi Kumagai
HL 18.2	Tue	10:00–10:30	H17	**Landau level Nanoscopy of charge and heat transport in low-dimensional heterostructures** — •Mengkun Liu
HL 18.3	Tue	10:30–11:00	H17	**Real space mapping of electrically tunable anisotropic THz plasmon polaritons in hBN encapsulated black phosphorus** — •Eva Pogna
HL 18.4	Tue	11:15–11:45	H17	**Ultra-confined THz hyperbolic phonon polaritons in a transition metal dichalcogenide** — Ryan A. Kowalski, Niclas S. Mueller, Gonzalo Alvarez-Perez, Maximilian Obst, Katja D. Granados, Giulia Carini, Aditha Senarath, Saurabh Dixit, Richarda Niemann, Ragu B. Iyer, Felix Kaps, Jakob Wetzel, J. Michael Klopf, Ivan I. Kravchenko, Deliang Bao, Sokrates T. Pantelides, Martin Wolf, Lukas Eng, Pablo Alonso-Gonzalez, Susanne Kehr, Thomas G. Folland, •Alexander Paarmann, Joshua D. Caldwell
HL 18.5	Tue	11:45–12:15	H17	**Programmable polariton nanophotonics using phase-change materials** — •Thomas Taubner
HL 30.1	Wed	9:30–10:00	H13	**Exploring semiconducting epigraphene grown by polymer-assisted sublimation growth** — •Teresa Tschirner, Julia Guse, Stefan Wundrack, Frank Hohls, Klaus Pierz, Hans Werner Schumacher
HL 30.2	Wed	10:00–10:30	H13	**Huge Enhancement of the Giant Negative Magnetoresistance with Decreasing Electron Density** — •Lina Bockhorn, Christian Reichl, Werner Wegscheider, Rolf J. Haug
HL 30.3	Wed	10:30–11:00	H13	**Ultrafast quantum optics with single-photon emitters in 2D materials** — •Steffen Michaelis de Vasconcellos
HL 30.4	Wed	11:15–11:45	H13	**Realistic simulation of quantum emitter dynamics made easy** — •Moritz Cygorek
HL 30.5	Wed	11:45–12:15	H13	**Data-driven Design of Next Generation 2D Materials and Their Heterostructures** — •Rico Friedrich
HL 34.1	Wed	9:30–10:00	H17	**From complex internal dynamics to emission characteristics control in quantum billiards** — •Martina Hentschel
HL 34.2	Wed	10:00–10:30	H17	**Positioning of microcavities around single emitters** — •Tobias Huber-Loyola
HL 34.3	Wed	10:30–11:00	H17	**Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities** — •Jan Wiersig

HL 34.4	Wed	11:15–11:45	H17	**Correlations and statistics in cavity embedded quantum dot sources of quantum light** — •Ana Predojevic
HL 34.5	Wed	11:45–12:15	H17	**Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum** — •Dario Ballarini
HL 42.1	Wed	16:45–17:15	H17	**Quantum key distribution with single photons from quantum dots** — Joscha Hanel, •Jingzhong Yang, Jipeng Wang, Vincent Rehlinger, Zenghui Jiang, Frederik Benthin, Tom Fandrich, Jialiang Wang, Fabian Klingmann, Raphael Joos, Stephanie Bauer, Sascha Kolatschek, Ali Hreibi, Eddy. Patrick Rugeramigabo, Michael Jetter, Simone. Luca Portalupi, Michael Zopf, Peter Michler, Stefan Kueck, Fei Ding
HL 46.1	Thu	9:30–10:00	H15	**Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System** — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, Manfred Bayer
HL 46.6	Thu	11:15–11:45	H15	**Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules** — •Annika Janssen
HL 47.1	Thu	9:30–10:00	H17	**Quantum-Dot Quantum Light Sources in Deployed Systems** — •Peter Michler
HL 47.2	Thu	10:00–10:30	H17	**Field test of semiconductor quantum light sources** — •Fei Ding
HL 47.3	Thu	10:30–11:00	H17	**Quantum dot based quantum communication in urban networks** — •Rinaldo Trotta
HL 47.4	Thu	11:15–11:45	H17	**Quantum communication protocols over a 14-km urban fiber link** — •Jürgen Eschner
HL 60.1	Fri	9:30–10:00	H17	**Constructing Artificial Matter in the Electron Microscope - Atomic Fabrication at Scale in CrSBr** — •Julian Klein
HL 60.2	Fri	10:00–10:30	H17	**Tuning the structure and magnetism in CrSBr via external pressure** — •Ece Uykur
HL 60.3	Fri	10:30–11:00	H17	**A theoretical perspective on exciton-magnon coupling and its implications** — •Akashdeep Kamra
HL 60.4	Fri	11:15–11:45	H17	**Exciton and valley properties of monolayer transition metal dichalcogenides on the van der Waals magnetic semiconductor CrSBr** — •Yara Galvao Gobato
HL 60.8	Fri	12:30–13:00	H17	**Electric field control of intra- and interlayer excitons in CrSBr** — •Nathan Wilson, Amine Ben Mhenni, Ferdinand Menzel, Alain Dijkstra, Zdenek Sofer, Jonathan Finley

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff, Matthias Florian, Frank Jahnke
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger, Julian Wiercinski, Moritz Cygorek

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

HL 1.1–1.13	Mon	9:30–13:00	H13	**Perovskite and Photovoltaics I (joint session HL/KFM)**
HL 2.1–2.13	Mon	9:30–13:00	H15	**2D Semiconductors and van der Waals Heterostructures I**
HL 3.1–3.8	Mon	9:30–13:00	H17	**Focus Session: Machine Learning of semiconductor properties and spectra**
HL 4.1–4.10	Mon	15:00–17:45	H3	**2D Materials and their Heterostructures I (joint session DS/HL)**
HL 5.1–5.12	Mon	15:00–18:00	H11	**2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
HL 6.1–6.14	Mon	15:00–18:45	H13	**Materials and Devices for Quantum Technology I**
HL 7.1–7.3	Mon	15:00–15:45	H14	**Semiconductor Lasers**
HL 8.1–8.5	Mon	15:00–16:15	H15	**2D Semiconductors and van der Waals Heterostructures II**
HL 9.1–9.6	Mon	15:00–16:30	H17	**Oxide Semiconductors I**
HL 10.1–10.9	Mon	15:00–17:15	H19	**Spin-Dependent Phenomena in 2D (joint session MA/HL)**
HL 11.1–11.10	Mon	16:00–18:45	H14	**Ultra-fast Phenomena I**
HL 12.1–12.6	Mon	16:45–18:15	H15	**Quantum Transport and Quantum Hall Effects (joint session HL/TT)**
HL 13.1–13.7	Mon	16:45–18:30	H17	**Heterostructures, Interfaces and Surfaces**
HL 14.1–14.11	Tue	9:30–13:00	H3	**2D Materials and their Heterostructures II (joint session DS/HL)**
HL 15.1–15.6	Tue	9:30–11:00	H13	**Quantum Dots and Wires: Growth and Properties**
HL 16.1–16.9	Tue	9:30–12:00	H14	**Organic Semiconductors**
HL 17.1–17.13	Tue	9:30–13:00	H15	**2D Semiconductors and van der Waals Heterostructures III**
HL 18.1–18.8	Tue	9:30–13:00	H17	**Focus Session: Nanoscale Light-matter Interaction I**
HL 19.1–19.9	Tue	9:30–13:15	H36	**Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)**
HL 20.1–20.25	Tue	10:00–12:30	P3	**Poster I**
HL 21.1–21.7	Tue	10:30–12:15	H6	**Graphene: Electronic Structure and Excitations (joint session O/HL)**
HL 22.1–22.10	Tue	10:30–13:00	H8	**2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)**
HL 23.1–23.7	Tue	11:15–13:00	H13	**Quantum Dots and Wires: Transport (joint session HL/TT)**
HL 24.1–24.3	Tue	12:15–13:00	H14	**Thermal Properties**
HL 25.1–25.8	Tue	13:30–15:30	P3	**Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)**
HL 26.1–26.5	Tue	13:30–15:30	P3	**Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
HL 27.1–27.5	Tue	13:30–15:30	P3	**Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)**
HL 28.1–28.5	Tue	14:00–15:15	H16	**Topological Insulators (joint session MA/HL)**
HL 29.1–29.96	Tue	18:00–20:00	P1	**Poster II**

HL 30.1–30.5	Wed	9:30–12:15	H13	**Focus Session: Young Semiconductor Forum**
HL 31.1–31.10	Wed	12:15–13:00	H13	**Focus Session: Young Semiconductor Forum Poster**
HL 32.1–32.6	Wed	9:30–11:00	H15	**Nitrides: Preparation and Characterization I**
HL 33.1–33.7	Wed	11:15–13:00	H15	**Nitrides: Devices**
HL 34.1–34.5	Wed	9:30–12:15	H17	**Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)**
HL 35.1–35.8	Wed	10:30–12:45	H11	**2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)**
HL 36.1–36.11	Wed	15:00–18:00	H13	**Materials and Devices for Quantum Technology II**
HL 37.1–37.2	Wed	15:00–15:30	H15	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)**
HL 38.1–38.3	Wed	15:00–15:45	H17	**Nanomechanical systems (joint session HL/TT)**
HL 39.1–39.25	Wed	15:00–18:00	P3	**Poster III**
HL 40.1–40.13	Wed	15:30–19:00	H15	**2D Semiconductors and van der Waals Heterostructures IV**
HL 41.1–41.3	Wed	15:45–16:30	H17	**Spin Phenomena in Semiconductors**
HL 42.1–42.6	Wed	16:45–18:30	H17	**Quantum Dots and Wires: Optics I**
HL 43.1–43.6	Wed	17:00–18:30	H31	**Twisted Materials / Systems (joint session TT/HL)**
HL 44.1–44.3	Wed	18:00–18:45	H13	**Focus Session: Quantum Technologies in Deployed Systems I**
HL 45.1–45.13	Thu	9:30–13:00	H13	**Perovskite and Photovoltaics II (joint session HL/KFM)**
HL 46.1–46.11	Thu	9:30–13:00	H15	**Optical Properties**
HL 47.1–47.7	Thu	9:30–12:30	H17	**Focus Session: Quantum Technologies in Deployed Systems II**
HL 48.1–48.7	Thu	9:30–12:45	H36	**Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)**
HL 49.1–49.8	Thu	10:30–12:30	H11	**2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)**
HL 50.1–50.11	Thu	15:00–17:45	H6	**2D Materials: Stacking and Heterostructures (joint session O/HL)**
HL 51.1–51.8	Thu	15:00–17:15	H13	**Transport Properties (joint session HL/TT)**
HL 52.1–52.8	Thu	15:00–17:15	H14	**Oxide Semiconductors II**
HL 53.1–53.8	Thu	15:00–17:15	H15	**2D Semiconductors and van der Waals Heterostructures V**
HL 54.1–54.8	Thu	15:00–17:15	H17	**Ultra-fast Phenomena II**
HL 55.1–55.13	Thu	15:00–18:30	H33	**Graphene and 2D Materials (joint session TT/HL)**
HL 56	Thu	17:30–19:00	H17	**Members' Assembly**
HL 57.1–57.13	Fri	9:30–13:00	H13	**Quantum Dots and Wires: Optics II**
HL 58.1–58.4	Fri	9:30–10:30	H14	**Nitrides: Preparation and Characterization II**
HL 59.1–59.8	Fri	9:30–11:45	H15	**2D Semiconductors and van der Waals Heterostructures VI**
HL 60.1–60.8	Fri	9:30–13:00	H17	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)**
HL 61.1–61.4	Fri	10:45–11:45	H14	**THz and MIR physics in semiconductors**
HL 62.1–62.5	Fri	11:45–13:00	H15	**2D Semiconductors and van der Waals Heterostructures VII**
HL 63.1–63.5	Fri	12:00–13:15	H14	**Focus Session: Nanoscale Light-matter Interaction II**

Members' Assembly of the Semiconductor Physics Division

Thursday 17:30–19:00 H17

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2026
- Verschiedenes

Sessions

– Invited Talks, Prize Talks, Topical Talks, Contributed Talks, and Posters –

HL 1: Perovskite and Photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00 Location: H13

HL 1.1 Mon 9:30 H13

Oxygen-Mediated (0D) Cs4PbX6 Formation during Open-Air Thermal Processing Improves Inorganic Perovskite Solar Cell Performance — Rafikul Ali Saha[1], •Wei-Hsun Chiu[2], Giedrius Degutis[1], Peng Chen[3], Matthias Filez[4], Eduardo Solano[5], Nikolai Orlov[6], Francesco De Angelis[7], Carlo Meneghini[7], Christophe Detavernier[4], Sawanta S. Mali[8], Minh Tam Hoang[2], Yang Yang[2], Erik C. Garnett[9], Lianzhou Wang[3], Hongxia Wang[2], Maarten B. J. Roeffaers[1], and Julian A. Steele[3] — [1]KU Leuven, Belgium — [2]Queensland University of Technology, Brisbane, Australia — [3]The University of Queensland, Brisbane, Australia — [4]Ghent University, Belgium — [5]ALBA synchrotron, Barcelona, Spain — [6]AMOLF, Amsterdam, The Netherlands — [7]Roma Tre University, Rome, Italy — [8]Chonnam National University, Gwangju, South Korea — [9]University of Amsterdam, The Netherlands

We highlight the beneficial role of ambient oxygen during the open-air thermal processing of metastable γ-CsPbI3-based perovskite thin films and devices. Physiochemical-sensitive probes elucidate oxygen intercalation and the formation of Pb-O bonds in the perovskite, entering via iodine vacancies at the surface, creating superoxide (O2-) through electron transfer reactions, which drives the formation of a zero-dimensional (0D) Cs4PbI6 protective capping layer during annealing (>330˚C). Applied to γ-CsPbI2Br perovskite solar cells, it boosts the operational stability and photo-conversion efficiency of champion devices from 12.7% to 15.4% when annealed in dry air.

HL 1.2 Mon 9:45 H13

Compositional Engineering of Mixed-Metal Chalcohalides for Photovoltaic Applications — •Pascal Henkel[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, P.O.Box 11100, 00076 AALTO, Finland — [2]School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China — [3]Technical University of Munich, 85748 Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaic's [1], that could overcome the stability and toxicity problems of halid perovskites [2], and still deliver high conversion efficiencies [3]. Compositional engineering enables the optimization of MMCH materials properties en route to commercialization.

We study the stability of MMCH alloys for three different compositional positions: the M(III), the Ch and the X site. We use a combination of density functional theory and machine learning to explore the compositional space of the alloys [4] and to compute their convex hulls. For x site alloying, for example $[Sn_2InS_2(Br_{1-c}I_c)_3]$, we obtained stable structures for $c = \frac{1}{3}$ and $c = \frac{2}{3}$ for the $Cmcm$ phase and for $c = \frac{1}{6}$ and $c = \frac{1}{3}$ for the $Cmc2_1$ phase, but not for $P2_1/c$. The energetically favored structures (at $c = \frac{1}{3}$) are highly symmetrical and exhibit a layered pattern. Every third halogen layer is fully occupied by iodine whereas the other two layers are filled with bromine.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Z. Anorg. Allg. Chem.* **468**, 91-98 (1980), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Phys. Rev. Materials* **6**, 113801 (2024).

HL 1.3 Mon 10:00 H13

Versatile Two-Step Process for Enhanced Stability and Efficiency in Perovskite Top Cells for Tandem Photovoltaics — •Ronja Pappenberger[1,2], Roja Singh[1,2], Alexander Diercks[2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany

To achieve highly efficient 2T perovskite/silicon (Si) tandem solar cells (TSCs), textured-front Si bottom cells provide superior light-harvesting capabilities, making higher short-circuit current densities of TSC possible. A promising approach to fabricating uniform, high-quality perovskite films on these textured Si cells is the solution-based two-step method. One of the main challenges for perovskite solar cells (PSCs) remains their long-term stability. While methylammonium (MA)-based PSCs have demonstrated some of the highest efficiencies, their instability continues to pose a major obstacle. In this work, a versatile two-step process is employed – replacing MA with formamidinium – which maintains high efficiency, improves open-circuit voltage and enhances stability. A further performance boost is achieved by implementing a dual passivation strategy using $PDAI_2$ and BAI for bulk and surface passivation. This leads to a stable power output exceeding 20.8% for E_g = 1.67 eV due to reduced non-radiative recombination at the perovskite/ETL interface and improved film crystallization, enhancing charge carrier extraction. The long-term stability is also distinctly improved. When implemented on textured Si bottom cells, this process delivers efficiencies exceeding 24% for lab-scale monolithic perovskite/Si TSCs with a 1 cm^2 active area.

HL 1.4 Mon 10:15 H13

Recombination at grain boundaries in Cd(Te,Se) thin films in comparison with other photovoltaic absorber layers — •Luka Blazevic[1], Sebastian Weitz[1], Elisa Artegiani[2], Alessandro Romeo[2], and Daniel Abou-Ras[1] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Universita di Verona, Italy

The role of grain boundaries on the device performance is of concern for all polycrystalline absorbers in photovoltaic solar cells. In the present work, recombination velocities s_{GB} at grain boundaries in Cd(Te,Se) thin-film absorbers were determined from cathodoluminescence (CL) intensity distributions, which were acquired together with electron backscatter diffraction (EBSD) and energy-dispersive X-ray spectroscopy (EDXS) maps. The resulting s_{GB} values exhibited ranges over several orders of magnitude (10^1–10^3 cm/s). These wide value ranges are in good agreement with those obtained on other photovoltaic absorber materials (multicrystalline Si, $Cu(In,Ga)Se_2$, $Cu_2ZnSn(S,Se)_4$). The present work suggests a model comprising the enhanced, nonradiative Shockley-Read-Hall recombination at grain boundaries as well as the upward/downward band bending (± several 10 meV) at these planar defects. This model can reproduce successfully the experimental s_{GB} values from various photovoltaic absorber materials and provides also ranges for the effective defect densities as well as their capture cross-sections at the grain boundaries. It will be shown that typical losses in the open-circuit voltage of the corresponding solar cells due to grain-boundary recombination in the absorbers are few 10 mV.

HL 1.5 Mon 10:30 H13

Microscopic origins of band-gap broadening and its relationship with Urbach tails in photovoltaic absorbers — •Daniel Abou-Ras — Helmholtz-Zentrum Berlin, Germany

The broadening of absorption edges is a general feature found in numerous semiconductors used as absorber layers for thin-film solar cells. Since this broadening gives rise to radiative losses of the open-circuit voltage, it is of importance to control the broadening by corresponding material design of the photovoltaic absorber materials. The present work provides an overview of the microscopic origins of band-gap broadening, addressing not only compositional aspects and microstrain, but also electrical and optoelectronic properties on the sub-μm scale. In addition, the Urbach energy extracted from absorptance or quantum efficiency spectra has been used broadly to quantify disorder in a material. However, up to date, it has not only not been clarified what the microscopic origins of Urbach tails are; the present contribution also shows that there is no direct correlation between the broadening of the absorption edge and the Urbach energy of a semiconductor, as verified for about 30 different photovoltaic absorbers.

HL 1.6 Mon 10:45 H13

Minimizing V_{OC} losses in high bandgap perovskite solar cells for the application in perovskite/perovskite/silicon triple-junction solar cells — •Athira Shaji[1,2], Minasadat Heydarian[1,3], Oliver Fischer[1,3], Michael Günthel[1], Orestis Karalis[4], Maryamsadat Heydarian[1], Alexander J. Bett[1], Hannes Hempel[4], Martin Bivour[1], Florian Schindler[1], Martin C. Schubert[1], Stefan W. Glunz[1,3], Andreas W. Bett[1,2], Juliane Borchert[1,3], and Patricia S. C. Schulze[1] — [1]Fraunhofer Institute for Solar Energy Systems ISE, Germany — [2]University Freiburg, Institute of Physics, Germany — [3]University of Freiburg, Department of Sustainable Systems Engineering, Germany — [4]Helmholtz-Zentrum Berlin, Solar Energy Division, Germany

The high bandgap (HBG) top cell is the main source of V_{OC} loss in perovskite/perovskite/silicon triple junction solar cells due to photoinduced phase segregation, non-radiative recombination at the perovskite bulk and interface with the charge transport layers (CTLs), as well as energetic misalignment between the perovskite layer and the CTLs. The starting point of this work was a triple-cation double-halide perovskite composition with a bandgap of 1.83 eV. By implementing a multi-faceted optimization approach, an average improvement in V_{OC} of 250 mV was achieved for HBG perovskite solar cells. Replacing the reference HBG perovskite with the optimised top cell in perovskite/perovskite/silicon triple-junction solar cells results in the improvement of V_{OC} by 124 mV, and the champion device achieves a voltage above 3 V.

15 min. break

HL 1.7 Mon 11:15 H13

The Effect of Overdamped Phonons on the Fundamental Band Gap of Perovskites — •Xiangzhou Zhu and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Different from conventional semiconductors, halide perovskites (HaPs) exhibit unique anharmonic fluctuations that strongly influence optoelectronic properties. Recent studies have shown that in specific temperature regimes, the strong phonon-phonon interactions in HaPs lead to overdamped phonons, where vibrational lifetimes drop below one oscillation period. However, the relationship between these overdamped phonons and atomic fluctuations, as well as their impact on optoelectronic properties, are not fully understood. Here, using molecular dynamics (MD) simulations and augmented stochastic Monte Carlo methods that account for phonon renormalization and imaginary modes, we contrast the band gap behavior of two anharmonic perovskite materials, $SrTiO_3$ and $CsPbBr_3$, of which only the latter exhibits overdamped phonons.[1] Our results show that the overdamped phonon dynamics in $CsPbBr_3$ drive slow atomic fluctuations that are not adequately captured by conventional phonon quasiparticle descriptions. Importantly, we show that these overdamped phonon lead to significant renormalization of the band gap. Our work disentangles the consequences of anharmonic effects on the optoelectronic properties and electron-phonon interactions in perovskites.

[1] Zhu, X. & Egger, D. A. arXiv:2406.05201 (2024).

HL 1.8 Mon 11:30 H13

Polymorphism at surface in $CsPbI_3$ from first principles — •Jasurbek Gulomov[1], Guido Roma[1], Jacky Even[2], and Marios Zacharias[2] — [1]Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif sur Yvette, 91191, France — [2]Université Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

Halide perovskites show great potential for optoelectronics and photovoltaics, but challenges with ion migration and phase stability remain.Atomic-scale phenomena at surfaces and interfaces must be understood to block ion migration and enhance passivation. A peculiar property of these materials is the tendency to gain energy by disordered structural distortions, dubbed polymorphism, in contrast to the view of a perfectly symmetric monomorphous structure. Using first-principles calculations, we investigate the electronic and structural properties of polymorphous bulk $CsPbI_3$ and its 100 surface with two terminations. For the bulk, we generate a dynamically stable polymorphous structure for the cubic high-temperature phase using the method recently proposed by M. Zacharias et al. [1]. The energy gain and band gap opening are essentially linked to the increased average length of Pb-I bonds. Then we extend the concept of polymorphism to the surface, analyzing surface dipoles and work functions by comparing monomorphous and polymorphous slabs with experimental data. Our results tend to confirm the occurrence of polymorphism at surfaces in $CsPbI_3$.

[1] Zacharias, M., et al., npj Comput. Mater. 9, 153 (2023).

HL 1.9 Mon 11:45 H13

Benchmarking approximations for the theoretical prediction of positron lifetimes in halide perovskites — Kajal Madaan[1], •Guido Roma[1], Jasurbek Gulomov[1], Pascal Pochet[2], Catherine Corbel[3], and Ilja Makkonen[4] — [1]Université Paris-Saclay, CEA, Service de recherches en Corrosion et Comportement des Matériaux, SRMP, 91191 Gif sur Yvette, France — [2]Department of Physics, IriG, Univ. Grenoble-Alpes and CEA, Grenoble, France — [3]LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, 91120, France — [4]Department of Physics, University of Helsinki, P.O. Box 43, FI-00014 Helsinki, Finland

Positron annihilation spectroscopy is a well recognized tool for probing vacancies in materials. Recent applications of this technique to $APbX_3$ halide perovskites are sparse, and the rare theoretical predictions of positron lifetimes in these materials, published in association with experiments, do not fully agree with each other. These works suggest that vacancies on the A site are not detected. In our theoretical study we thoroughly revisit and compare several approximations for the electron-positron correlation functional, applied to methylammonium lead iodide ($MAPbI_3$) and $CsPbI_3$ and their vacancies. The discrepancies between the approaches make it difficult to unequivocally exclude the presence of methylammonium vacancies in $MAPbI_3$. Moreover, when using a truly nonlocal electron-positron correlation functional, the predicted positron density in a vacancy presents peculiar features and a much lower binding energy to the vacancy with respect to semilocal approximations.

HL 1.10 Mon 12:00 H13

Dynamics of electronic surface states in halide perovskites using machine-learning force fields — •Frederico Delgado[1], Frederico Simões[1], Waldemar Kaiser[1], Leeor Kronik[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The photovoltaic performance exhibited by bulk halide perovskites (HaPs) hinges on their excellent optoelectronic properties, which have been extensively investigated. Nonetheless, extended defects like surfaces are ubiquitous, and as such, their impact on such properties requires further, careful investigation. Rigorous examination of dynamics in this context through ab-initio molecular dynamics implies large computational costs, which are here circumvented by the use of machine learning (ML) force fields. In this study, we demonstrate the transient and shallow nature of surface states in $CsPbBr_3$. We shed light on the mechanisms which underpin the behaviour of such states through the framework of local, internal dipoles. Our results aid in rationalizing the benign nature of surfaces in $CsPbBr_3$, and further the understanding of the correlation between structural dynamics and optoelectronic properties of HaP surfaces.

HL 1.11 Mon 12:15 H13

Comprehensive High-Throughput DFT Study of Intrinsic Defects and Dopability in p-type Zn3P2 for Photovoltaic Applications — •Nico Kawashima[1,2,3] and Silvana Botti[1,3] — [1]Ruhr-Universität, Bochum, Germany — [2]Friedrich-Schiller-Universität, Jena, Germany — [3]RC FEMS, Bochum, Germany

Zn_3P_2 has attracted significant interest as a thin-film absorber material for photovoltaic applications due to its intrinsic p-type conductivity and earth-abundant constituents. However, the nature of the dominant native defects – whether phosphorus interstitials (P_i) or zinc vacancies (V_{Zn}) – remains a subject of debate, with implications for the material's electronic structure and dopability through mechanisms such as Fermi-level pinning and defect compensation.

We perform a high-throughput density functional theory (DFT) analysis to systematically investigate both intrinsic point defects and potential extrinsic dopants. By resolving the ground-state configurations and formation energies of key native defects, we provide a clearer understanding of their impact on the electronic landscape. This insight is then applied to evaluate a range of extrinsic dopants, predicting their incorporation and activation potentials in the presence of native defects.

Our study offers a comprehensive framework that links intrinsic defect behavior with extrinsic doping strategies, providing critical guidance for tuning the electrical properties of Zn_3P_2. The findings present experimentally actionable insights that can drive the optimization of Zn_3P_2 for next-generation photovoltaic devices.

HL 1.12 Mon 12:30 H13

Density functional theory study of hydrogen passivation mechanisms in defective silicon — •Hania Azzam[1], Tobias Binninger[1], and Michael Eikerling[1,2] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Silicon heterojunction (SHJ) solar cells offer high-effeciency energy conversion, with reported efficiencies up to 27%. Their performance and durability depend on effective passivation of dangling bonds at the amorphous/crystalline silicon interface, where electron-hole recombination reduces efficiency. Hydrogen atoms play a crucial role in passivating those dangling bonds, minimizing recombination loses. Recent experimental studies by IMD-3 at Forschugnszentrum Jülich showed performance improvements after light soaking, a process where solar cells are exposed to intensive light at elevated temperatures. It is hypothesized that light soaking activates hydrogen migration toward defect sites. This theoretical study explores hydrogen passivation mechanisms in defective silicon for SHJ solar cells. Using Density Functional Theory (DFT), we analyze how silicon vacancies alter the electronic structure of Si-H systems, introducing localized defect states within the band gap and shifts in Fermi level, and subsequently investigate the changes induced by hydrogen passivation. These insights contribute to understanding the beneficial effects of light soaking on SHJ solar cells.

HL 1.13 Mon 12:45 H13

First principles theory of nonlinear long-range electron-phonon interaction — •Matthew Houtput[1,2], Luigi Ranalli[2], Jacques Tempere[1], and Cesare Franchini[2] — [1]University of Antwerp, Belgium — [2]University of Vienna, Austria

Electron-phonon interactions in a solid are crucial for understanding many interesting material properties, such as transport properties and the temperature dependence of the electronic band gap. For harmonic materials, the linear interaction process where one electron interacts with one phonon is sufficient to quantitatively describe these properties. However, this is no longer true in anharmonic materials with significant electron-phonon interaction, such as quantum paraelectrics and halide perovskites. Currently, the only available models for nonlinear electron-phonon interaction are model Hamiltonians, written in terms of phenomenological parameters. Here, we provide a microscopic semi-analytical expression for the long-range part of the 1-electron-2-phonon matrix element, which can be interfaced with first principles techniques. We show that

unlike for the long-range 1-electron-1-phonon interaction, the continuum approximation is not sufficient and that the entire phonon dispersion must be taken into account. We calculate an expression for the quasiparticle energies and show that they can be written in terms of a 1-electron-2-phonon spectral function. To demonstrate the method in practice, we calculate the 1-electron-2-phonon spectral function for $KTaO_3$ from first principles. The framework in this article bridges the gap between model Hamiltonians and first-principles calculations for the 1-electron-2-phonon interaction.

HL 2: 2D Semiconductors and van der Waals Heterostructures I

The session covers the photonic properties and corresponding devices made from 2D semiconductors and van der Waals heterostructures.

Time: Monday 9:30–13:00 Location: H15

HL 2.1 Mon 9:30 H15

Probing strong electron-phonon coupling in graphene by resonance Raman spectroscopy with infrared excitation energy — •Simone Sotgiu[1,2], Tommaso Venanzi[1], Lorenzo Graziotto[1], Francesco Macheda[1], Taoufiq Ouaj[2], Elena Stellino[1], Bernd Beschoten[2], Christoph Stampfer[2], Francesco Mauri[1], and Leonetta Baldassarre[1] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

Resonance Raman spectroscopy (RRS) has been a key asset to study the interplay between electronic and vibrational properties of graphene. We report on RRS measurements with an excitation photon energy down to 1.17 eV on mono (MLG) and bilayer (BLG) graphene, to study how low-energy carriers interact with lattice vibrations. Thanks to the excitation energy close to the Dirac point, we unveil in the MLG a giant increase of the intensity ratio between the double-resonant 2D and 2D* Raman peaks with respect to graphite [1]. In BLG, the low excitation energy hampers some of the resonant Raman processes giving rise to the 2D peak. Consequently, the sub-features composing the 2D mode are spectrally more separated with respect to visible excitations. We compare experimental measurements on BLG with ab initio theoretical calculations and we trace back such modifications on the joint effects of probing the electronic dispersion close to the band splitting and enhancement of electron-phonon matrix elements [2]. [1] T. Venanzi et al., Phys. Rev. Lett. 2023, 130, 256901 [2] L. Graziotto et al., Nano Lett. 2024, 24, 1867

HL 2.2 Mon 9:45 H15

Nonlinear Probing of Ultrafast Bandgap Modulations in Atomically Thin Semiconductors — •Sebastian Klimmer[1,2], Thomas Lettau[3], Jan Wilhelm[4,5], Dragomir Neshev[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]ARC Centre of Excellence for Transformative Meta-Optical Systems, Department of Electronic Materials Engineering, Research School of Physics, The Australian National University, Canberra, Australia — [3]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Jena, Germany — [4]Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [5]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany

Bandgap modulations are pivotal for semiconductor based applications, typically achieved by permanent modifications of material composition or size. Recently, dynamic, ultrafast bandgap modulations have been demonstrated in transition metal dichalcogenides, exploiting the valley exclusive optical Stark (OS) and Bloch-Siegert (BS) shifts. However, their detection requires state of the art two-color pump-probe schemes. Here, we show a simplified method by measuring the second-harmonic (SH) power dependence in monolayer WSe_2. The fundamental beam (FB) blue-shifts the bandgap by OS/BS shifts, which scale linearly with intensity, resulting in a enhanced (reduced) SH signal, depending on the detuning $E_g - 2\hbar\omega_{FB}$. Our experimental data are fully explained by an analytical SBE model, which allows us to extract values for the transition dipole element and dephasing time.

HL 2.3 Mon 10:00 H15

Detecting out-of-plane polarized luminescence in TMDs with laser-written waveguide circuits — •Alina Schubert[1], Karo Becker[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Matthias Heinrich[1], and Tobias Korn[1] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]2Ferdinand Braun Institut, Leibnitz Institut für Höchstfrequenztechnik, Berlin, Germany

Photoluminescence (PL) spectroscopy is used widely to investigate the outstanding excitonic properties of two-dimensional crystals. However, since these measurements are typically performed in vertical incidence, the sample is excited with light polarized in the plane of its layer. Despite, these detection schemes systematically neglect the out-of-plane polarized components of the emitted signal that propagate along the layer and therefore are only accessible by side-on detection.

Here, a side-on detection is achieved by using femtosecond laser direct written waveguides in fused silica glass as substrates [1]. By inscribing the waveguides directly under the surface of the glass, interactions of the waveguide's evanescent field and the sample are enabled in a controlled fashion. Therefore, the sample can be excited due to its proximity to the waveguide, while, in turn, the excitonic emission can be coupled into the waveguide and subsequently be detected.

In this work, the in-plane propagating luminescence in TMDs is analyzed with a particular focus on determining influences on the signal resulting from combining TMDs and surface waveguides.

[1] A. Szameit et al., J. Phys. B.: At. Mol. Opt. Phys., 43 (2010).

HL 2.4 Mon 10:15 H15

Current-induced second-harmonic generation in monolayer graphene-devices — •Nele Tornow[1], Friederike Renz-Wieland[1], Omid Ghaebi[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

In pristine and isolated graphene, second-order nonlinear optical processes are, within the dipole approximation, forbidden due to the invariance under space inversion symmetry. Few studies have suggested that inversion symmetry can be broken by in-plane currents, leading to a measurable second-harmonic generation (SHG) [1,2]. In particular, investigations have shown that interfacial charge trapping between a monolayer graphene and silicon dioxide (SiO_2) on silicon substrate results in electrically tunable SHG when driving in-plane currents [2]. To further verify this hypothesis, we study current-tunable second-harmonic emission in two graphene based devices: one high-quality double-encapsulated hexagonal boron nitride/graphene field-effect transistor and one with a graphene-SiO_2 interface, finding SHG only in the latter one.

Our findings provide insights into the origin of current-tunable SHG and the mechanisms underlying space inversion symmetry breaking in graphene.

[1] Dean, J. et al., Appl. Phys. Lett. 26, 261910 (2009)

[2] An, Y. et al., Nano Lett. 13, 2104-2109 (2013)

HL 2.5 Mon 10:30 H15

Electron-phonon coupling across the TMD/hBN van der Waals interface — •Gianmarco Gatti[1,2], Christophe Berthod[3], Julia Issing[2], Michael Straub[2], Salony Mandloi[2], Yann Alexaniann[2], Anna Tamai[2], and Felix Baumberger[2] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland — [3]Department of Theoretical Physics, University of Geneva, Geneva, Switzerland

The lattice mismatch at van der Waals interfaces is widely used to engineer single particle band structures supporting complex quantum phases in two dimensions. Electronic states in van der Waals heterostructures may also couple to bosonic excitations in an adjacent substrate. These interfacial interactions are difficult to identify, and it is commonly assumed that they play a marginal role. Here, we reveal that quasiparticles in monolayer transition metal dichalcogenides (TMDs) are dressed by a remote cloud of phonons in the adjacent hexagonal boron nitride slab. Using angle resolved photoemission, we identify replica bands in the TMDs which are a clear fingerprint of a long-range electron-phonon interaction. We develop a modified Fröhlich model that shows quantitative agreement with the experimental spectral functions and discuss the properties of this model. Our analysis shows that remote electron-phonon coupling is a generic property of interfaces with hBN. This has implications for electron mobilities in 2D materials, for superconductivity and possibly for moiré correlated phases.

HL 2.6 Mon 10:45 H15

Polaron spectroscopy of many-body systems — •Ivan Amelio — Université Libre de Bruxelles, Brussels, Belgium

When an impurity is immersed in a many-body background, it is dressed by the excitations of the bath, and forms "a polaron".

As a result, the injection spectrum of the impurity carries the hallmarks of the correlations present in the bath. This physics is relevant for excitons optically injected in a few layer heterostructure, or for cold atomic mixtures.

In this talk, we will first review the basic theoretical framework and recent experimental progress.

Then, we will theoretically analyze a few cases of correlated many-body states: the impurity injection spectra are predicted to display peculiar features, that al-

low to distinguish whether the bath features BCS pairing, charge density waves, topological phases, the BKT transition, etc.

15 min. break

HL 2.7 Mon 11:15 H15

Ultrafast All-Optical Probe of Broken Time-Reversal Symmetry in Monolayer WSe_2 — •Paul Herrmann[1], Sebastian Klimmer[1], Thomas Lettau[1], Till Weickhardt[1], Anastasios Papavasileiou[2], Kseniia Mosina[2], Zdeněk Sofer[2], Jan Wilhelm[3], and Giancarlo Soavi[1] — [1]Friedrich Schiller University Jena, Germany — [2]University of Chemistry and Technology, Prague, Czech Republic — [3]University of Regensburg, Germany

The combination of broken space inversion and preserved time-reversal symmetry (TRS) underlies the spin-valley degree of freedom in monolayer transition metal dichalcogenides (TMDs). Introduction of an imbalance between the energy degenerate, but non-equivalent valleys (local extrema of the bandstructure) at the ±K points of the Brillouin zone breaks TRS. We probe broken TRS and a valley imbalance on ultrashort time scales by comparing the second harmonic (SH) intensity for a circularly *vs.* linearly polarized fundamental beam (FB). By numerically and analytically solving the semiconductor Bloch equations, we show that a two-photon resonant right/left circularly polarized FB interacts exclusively with the ±K valley. Thus, a circularly polarized FB probes the C_{3h} wave vector group of the ±K valleys, in contrast to a linearly polarized FB probing the D_{3h} group of the Γ point. This difference between wave vector groups at K and Γ fully captures and explains the experimentally measured deviation from the otherwise expected ratio of 2 in the circular *vs.* linear SH intensities.

HL 2.8 Mon 11:30 H15

Layer number sensitive Raman modes of atomically thin layered MoS_2 — •Henry Hübschmann[1], Gerhard Berth[1], Klaus Jöns[1], Katharina Burgholzer[2], and Alberta Bonanni[2] — [1]PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany — [2]Johannes Kepler University Linz, Linz, Austria

The material group of TMDCs like molybdenum disulfide has gained great attention in the fields of quantum technologies over the last decade due to their particular electronic and optical properties [1]. 2D-MoS_2 has found many applications in optoelectronics and photonics, where the tunable electronic band gap exhibiting strong strutural dependency is an essential feature [2]. Here Raman spectroscopy represents the method of choice for the layer number identification of such 2D structures [3].

This work deals with layer structure sensitive phonon modes of mechanically exfoliated 2D-MoS_2 utilizing Raman analysis. Regarding the two main phonon modes occuring we successfully observed corresponding Raman shifts for monolayer to nine-layer configurations showing a specific dependency on the layer number, enabling the unambiguous determination of the layer number. Besides the two dominant vibrations many other phonon modes are identified, assigned to the symmetry and analyzed in the same manner. Within our comprehensive study we found other structure sensitive phonon modes, showing specific dependency on the layer number, expanding the set of Raman modes for the investigation of 2D-MoS_2 and its properties.

HL 2.9 Mon 11:45 H15

Universal and ultrafast probe of broken time-reversal symmetry — •Florentine Friedrich[1], Paul Herrmann[1], Sebastian Klimmer[1], Zdeněk Sofer[2], Shridhar Sanjay Shanbhag[3], Jan Wilhelm[3], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [3]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Germany

Time-reversal symmetry (TRS) defines some of the most fundamental properties of condensed matter, such as the relation between energy, spin and Berry curvature, therefore influencing features like topology or non-trivial spin textures. Two-dimensional transition metal dichalcogenides (TMDs) offer the possibility to engineer TRS and space-inversion symmetry independently, rendering them excellent model systems. TRS in TMDs can be lifted *via*, *e.g.* valley-selective bandgap opening. Nonlinear optics (NLO) as a probe of TRS is non-invasive and ultrafast; however, detection *via* second harmonic generation is limited to non-centrosymmetric systems. In this work, we make the nonlinear all-optical probe of broken TRS universal by utilizing polarization-resolved third harmonic generation (THG), which is always present also in centro-symmetric crystals. As a proof of principle, we probe broken TRS in a TMD monolayer, by using elliptically polarized light, leading to valley and spin asymmetric gap opening. We then test our method on a TMD bilayer, probing broken TRS in a centrosymmetric system with THG for the first time.

HL 2.10 Mon 12:00 H15

Ultrafast pump-probe spectroscopy of WSe_2 multilayer bubbles — •Jens-Christian Drawer, Henri Melchert, Marti Struve, Christian Schneider, and Martin Esmann — Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Heterostructures of van der Waals materials have recently emerged as a versatile platform for the tailored generation and detection of coherent acoustic phonons in the GHz up to THz frequency range [1]. In this work, we investigate WSe_2 layers of different thicknesses by ultrafast pump-probe spectroscopy and observe thickness-dependent breathing-type acoustic phonon modes up to 850 GHz in frequency in the bilayer case. Under suitably chosen conditions for the dry-gel stamping preparation, 40 nm thick WSe_2 flakes form nanobubbles. For these bubbles, our pump-probe measurements reveal a significant improvement in the quality factor of their fundamental 29 GHz acoustic Fabry-Pérot mode from $Q = 13.9 \pm 0.7$ to $Q = 141 \pm 5$. We then tailor these high-Q modes by encapsulating the bubbles with hBN, introducing new spectral features attributed to coupled acoustic modes between WSe_2 and hBN. For example, our approach may enable the ultrafast modulation of strain-defined quantum emitters found in WSe_2.

[1] Yoon, Y. et al.. Nature 631, 771–776 (2024).

HL 2.11 Mon 12:15 H15

Polarized optical contrast spectroscopy of in-plane anisotropic van-der-Waals heterostructures — Ernst Knöckl[1,2], •Alexandre Bernard[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany

To properly exploit interfacial symmetry breakings in van der Waals (vdW) heterostructures, giving rise to emergent behaviors, it is crucial to determine the symmetry axes of the individual layers.

I will discuss polarized optical contrast spectroscopy as a simple and non-destructive approach to characterize the crystalline anisotropy and orientation of 2D materials in vdW heterostructures. We developed a 3D-printed motorized polarization module compatible with typical microscope platforms, allowing broadband polarization-resolved reflectance spectroscopy. We investigated the in-plane birefringence of exfoliated MoO3 thin films (optically transparent) and few-layer WTe2 crystals (semi-metallic). We compared the measured spectra to a model based on a transfer matrix formalism.

Contrasting with other polarization-sensitive approaches, such as Raman or second harmonic generation spectroscopy, this method requires orders of magnitude less excitation power densities, avoiding degradation of delicate layers. Furthermore, it allows quick and simple polarization-sensitive absorbance measurements to resolve anisotropic excitonic properties in symmetry-breaking heterostructures or anisotropic semiconductors.

HL 2.12 Mon 12:30 H15

Microscopic comparison of TMD and QW laser capabilities — •Tommy Schulz, Daniel Erben, Alexander Steinhoff, and Frank Jahnke — Institut für theoretische Physik, Bremen, Germany

The lasing capabilities of monolayer transition metal dichalcogenides (TMDs) are compared to quantum wells (QWs). For material-realistic calculations of the optical gain we connect tight-binding bandstructures for TMDs and $\vec{k} \cdot \vec{p}$ band structures for QWs and the respective interaction matrix elements with state of the art many-body theory. The semiconductor Bloch equations are solved for highly excited materials, where Coulomb interaction is treated selfconsistently on a GW level together with carrier-phonon interaction. While TMDs provide larger material gain, they also exhibit large shifts of the peak gain with increasing high excitation densitiy, thereby limiting the lasing capabilities.

HL 2.13 Mon 12:45 H15

Strong coupling between light confined in a dielectric nanocavity and excitons in a monolayer TMDC — •Frederik Schröder[1,2], Paweł Wyborski[1], Meng Xiong[1,2], George Kountouris[1,2], Battulga Munkhbat[1], Martijn Wubs[1,2], Philip T. Kristensen[1,2], Jesper Mørk[1,2], and Nicolas Stenger[1,2] — [1]Department of Electrical and Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]NanoPhoton - Center for Nanophotonics, Technical University of Denmark, Ørsteds Plads 345A, DK-2800 Kgs. Lyngby, Denmark

Enhancing light-matter interactions with optical nanocavities is essential for many applications, such as nanolasers and quantum technologies. Recently, advances in the design and fabrication of extreme dielectric confinement (EDC) cavities enabled the confinement of electromagnetic fields in InP on the tens of nanometer scale without being limited by absorption losses [1]. We demonstrate experimentally strong light-matter interactions between excitons in a single layer of $MoTe_2$ and light confined in an EDC nanocavity. The avoided crossing of the system is verified with both photoluminescence and reflection measurements. The observed Rabi-energy of 10.1 meV exceeds the averaged losses in the system [2]. These results pave the way for future studies on nonlinearities at the single-photon level [3].

[1] M. Xiong et al., *Opt. Mater. Express*, 14, 397 (2023), [2] F. Schröder et al., *in preparation*, [3] E. V. Denning et al., *Phys. Rev. Res.*, 4, L012020 (2022)

HL 3: Focus Session: Machine Learning of semiconductor properties and spectra

The focus session highlights recent advances of machine learning concepts for the characterization of semiconductors. It particularly spotlights ML-driven advances in the prediction of key semiconductor properties, such as band gaps, dielectric constants and optical spectra, which are critical for the design of next-generation energy materials.

The focus session is organized by Erich Runge (TU Ilmenau).

Time: Monday 9:30–13:00 Location: H17

Invited Talk HL 3.1 Mon 9:30 H17

Alexandria Database - Improving machine-learning models in materials science through large datasets — •Jonathan Schmidt[1], Tiago Cerqueira[3], Aldo Romero[4], Silvana Botti[2], and Miguel Marques[2] — [1]Department of Materials, ETH Zürich, Zürich, CH-8093, Switzerland — [2]Research Center Future Energy Materials and Systems of the University Alliance Ruhr and ICAMS, Ruhr University Bochum, D-44801, Bochum, Germany — [3]CFisUC, Department of Physics, University of Coimbra, Coimbra, PortugalLarga, 3004- — [4]Department of Physics, West Virginia University, Morgantown, WV, 26506, USA

Accurate machine learning models hinge on the availability of large, high-quality datasets for both training and validation - a need that is particularly acute in materials science due to the scarcity of robust datasets. To address this gap, we present Alexandria, an open-access database generated through high-throughput studies using crystal-graph-attention networks to identify novel, stable crystal structures. The database includes over five million density-functional theory calculations for periodic compounds spanning one, two, and three dimensions.

Leveraging data generated with higher fidelity exchange-correlation functionals, we also explore the effectiveness of transfer learning strategies in detail. Finally, we assess to what extent incorporating experimental data can further enhance predictions of DFT band gaps.

Schmidt, Jonathan, et al. Materials Today Physics 48 (2024): 101560.

Invited Talk HL 3.2 Mon 10:00 H17

Generative Models on the Rise - Which one shall I pick for my Inverse Design Problem? — •Hanna Türk[1,2], Elisabetta Landini[2], Christian Kunkel[2], Patricia König[2], Christoph Scheurer[2], Karsten Reuter[2], and Johannes Margraf[2,3] — [1]EPFL, Lausanne, Switzerland — [2]Fritz-Haber-Institut der MPG, Berlin, Germany — [3]Universität Bayreuth, Bayreuth, Germany

The pursuit of novel materials through computational discovery appears endless due to the vast space of potential structures and compositions. For inorganic materials, this complexity is heightened by the combinatorial possibilities presented by the periodic table, where even a single-crystal structure can theoretically exhibit millions of compositions.

Recently, generative machine learning models have emerged as method for direct exploration of the material design space. Here, we evaluate the efficacy of various conditioned deep generative models, including reinforcement learning, variational autoencoders, and generative adversarial networks, in the prototypical task of designing Elpasolite compositions with low formation energies. Utilizing the fully enumerated space of 2 million main-group Elpasolites, we rigorously assess the precision, coverage, and diversity of the generated materials. Furthermore, we develop a hyperparameter selection scheme tailored for generative models in chemical composition space. Finally, we demonstrate the power of these machine learning models on a realistic application.

[1] Chem. Mater. 2022, 34, 9455-9467.

Invited Talk HL 3.3 Mon 10:30 H17

Machine-learning accelerated prediction of two-dimensional conventional superconductors — Thalis H. B. da Silva[2], Théo Cavignac[1], Tiago F. T. Cerqueira[2], •Haichen Wang[1], and Miguel A. L. Marques[1] — [1]Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstraße 150, Bochum, Germany — [2]CFisUC, Department of Physics, University of Coimbra, Rua Larga, Coimbra, Portugal

We perform a large-scale search for two-dimensional (2D) superconductors, by using electron-phonon calculations with density-functional perturbation theory combined with machine learning models. In total, we screened over 140 000 2D compounds from the Alexandria database. Our high-throughput approach revealed a multitude of 2D superconductors with diverse chemistries and crystal structures. Moreover, we find that 2D materials generally exhibit stronger electron-phonon coupling than their 3D counterparts, although their average phonon frequencies are lower, leading to an overall lower T_c. In spite of this, we discovered several out-of-distribution materials with relatively high-T_c. In total, 105 2D systems were found with $T_c > 5$ K. Some interesting compounds, such as CuH_2, NbN, and V_2NS_2, demonstrate high T_c values and good thermodynamic stability, making them strong candidates for experimental synthesis and practical applications. Our findings highlight the critical role of computational databases and machine learning in accelerating the discovery of novel superconductors.

15 min. break

Invited Talk HL 3.4 Mon 11:15 H17

Machine Learning for Design, Understanding, and Discovery of (Semiconducting) Materials — •Pascal Friederich — Karlsruher Institut für Technologie

Machine learning can accelerate the screening, design and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on graph neural networks for property prediction [1] and understanding of structure-property relations [2], as well as on the use of machine learning for automated data analysis and autonomous decision-making in self-driving labs, especially in the area of semiconductor optimization for photovoltaics [3,4].

[1] Reiser et al., Communications Materials 3 (1) (2022), https://www.nature.com/articles/s43246-022-00315-6

[2] Teufel et al., xAI (2023), https://arxiv.org/abs/2211.13236

[3] Wu et al., JACS 2023, https://pubs.acs.org/doi/full/10.1021/jacs.3c03271

[4] Wu et al., Science 2024

Invited Talk HL 3.5 Mon 11:45 H17

OptiMate: Artificial intelligence for optical spectra — •Malte Grunert and Max Grossmann — Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Machine Learning (ML) is currently transforming computational materials science - many material properties can now be predicted to *ab initio* accuracy almost instantly using modern ML techniques. Until recently, optical properties such as absorption in the UV/VIS region were excluded from the ever-growing list of machine-learned properties, due to lack of high-quality training data for electronic excitations. To address this missed opportunity, we present OptiMate [1], a graph attention neural network trained on the largest high-quality, high-throughput dataset of optical properties available to date – a dataset that we have independently generated. OptiMate is capable of predicting the complex optical properties of a wide class of materials up to the XUV range with quantitative accuracy. In addition, OptiMate learns physical properties of spectra like continuity and causality directly from high-quality data, without such properties being enforced by constraints in the model architecture or with penalties during training. We detail the workings of OptiMate, show that it (and probably other complex models) learns a surprisingly meaningful representation of the material space, and preview current developments such as transfer learning to higher levels of theory.

[1] M. Grunert *et al.*, Phys. Rev. Mater. **8**, L122201 (2024)

HL 3.6 Mon 12:15 H17

Mechanical Properties of Hybrid Perovskites study using explainable Machine Learning — •Yuxuan Yao[1,2], Dan Han[3], and Harald Oberhofer[2] — [1]Chair for Theoretical Chemistry, Technical University of Munich — [2]Chair for Theoretical Physics VII, University of Bayreuth — [3]School of Materials Science and Engineering, Jilin University

Lead-based halide perovskite photovoltaics are of great interest for use in optoelectronic devices due to the high power conversion efficiency and low cost. 2D hybrid organic and inorganic perovskites (HOIPs) have been utilized as capping layers on top of 3D perovskites to increase the stability. On top of that, soft and stable HOIPs are an attractive material for use in flexible electronic devices. We utilize explainable machine learning (ML) techniques to accelerate the in silico prediction of elasticities of 2D perovskites, based on their Young's moduli. Our ML models allow us to distinguish between stiff and nonstiff HOIPs and to extract the materials' features most strongly influencing their elasticities. The Pb-halogen-Pb bond angle and the cations' steric effect indices (STEI) emerge as the dominant physical feature with an inverse correlation to the structural non-stiffness. The deformation of the octahedra strongly affects the material's mechanical properties, which allows us to perform the transferability test from single-layered to multi-layered 2D perovskites. Overall, our work thus points the way towards future design efforts of HOIPs with regards to their elasticity.

HL 3.7 Mon 12:30 H17

Exploring Strongly Anharmonic Thermal Insulators with Machine-Learned Interatomic Potential using an Active Learning Scheme — •Shuo Zhao, Kisung Kang, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max Planck Society

Thermal insulating semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as defect creation and phase-transition precursors [1]. These phenomena disrupt the conventional phonon picture and render perturbative methods ineffective or even incorrect for describing heat transport, leading to a substantial challenge for reliable prediction of thermal conductivity. This work presents a framework that combines the Green-Kubo formalism with machine-learned interatomic potentials, enhanced by a sequential active learning scheme [2]. Equivariant neural networks `NequIP` [3] and `So3krates` [4] are employed and systematically compared for this purpose. Based on this framework, we examine 15 materials that possibly have ultra-low thermal conductivity previously, predicted by a symbolic regression machine-learning model [5]. Our demonstrations and results not only provide precise thermal conductivity predictions for strongly anharmonic systems but also pave the way for accelerated exploration and design of novel thermal insulators.

[1] F. Knoop, *et al.*, *Phys. Rev. Lett.* **130**, 236301 (2023). [2] K. Kang, *et al.*, arXiv:2409.11808 (2024). [3] S. Batzner, *et al.*, *Nat. Commun.* **13**, 2453 (2022). [4] J.T. Frank, *et al.*, *Nat. Commun.* **15**, 6539 (2024). [5] T.A.R. Purcell, *et al.*, *Npj Comput. Mater.* **9**, 112 (2023).

HL 3.8 Mon 12:45 H17

Learning an effective Hamiltonian for large-scale electronic-structure calculations — •Martin Schwade and David A. Egger — TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale systems across various temperatures using conventional density functional theory (DFT) often encounters significant computational challenges. Recent advancements in machine learning force fields (ML-FFs) have made it easier to generate atomic trajectories at different temperatures. However, determining the electronic structure with temperature dependence remains a difficult task. Building on our earlier work involving a temperature-transferable tight-binding (TB) model [1] to learn an effective Hamiltonian, we introduce an extension of this method that leverages machine learning techniques to increase the accuracy and transferability of this approach. By integrating ML with TB models, this strategy offers a promising pathway to evaluate temperature-dependent material properties with reduced computational demands. [1] M. Schwade, M.J. Schilcher C. Reverón Baecker, M. Grumet, D. A. Egger, J. Chem. Phys. 160, 134102 (2024)

HL 4: 2D Materials and their Heterostructures I (joint session DS/HL)

Time: Monday 15:00–17:45 Location: H3

See DS 3 for details of this session.

HL 5: 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Monday 15:00–18:00 Location: H11

See O 14 for details of this session.

HL 6: Materials and Devices for Quantum Technology I

Time: Monday 15:00–18:45 Location: H13

HL 6.1 Mon 15:00 H13

First-Principles Investigation of NV Centers in Silicon Carbide Polytypes — •Timur Biktagirov, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Optically addressable spin defects in semiconductors offer versatile platforms for quantum applications, including computing, communication, and sensing. Among these, nitrogen-vacancy (NV) centers in silicon carbide (SiC) polytypes have emerged as a promising class of quantum defects, analogous to the NV center in diamond. In contrast to diamond, SiC is a technologically mature material with large-scale production capabilities, advanced doping techniques, and compatibility with CMOS fabrication methods. Additionally, the emission wavelengths of NV centers in SiC lie in the near-infrared range, making them particularly suitable for applications in single-photon emission. In this work, we discuss recent advancements in the ab initio investigation of NV centers in the 4H, 6H, and 3C polytypes of SiC. Simulating the magneto-optical properties of these spin centers, which are crucial for quantum applications, requires a detailed and accurate description of both the host material and the embedded defect. Accordingly, we demonstrate how supercell density functional theory (DFT) and recent implementations based on DFT can be employed to model key properties, including intra-defect optical transition energies, electron-electron and electron-nuclear spin interactions, and electron-phonon coupling. These theoretical insights provide a foundation for optimizing NV centers in SiC for next-generation quantum technologies.

HL 6.2 Mon 15:15 H13

tunable superconductivity in Ga-doped SixGe1-x via ion implantation and flash lamp annealing — •yu cheng[1,2], yi li[1,2], oliver steuer[1], mao wang[3], artur erbe[1,2], manfred helm[1,2], shengqiang zhou[1], and slawomir prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Laboratory of Micro-Nano Optics, College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu, PR China

Group-IV superconducting semiconductors offer promising opportunities for scalable superconductor-semiconductor platforms in quantum computing. However, realizing a superconducting phase in semiconductors requires doping concentrations beyond the metal-insulator transition (MIT). Achieving such high doping levels in silicon (Si) and germanium (Ge) is challenging due to the limited solid solubility of acceptors in these materials. Various advanced techniques have been developed to overcome this problem, such as gas immersion laser doping or ns-pulsed laser melting [1]. Here, we explore tunable superconducting states in Ga-hyperdoped SixGe1-x alloys by applying ion implantation followed by ms-range flash lamp annealing. We observed that the critical temperature depends on the Ge-concentration. Samples with the highest Ge content demonstrate the transition temperature (Tc) of 1.2 K, attributed to increased Ga solubility, while samples with 70% of Si shows Tc around 100 mK. Notably, all samples achieved carrier concentrations over solid solubility, illustrating the effects of hyperdoping on superconductivity.

HL 6.3 Mon 15:30 H13

Direct printing of microlenses on hexagonal boron nitride to improve light outcoupling — •Daniel Klenkert[1,2], Paul Konrad[2], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]1Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg

Optically active defects in hexagonal boron nitride (hBN) have attracted wide research interest in the field of quantum technology. Solid immersion lenses can be employed in order to increase light outcoupling and thus the external quantum efficiency (EQE) of such defects. These lenses are, however usually created by etching them into the surface of the host material, which makes them rather unsuitable for 2D materials such as hBN.

Here we present an alternative approach: direct printing of polymer microlenses onto hBN using the two-photon polymerization technique. This strategy is not limited to bulk crystals, but can also be applied to thin films. Using a ceramic hybrid polymer with low fluorescence and high optical transparency, hemispherical lenses were directly printed on macroscopic hBN crystals and on thin flakes to demonstrate the feasibility and EQE enhancement of this approach.

HL 6.4 Mon 15:45 H13

Dynamical reorientation of spin multipoles in silicon carbide by transverse magnetic fields — •Alberto Hernández-Mínguez[1], Alexander V. Poshakinskiy[2], Michael Hollenbach[3], Paulo V. Santos[1], and Georgy V. Astakhov[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]ICFO-Institut de Ciències Fotòniques, Castelldefels, Spain — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The long-lived and optically addressable high-spin state of the negatively charged silicon vacancy (V_{Si}) in silicon carbide makes it a promising system for applications in quantum technologies. Most studies of its spin dynamics have been performed under external magnetic fields applied along the symmetry axis of the V_{Si} center. Here, we show that the application of a weak magnetic field perpendicular to the symmetry axis leads to a non-trivial behavior of the optically detected magnetic resonances (ODMRs) caused by the dynamical reorientation of the spin multipole under optical excitation. Particularly, we observe the inversion of the quadrupole-spin polarization in the excited state and the appearance of a dipole-spin polarization in the ground state. The latter is much higher than the thermal polarization and cannot be induced solely by optical excitation. Our theoretical model reproduces well all sharp features in the ODMR spectra and shine light on the complex dynamics of spin multipoles in these kinds of solid-state systems.

[1] A. Hernández-Mínguez *et al.*, Phys. Rev. Appl. **22**, 044021 (2024)

HL 6.5 Mon 16:00 H13

The hBN defects database for quantum applications — •Chanaprom Cholsuk[1,2], Asli Cakan[1,2], Sujin Suwanna[3], and Tobias Vogl[1,2,4] — [1]Department of Computer Engineering, School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [3]Optical and Quantum Physics Laboratory, Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand — [4]Abbe Center of Photonics, Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany

Hexagonal boron nitride (hBN) has emerged as a solid-state platform for hosting a variety of defects for quantum applications. Identifying optimal defects for specific quantum applications has been challenging as some defects exhibit similar properties while others encounter strain. Comprehensive properties are therefore required. This work addresses this gap by utilizing density functional theory and open quantum system approaches to thoroughly characterize the properties of 257 defects and evaluate their potential for quantum emitter and quantum memory applications. This enables matching defects with suitable quantum applications. Furthermore, all findings are compiled into an accessible online database at https://h-bn.info, allowing one to compare our calculated optical fingerprints with experiments and other simulations. Consequently, this work enriches hBN defect resources, supporting progress in quantum technologies and defect identification.

HL 6.6 Mon 16:15 H13

Scanning NV center thermometry — Elias Sfeir[1], Maxime Rollo[1], Yoann Baron[2], Felipe Favaro de Oliveira[3], Gediminas Seniutinas[3], Marcelo Gonzàlez[3], Mathieu Mathieu[3], Patrick Maletinsky[3,4], Jean-Baptiste Jager[5], Jean-Michel Gérard[5], Vincent Jacques[1], •Aurore Finco[1], and Isabelle Robert-Philip[1] — [1]Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France — [2]Univ. Grenoble Alpes, CEA, LETI, Grenoble, France — [3]Qnami, Muttenz, Switzerland — [4]Department of Physics, University of Basel, Basel, Switzerland — [5]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, Grenoble, France

Scanning NV center microscopy relies on a single nitrogen-vacancy (NV) defect in diamond as a quantum sensor for scanning probe experiments. It is now routinely used as a powerful magnetometry technique, and its functionalities can be extended to temperature measurements by exploiting the temperature dependence of the NV electron spin resonance (ESR) frequency. In this work, we show how to simultaneously map the Joule heating and the Oersted field generated by an electrical current flowing through a semiconductor nanowire with a scanning NV center microscope. Our results highlight that the component of the magnetic field perpendicular to the NV center quantization axis competes with the effect of temperature on the NV ESR frequency, making quantitative temperature measurements challenging. Therefore, we finally propose solutions to improve the overall performances of the technique through the design of optimized diamond probes.

15 min. break

HL 6.7 Mon 16:45 H13

Luminescence of electron and ion beam irradiated hBN — •Jan Böhmer, Annkathrin Köhler, Christian T. Plass, and Carsten Ronning — Friedrich Schiller University, Jena, Germany

Defect centers in solid state materials have emerged as promising candidates for quantum emitters. Here, hexagonal boron nitride (hBN) has attracted much interest as an interesting material for the realization of room temperature single photon emitters (SPEs). Emitting defects can be specifically created by irradiation of hBN flakes and nanoparticles with (focused) electron and ion beams, which allows to modify the luminescence properties of the hBN samples and fabricate targeted localized SPEs. The effects of the irradiation on the luminescence spectrum were investigated using micro photoluminescence (μPL). The nature and applicability for SPEs were determined by $g_{(2)}$-autocorrelation measurements as a function of the irradiation parameters.

HL 6.8 Mon 17:00 H13

Strain-induced tuning of quantum emitters in hexagonal boron nitride — •Tjorben Matthes[1,2], Anand Kumar[1,2], Mohammad Nasimuzzaman Mishuk[1,2], and Tobias Vogl[1,2] — [1]Department of Computer Engineering, TUM School of Computation, Information and Technology, Technical University of Munich, 80333 Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

In this talk, we will show our recent progress in controlling the emission characteristics of our single photon emitters in hexagonal boron Nitride (hBN).

We have previously demonstrated our results on the polarisation characteristics of both the absorption and the emission characteristics of our single photon emitters. By conducting a statistical analysis of a large array of emitters, we found some unexpected results that indicate a shift of the emission axes in one direction compared to the crystal axes. We suspected a strain induced by the exfoliation process as the cause. We, therefore, conduct now further tests deliberately inducing strain into the hBN flakes in which the emitters are embedded.

HL 6.9 Mon 17:15 H13

Impact of a magnetic field on low-temperature photoluminescence of indium-doped silicon — •Kevin Lauer[1,2], Mario Bähr[1], Richard Grabs[1], Frank Long[1,3], Martin Kaleta[1], Andreas Frank[1], Thomas Ortlepp[1], Katharina Peh[2], Noah Stiehm[2], Rüdiger Schmidt-Grund[2], Dirk Schulze[2], and Stefan Krischok[2] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [3]Universität Göttingen, Göttingen, Germany

Acceptor-interstitial silicon (ASi-Sii)-defects [1] were proposed to be responsible for a gain loss in low-gain avalanche detectors (LGAD) and for an efficiency loss in silicon solar cells. Recently, it was speculated that this defect category could be relevant for silicon-based quantum technology, as well. To advance the understanding of these defects in silicon with respect to their potential use as qubits, low-temperature photoluminescence (PL) measurements are performed while subjecting the sample to magnetic fields. Silicon samples with and without indium doping were treated by a temperature quenching step to generate ASi-Sii-defects. The ASi-Sii-defect generation was done using a local laser quenching method as well as using a Bunsen burner with subsequent water quenching. As expected, the integrated PL intensity increased after this generation process. While the sample is subjected to magnetic fields, the integrated PL intensity changes significantly. Differences between samples with and without indium doping will be discussed. [1]K. Lauer et al., Phys. Status Solidi A, 219 (2022) 2200099

HL 6.10 Mon 17:30 H13

Fabrication, characterization and deformation of Si/SiGe membranes for spin qubit devices — •Lucas Marcogliese[1], Ouviyan Sabapathy[1], Rudolf Richter[2], Dominique Bougeard[2], and Lars R. Schreiber[1,3] — [1]JARA-FIT Institute for Quantum Information, Aachen, Germany — [2]University of Regensburg, Regensburg, Germany — [3]ARQUE Systems GmbH, Aachen, Germany

The energy separation between the two lowest lying energy states in silicon, known as valley splitting, has been shown to have a significant impact on dephasing times, readout and shuttling fidelities of spin qubits in Si/SiGe. Greater control over the strain tensor field may be decisive for deterministic valley splitting enhancement in the presence of alloy disorder. Here, we demonstrate the fabrication of SiGe/Si/SiGe quantum well membranes suspended by the handle wafer via wet etching. Relying on SiGe as an etch stop, the robust and reproducible process yields membranes down to micrometer thicknesses. Raman maps confirm that etching preserves epitaxial tensile strain in the quantum well. Remarkably, they reveal that the in-plane strain components generated by the cross-hatch pattern typical of Si/SiGe heterostructures on bulk substrates disappear on etched membranes. To probe their elastic properties, the membranes are stressed by loading with a profilometer stylus at room temperature. We envision the Si/SiGe membrane as a flexible scientific platform for investigating novel, advanced valley splitting enhancements techniques, required for scalable Si/SiGe quantum computing with electron spins.

HL 6.11 Mon 17:45 H13

Design and optimization of bimodal cavities coupled to multi-level quantum systems — •Oscar Camacho Ibarra, Jan Gabriel Hartel, Atzin Ruiz Perez, Sonja Barkhofen, and Klaus Jöns — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany

Photonic integrated cavities are essential building blocks for qubit-controlled switches, routers, and gates in quantum networks and quantum information

processing. These devices rely on the integration of multi-level quantum systems coupled to multiple photonic modes inside a cavity. Thus, the present work introduces a systematic workflow for the design of bimodal cavities by employing one-dimensional crossed photonic crystal nanobeam cavities with non-zero cavity lengths. By optimizing three key parameters*the periodicity, a single feature size of the hole shape, and the central cavity length*we establish a robust methodology for designing crossed nanobeam cavities. This approach supports configurations with either matching or mismatched resonance frequencies, offering flexibility for diverse quantum applications. References [1]* Mikkel Heuck, Kurt Jacobs and Dirk R. Englund. Controlled-Phase Gate Using Dynamically Coupled Cavities and Optical Nonlinearities. Phys. Rev. A 109, 062620 (2024). [2]* Luiz O. R. Solak, Daniel Z. Rossatto, and Celso J. Villas-Boas, Universal quantum computation using atoms in cross-cavity systems. Phys. Rev. A 109, 062620 (2024).

HL 6.12 Mon 18:00 H13

In Situ Defect Density Determination of Spin Defects in Hexagonal Boron Nitride — Atanu Patra[1], •Paul Konrad[2], Andreas Sperlich[2], Timur Biktagirov[3], Thinh Tran[4], Igor Aharonovich[4], Sven Höfling[1], and Vladimir Dyakonov[2] — [1]Technische Physik, Julius-Maximilians-University Würzburg, 97074 Würzburg — [2]Experimentelle Physik 6, Julius-Maximilians-University Würzburg, 97074 Würzburg — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [4]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

In recent years, the negatively charged boron vacancy (V_B^-) spin defects in hexagonal boron nitride (hBN) caught attention for their sensitivity to environmental parameters such as magnetic field, temperature, and pressure, making them ideal for quantum sensing. The optical emission from these defects, crucial for applications, depends on their density, which could -so far- not be determined directly for thin flakes. Our study identifies distinct Raman modes alongside the E_{2g} peak in defect-enriched hBN. Polarization-dependent Raman measurements reveal that these modes arise from atomic vibrations associated with the V_B^- defects. Additionally, we corroborate this result by density functional theory. We investigate the interdependent relationship between the vibronic states and defect density and obtain a universally applicable method to directly determine the absolute spin-defect density in flakes by Raman spectroscopy alone.

HL 6.13 Mon 18:15 H13

Electric-circuit realization of the Floquet-SSH-Model — •Christine Barko[2], Alexander Stegmaier[1], Alexander Fritzsche[1], Riccardo Sorbello[1], Martin Greiter[1], Hauke Brand[2], Maximilian Hofer[2], Udo Schwingenschlögl[3], Roderich Moessner[4,5], Ching Hua Lee[6], Alexander Szameit[5,7], Andrea Alù[8,9], Tobias Kiessling[2,5], and Ronny Thomale[1,5] — [1]Physikalisches Inst. (TP1), Universität Würzburg, Würzburg, Germany — [2]Physikalisches Inst. (EP3), Universität Würzburg, Würzburg, Germany — [3]Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, Dresden, Germany — [5]Würzburg-Dresden Cluster of Excellence ct.qmat, Würzburg, Germany — [6]Department of Physics, National University of Singapore, Singapore — [7]Institute of Physics, University of Rostock, Rostock, Germany — [8]Photonics Initiative, Advanced Science Research Center, City University of New York, New York, USA — [9]Physics Program, Graduate Center, City University of New York, New York, USA

We build Floquet-driven capactive circuit networks to realize topological states of matter in the frequency domain. We find the Floquet circuit network equations of motion to reveal a potential barrier which effectively acts as a boundary in frequency space. By implementing a Su-Shrieffer-Heeger Floquet lattice model and measuring the associated circuit Laplacian and characteristic resonances, we demonstrate how topological edge modes can nucleate at such a frequency boundary.

HL 6.14 Mon 18:30 H13

Erbium dopants in nanophotonic resonators — •Andreas Gritsch, Alexander Ulanowski, Stephan Rinner, Johannes Früh, Jakob Pforr, and Andreas Reiserer — Technical University of Munich, TUM School of Natural Sciences and Munich Center for Quantum Science and Technology (MCQST), 85748 Garching, Germany

Optically addressable spin qubits are pristine candidates for large-scale quantum networks [1] and modular quantum computing architectures [2]. Erbium dopants are the only emitter with a coherent optical transition in the minimal-loss-band of optical fibers. In silicon, erbium integration is compatible with industrial-grade nanofabrication processes [4]. In nanophotonic resonators efficient spin-photon interfaces can be realized, in which about ten single dopants can be resolved with Purcell enhancement up to 177. Their spin state can be initialized and read out with a combined fidelity of 87%. This spin further exhibits a second-long lifetime and a Hahn-echo coherence time of 48 s [4]. We further investigate the optical coherence and the spectral multiplexing capabilities in our silicon devices, which allows a detailed comparison to our experiments with YSO membranes integrated into Fabry-Perot resonators [5].

[1] A. Reiserer, Rev. Mod. Phys. 94, 041003 (2022). [2] S. Simmons, PRX Quantum 5, 010102 (2024). [3] S. Rinner, et al., Nanophotonics 12 (2023). [4] A. Gritsch, et al., arXiv:2405.05351 (2024), Nat. Commun., (in press). [5] A. Ulanowski, et al., Advanced Optical Materials 12 (2024).

HL 7: Semiconductor Lasers

Time: Monday 15:00–15:45 Location: H14

HL 7.1 Mon 15:00 H14

Development and Analysis of a VECSEL based on InGaAs Quantum Dots for Emissions in the Telecom O-Band — •Justus Unfried, Philipp Noack, Rebecca Rühle, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The advancement of sophisticated laser technologies for high-resolution spectroscopy and sensing applications has stimulated interest in versatile, high-performance light sources. Vertical External-Cavity Surface-Emitting Lasers (VECSELs) based on InGaAs quantum dots (QDs) are promising for emissions in the telecommunications O-band and offer broad wavelength tunability, high output power, and excellent beam quality. This study focuses on optimizing QD layers through metal-organic vapor-phase epitaxy (MOVPE), utilizing the Stranski-Krastanov growth mode, followed by laser performance characterization. To enhance QD density and emission characteristics, the gallium precursor was substituted with TEGa, exhibiting a higher decomposition rate at lower growth temperatures. The indium supply was modified, and the duration of the arsine interruption following QD deposition was examined to increase density and reduce large In-clusters. Subsequently, 12 of these high-density QD layers are deposited on a distributed Bragg reflector (DBR) structure, completing the VECSEL. This laser development is accompanied by structural and performance characterizations.

HL 7.2 Mon 15:15 H14

Comparison between a 675nm and 532nm pumped 4x3 InGaAsP QW VECSEL emitting at around 760nm in a V-Shaped resonator — •Rebecca Rühle[1], Maxim Leyzner[2], Marwan Abdou Ahmed[2], Thomas Graf[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Strahlwerkzeuge, Universität Stuttgart, Pfaffenwaldring 43, 70569 Stuttgart, Germany

The quantum defect between the emission and the pump wavelengths has a substantial impact on the performance of a vertical external-cavity surface-emitting lasers (VECSEL). An increase in the wavelength of the pump laser should result in an improvement in thermal behavior and the laser performance. One disadvantage is that the pump absorption is reduced, given that the pump energy is typically below the barrier bandgap. In our previous studies, the GaInP barrier of our InGaAsP VECSEL structure was modified to absorb pump light at a wavelength of 675nm. Power measurements were conducted with a 675nm pump laser and a 532nm pump laser, employing the aforementioned adapted structure. By varying the reflectivity of the outcoupling mirror in the V-shaped resonator, we gain further insight into the absorption characteristics within the active region of the VECSEL. Due to the specifications of the laser source, the pump spot size was approximately 310μmx230μm, resulting in a multimode emission from the VECSEL rather than single mode for both pumplasers.

HL 7.3 Mon 15:30 H14

Quantum optical validation of high-β lasing in monolayer-based self-assembled photonic-defect nanocavities — •Aris Koulas-Simos[1], Chirag Palekar[1], Kartik Gaur[1], Imad Limame[1], Bárbara Rosa[1], Cun-Zheng Ning[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Teschnische Universität Berlin, 10623 Berlin, Germany — [2]College of Integrated Circuits and Optoelectronic Chips, Shenzhen Technology Univesity, Shenzhen 518118, China

Nanolasers based on transition metal dichalcogenides have garnered substantial research interest for innovative photonic applications. This study presents the

fabrication of multiple self-assembled photonic defect nanocavities within a single, fully encapsulated WSe_2 monolayer integrated into a dielectric distributed Bragg reflector (DBR) structure. Spontaneously formed bubbles during the encapsulation process lead to the generation of photonic-defect nanocavities in the DBR. These structures achieve strong optical lateral confinement and exhibit size-dependent optical characteristics, as confirmed by μPL-measurements in both the real and k-space and numerical cavity simulations. Optical power-dependent investigations conducted at cryogenic temperatures reveal lasing behavior, evidenced by a distinct kink in the input-output curve, accompanied by slight linewidth narrowing and a lineshape transition in two specific devices. Finally, photon-autocorrelation measurements performed on one of these devices provide unequivocal confirmation of a lasing transition [1].

[1] A. Koulas-Simos et al., Laser & Photonics Rev., 2400271 (2024).

HL 8: 2D Semiconductors and van der Waals Heterostructures II

The session covers the physics of emerging 2D materials.

Time: Monday 15:00–16:15 Location: H15

HL 8.1 Mon 15:00 H15

atomic and electronic structures of colloidal ultrathin PbSe nanoplatelets — •Huu Thoai Ngo[1,2], Leon Biesterfeld[3], Ahmed Addad[1], Bruno Grandidier[1], Christophe Deere[1], Jannika Lauth[3], and Louis Biadala[1] — [1]Université de Lille, CNRS, Centrale Lille, Université Polytechnique Hauts-de-France, Junia-ISEN, UMR 8520-IEMN, INRAE, UMR-8207, UMET- Unité Matériaux et Transformations, F-59000 Lille, France. — [2]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany. — [3]Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Callinstr. 3A, D-30167 Hannover, Germany

Two-dimensional (2D) PbSe nanoplatelets (NPLs) are promising materials for lighting technologies due to their efficient and tunable photoluminescence (PL), such as narrow PL emission reaching telecom bands. However, the electronic properties of single NPLs remain underexplored, limiting insights into quantum confinement effects. Here, we investigate the structural and electronic properties of ultrathin PbSe NPLs using low-temperature scanning tunneling microscopy (LT-STM). STM images confirm flat 2D morphologies at various thicknesses while tunneling spectra reveal pronounced quantum confinement along the thickness, resulting in bandgap shifts. High-angle annular dark-field scanning transmission electron microscopy confirms the rock-salt crystal structure, providing atomic-level insights. Additionally, tight-binding calculations demonstrate lateral quantum confinement effects, showing that in-plane dimensions influence electronic properties.

HL 8.2 Mon 15:15 H15

Modifying properties of 2D transition metal dichalcogenides by confined-space annealing — •Christian Tessarek, Christian Petersen, Tim Grieb, Florian F. Krause, Alexander Karg, Christian Habben, Andreas Rosenauer, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

2D transition metal dichalcogenides (TMDs) can be grown by different methods, e.g. chemical vapor or atomic layer deposition (ALD) [1]. Subsequent annealing is often applied to improve the properties of the as-grown 2D layers. Decomposition of TMD layers due to desorption of chalcogenides usually limits the temperature range. Higher annealing temperatures are possible in a chalcogene containing atmosphere but require special safety requirements of the annealing equipment.

In this study, a confined-space annealing (CSA) approach is demonstrated and realized by a close contact face-to-face sample arrangement of TMD layers on SiO_2/Si or graphene substrates. CSA is performed in vacuum or in an inert gas atmosphere without using additional chalcogene containing precursors. Such sample arrangement strongly reduces chalcogene outdiffusion from the confined space and allows annealing at higher temperatures and longer durations. The influence of CSA parameters is investigated with respect to structural and optical properties of the TMDs and compared to a standard annealing process of uncovered layers. It will also be shown that CSA can be used for conversion of MoS_2 to ternary $Mo(S,Se)_2$ and binary $MoSe_2$.

[1] C. Tessarek et al., 2D Mater. **11**, 025031 (2024).

HL 8.3 Mon 15:30 H15

Mapping the lateral homogeneity of semiconducting monolayer 2D polar Ag using spectroscopic imaging ellipsometry — •Ulrich Limberg[1], Jakob Henz[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua Robinson[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Muenster, Germany — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

2D polar metals are a novel family of atomically thin plasmonic quantum materials, which are synthesized by confinement heteroepitaxial growth (CHet)[1]. Hereby, metal atoms such as silver or gallium are intercalated between bilayer graphene and a silicon carbide substrate. In the case of 2D polar silver, a stable monolayer structure forms which has been shown to be an indirect bandgap semiconductor[2]. However, Raman imaging seems to indicate the existence of a second, possibly metallic, phase[3].

We investigated 2D polar silver samples of varying growth conditions via spectroscopic imaging ellipsometry, in order to access lateral inhomogeneities by modifications in the dielectric functions sensitive to different phases.

1 N. Briggs, et al. Nature materials 19.6 (2020): 637-643.
2 W. Lee, et al., Nano letters, 22(19) (2022): 7841-7847.
3 M. Wetherington et al., 2D Materials, 8.4 (2021): 041003.

HL 8.4 Mon 15:45 H15

Biaxial Compressive Strain Tuning of Quantum Properties in 2D Materials — •Eudomar Rafael Henriquez Guerra[1,3], Lisa Almonte[1,3], Hao Li[4], Daniel Elvira[3], Reyes Calvo[1,2,3], and Andres Castellanos Gomez[4] — [1]BCMaterials, Basque Center for Materials, Applications and Nanostructures — [2]Ikerbasque, Basque Foundation for Science — [3]Depto. de Física Aplicada, Instituto Universitario de Materiales, Universidad de Alicante — [4]2D Foundry Group, Instituto de Ciencia de Materiales de Madrid, CSIC

This study investigates the impact of biaxial compressive strain on 2D materials at cryogenic temperatures, focusing on single-layer transition metal dichalcogenides (TMDs) and multilayered NbSe2. While tensile strain has been widely explored, compressive strain at low temperatures remains underexplored, despite its potential to significantly alter quantum properties such as magnetic and superconducting phase transitions. We show that biaxial compressive strain, induced by the thermal expansion mismatch between the polymer substrates and TMDs, leads to dramatic shifts in exciton energy and gauge factors, surpassing previous compressive strain effects. Moreover, we observe a consistent reduction in the superconducting critical temperature of NbSe2 flakes, with the most pronounced changes in thinner samples. Remarkably, this effect is still noticeable even for NbSe2 flakes as thick as 86 nm. These results highlight a powerful and cost-effective method for tuning phase transitions and other quantum phenomena in 2D materials at low temperatures.

HL 8.5 Mon 16:00 H15

Two-dimensional semiconductor with tunable bandgap close to the full visible spectrum: a MOCVD study — •Nils Langlotz, Robin Günkel, Tigmanshu Sundiyal, Oliver Massmeyer, Jürgen Belz, and Kerstin Volz — Department of Physics and Material Sciences Center, Philipps-University Marburg, Germany

Two-dimensional (2D) semiconductors have attracted considerable attention due to their extraordinary thickness-dependent properties. III-VI compounds such as GaSe or GaS exhibit a unique Mexican hat band structure with a van Hove singularity near the valence band maxima (VBM) at the Γ point. Furthermore, 2D GaSe and GaS as bulk material have a direct band gap of 2.0 eV and 2.5 eV, respectively, making a dilute $GaSe_xS_{1-x}$ system a tunable LED in the visible regime. Tuning the band gap in the few layer regime is also possible, but the indirect band gap has to be overcome, which is suggested by doping. Metal organic chemical vapour deposition (MOCVD) is used for the growth of bulk GaSe, GaS and $GaSe_xS_{1-x}$ on sapphire (0001). Growth for all materials was performed in an AIX200GFR at 50 mbar at 500°C in a flow modulated growth mode where the first pulse is 30 s of the gallium species and the second pulse is 30 s of selenium or sulphur, repeated for 150 cycles for the pure crystals. For the diluted crystal the second pulse is replaced by $(30-x)$ s of selenium followed by x seconds of sulphur. The organometallic precursors used were tri-tertiary-butyl-gallium (TTBGa), di-iso-propyl-selenide (DiPSe) and tertiary-butyl-sulphide (TBS). Raman spectroscopy is used to verify the selenium/sulphur incorporation.

HL 9: Oxide Semiconductors I

Time: Monday 15:00–16:30 Location: H17

HL 9.1 Mon 15:00 H17

Nitrogen Doping of Sputtered $BiVO_4$ Thin Films — •Hannah Sassenfeld[1,2], Tsedenia Zewdie[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, D-85748 Garching, Germany

Bismuth vanadate ($BiVO_4$) is a promising photoanode material for photoelectrochemical (PEC) water splitting, given its suitable band gap (≈2.5 eV) and valence band maximum position relative to the water oxidation potential. Reducing the band gap of $BiVO_4$ can lead to a more effective utilization of the solar spectrum. One strategy towards band gap reduction is nitrogen incorporation, as previously reported by Irani et al. [1] and Kim et al. [2]. While both studies observe reduced band gaps, they do not agree on how nitrogen is incorporated into $BiVO_4$ and whether it improves or deteriorates PEC performance. To shed light onto the nature and effects of nitrogen incorporation, we use well-controlled reactive co-sputter deposition of $BiVO_4$ in nitrogen-containing environments (N:$BiVO_4$). Adjusting the amount of nitrogen in the reactive gas mixture and post-annealing treatments allow us to control the amount of incorporated nitrogen. Using this systematic sample library of N:$BiVO_4$, we interrogate the optical and structural properties of N:$BiVO_4$, its composition and electronic structure, and evaluate the impact of nitrogen incorporation on PEC performance.

[1] Irani et al. Solar RRL 4.1 (2020): 1900290. [2] Kim et al. Nature communications 6.1 (2015): 8769.

HL 9.2 Mon 15:15 H17

Plasma Plume Deflection and Target Surface Roughness During Pulsed Laser Deposition of Functional Oxides — •Jonas Elz, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Pulsed laser deposition (PLD) is a highly flexible, fast and reproducible physical vapor deposition technique that uses a pulsed laser to evaporate a target material, producing an excited laser-induced plasma. Although simple in set-up, modeling the ablation process is difficult because of its non-equilibrium nature due to the high pulse energy incident on a short time scale (20 ns laser pulse width). Ablation of any target material requires optimization of the process parameters. Some targets used in PLD develop a rough surface structure upon longer use that causes the plasma plume to deflect toward the incoming laser beam during the ablation process. Typically, the plume deflection increases until a stable surface morphology is reached. In this work, we present a comparison of the plasma plume deflection with surface roughness and morphology of different PLD targets as measured by laser scanning microscopy. A Python script is used to evaluate plume images to determine the deflection angle.

HL 9.3 Mon 15:30 H17

Analysis of film thickness distributions for combinatorial pulsed laser deposition — •Clemens Petersen, Marius Grundmann, and Holger von Wenckstern — Universität Leipzig Felix-Bloch-Institut für Festkörperphysik, Leipzig, Deutschland

Recently combinatorial deposition methods have increasingly gained scientists* attention, due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. They enable fast screening of material properties of multinary material systems using just a single sample. By employing pulsed laser deposition with our segmented target approach [1] we realized the deposition of α-$(Al_xGa_{1-x})_2O_3$ with continuous composition spread over the whole composition range on a single 2-inch sapphire wafer [2]. Accompanied by the usage of high-throughput measurements such as spectroscopic ellipsometry and X-ray diffraction, the characterization of physical properties with high chemical resolution and comparably low efforts becomes feasible.

Here we utilize a predictive numerical model, based on the corrected plasma expansion description of Anisimov *et al.* [3], for the calculation of binary growth rates of group-IIII and transition metal sesquioxides. Further the model can be applied to predict and model elemental composition and thickness distributions of ternary alloys for these materials. [1] H. von Wenckstern *et al.*, pss(b), Vol. 257, 1900626 [2] A. Hassa *et al.*, pss(b), Vol. 258, 2000394 [3] S. I. Anisimov *et al.*, Phys. rev. B, Vol 48, 12076.

HL 9.4 Mon 15:45 H17

Influence of different gate metals on α-Ga_2O_3 MESFET device performance — •Sebastian Köpp, Clemens Petersen, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

We present metal-semiconductor field effect transistors (MESFET) on α-Ga_2O_3 grown by pulsed laser deposition in a two-step process on Al_2O_3 [5]. The MESFETs exhibit high on/off ratios above 9 orders of magnitude and subthreshold swings as low as 100 mV/dec. We evaluate different gate materials in an effort to optimize device switching and breakdown behaviour.

With its ultra-wide bandgap of 5.3 eV to 5.6 eV [1,2] and a high predicted breakdown field of 10 MV/cm [3], α-Ga_2O_3 is a promising material for high-power devices, as well as deep-UV photodetectors. α-Ga_2O_3, being isostructural to aluminium oxide, allows for heteroepitaxial growth on cost-efficient sapphire substrates, and also opens up the option of α-$(Al_xGa_{1-x})_2O_3$ alloys [4], potentially pushing device performance even further.

[1] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[2] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)
[3] M. Biswas and H. Nishinaka, APL Mater. 10, 060701 (2022)
[4] J. Steele *et al.*, APL Mater. 12, 041113 (2024)
[5] S. Vogt *et al.*, Phys. Status Solidi A, 220 2200721 (2023)

HL 9.5 Mon 16:00 H17

Adsorption-controlled growth of κ-Ga2O3 — •Alexander Karg[1], Niklas Krantz[1], Manuel Alonso-Orts[1,2], Marco Schowalter[1,2], Patrick Vogt[1,3], Andreas Rosenauer[1,2], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany — [3]Max Planck Institute for solid state research, Heisenbergstraße 1, 70569 Stuttgart, Germany

The ultra-wide band gap semiconductor Ga2O3 can crystallize in at least 5 different polymorphs. For one of these, the metastable κ-Ga2O3, a spontaneous polarization along the c-axis is predicted [1]. Utilizing this property in heterostructure devices requires the formation of sharp, distinct interfaces between different alloyed layers to achieve high sheet carrier densities.

The recent development of suboxide MBE (S-MBE) has enabled the adsorption-controlled growth of Ga2O3 thin films [2]. In this contribution, S-MBE is specifically applied to the growth of metastable, orthorhombic κ-Ga2O3. The growth process, phase stabilization, and their impact on layer properties are analyzed in detail. This is combined with the use of indium as surfactant. Additionally, the study is complemented by the realization of κ-Ga2O3-based heterostructures using suboxide MBE [3].

[1] Maccioni et al., Appl. Phys. Express 9, 041102 (2016);[2] Vogt et al., U.S. Patent No. 11,462,402 (2022);[3] Karg et al., APL Mater. 11, 091114 (2023)

HL 9.6 Mon 16:15 H17

Realization of highly rectifying pn-heterojunctions on pulsed laser deposited α-Ga_2O_3 thin films — •Paul Bokemeyer, Sofie Vogt, Clemens Petersen, Holger von Wenckstern, and Marius Grundmann — University Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnestr. 5, Leipzig, Germany

The wide band gap of about 5.3 eV[1], the possibility for adjusting the band gap energy by alloying with isostructural aluminum oxide or indium oxide[1] and a high expected breakdown field of up to 10 MV/cm[2], renders the corundum α-phase of Ga_2O_3 interesting for high power applications. We present lateral p^+n-heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition(PLD) using a two step approach[3]. Room temperature deposited ZnCoO(ZCO) (PLD), NiO (PLD) and CuI (PLD and sputtering) were used as p^+-type materials. We further investigated the influence of a remote oxygen plasma treatment prior to the deposition of the p-type layers on the device performance. High current rectification ratios of of 8.2 (ZCO), 7.8 (NiO), and 5.1 (CuI) orders of magnitude at ± 3V were achieved. Additionally, α-Ga_2O_3:Zr junction-field-effect-transistors(JFETs) with ZCO and NiO as gate materials were fabricated, yielding on/off ratios of more than 9 orders of magnitude and sub-threshold-swings down to 119 mV/dec.

[1] A. Hassa et.al., J.Phys. D: Appl. Phys. **54**, 223001 (2021)
[2] M. Biswas et al., APL Mater. **10**, 060701 (2022)
[3] S. Vogt et al., Phys. Status Solidi A, **220** 2200721 (2023)

HL 10: Spin-Dependent Phenomena in 2D (joint session MA/HL)

Time: Monday 15:00–17:15 Location: H19

See MA 8 for details of this session.

HL 11: Ultra-fast Phenomena I

Time: Monday 16:00–18:45 Location: H14

HL 11.1 Mon 16:00 H14

Femtosecond Photocurrents in 2D materials — •Björn Sinz[1,2], Johannes Schmuck[1,2], Johannes Gröbmeyer[1,2], Nina Pettinger[1,2], Sergey Zherebtsov[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, TU Munich, Munich, Germany — [2]Munich Center of Quantum Science and Technology (MCQST), Munich, Germany

Light-field-driven currents have already been investigated in graphene by ultrashort laser pulses. In the strong-field regime, the electric field directly generates such photocurrents on a time scale of femtoseconds, whereas in the weak-field regime other photogeneration processes like the photo-thermoelectric effect dominate [1]. The different photocurrents are not limited to graphene but are also predicted for transition metal dichalcogenide (TMDC) monolayers. We report on femtosecond-pulse driven photocurrents in monolayer TMDC samples.

[1]: J. Gröbmeyer, P. Zimmermann, B. Huet, J. A. Robinson, A. W. Holleitner; Space-charge limited and ultrafast dynamics in graphene-based nano-gaps. Appl. Phys. Lett. 3 July 2023; 123 (1): 013504. https://doi.org/10.1063/5.0154152

HL 11.2 Mon 16:15 H14

Hot-Electron-Induced Substrate Response in Transient Absorption Spectroscopy of Tantalum — •Erik Willem de Vos[1,2], Sergej Neb[1], Marko Hollm[1], Florence Burri[1], Lukas Gallmann[1], and Ursula Keller[1] — [1]Department of Physics, Institute for Quantum Electronics, ETH Zurich, Switzerland — [2]Department of Materials, ETH Zurich, Zurich, Switzerland

We show that for extreme ultraviolet transient absorption spectroscopy measurements on thin-film metals, the substrate can significantly contribute to the observed change in absorption even if the substrate is transparent to the excitation wavelengths of the pump pulse and does by itself not produce a transient signal. Irradiation of a thin-film tantalum layer deposited on a silicon nitride substrate by a near-infrared femtosecond pulse is found to excite a coherent acoustic phonon in both the tantalum as well as the substrate. The response in the substrate rises on sub-picosecond timescales and is the result of direct excitation by the hot-electron distribution in the metal layer.

HL 11.3 Mon 16:30 H14

Nonequilibrium electron-phonon dynamics: dynamical control of quantum matter — •Yaxian Wang — Institute of Physics, Chinese Academy of Sciences

Electron-phonon interaction is an old yet evergreen problem in condensed matter physics. It is closely related to many quantum states we are concerned with, such as superconductivity, charge density waves, and polarons. It also profoundly affects, or often accompanies, critical phenomena such as the formation of excitonic insulators and metal-insulator transitions. When the system is driven out of equilibrium, for example pumped by an ultrafast laser pulse, the potential energy surface and thus the coupling in the excited states can be greatly reshaped, and this may open up a new avenue of ultrafast coherent control of quantum phases and topological orders. However, theoretical approaches often fail to capture the coupled dynamics of the non-thermal excited carriers and the nonequilibrium lattice order. In this talk, I will introduce how light-induced coherent phonons can cause a quasi-static lattice distortion and result in a Lifshitz transition in a nodal-line semimetal. We also demonstrate how the laser energy can shift the quasi-equilibrium lattice structure towards opposite directions, thus engineering the electronic structure via different regimes. Moreover, I will discuss our recent discovery on how nonequilibrium electron-phonon interaction can interact with the spin degree of freedom, causing ultrafast demagnetization and excitation of chiral phonons in a monolayer ferromagnet.

HL 11.4 Mon 16:45 H14

Nonequilibrium control of the ultrafast electron dynamics in semiconductors via light-driven coherent phonons — •Chenyu Wang[1,2], Yaxian Wang[1], and Sheng Meng[1,2,3] — [1]Institute of physics, Chinese Academy of Sciences — [2]School of physical sciences, University of Chinese Academy of Sciences — [3]Songshan Lake Materials Laboratory

Driving lattice vibration with a high degree of spatial and temporal coherence via strong light-matter interactions has emerged as a unique knob to control the out-of-equilibrium quantum states and the exotic ultrafast phenomena.

In this talk, I will present our recent theoretical works on the exploration and understanding of how the coherent phonon excitation can be utilized to control the electronic behaviors on ultrafast timescales, for example to engineer the carrier transport in monolayer WSe2 and to manipulate the nonrelativistic spin splitting in the prototypical altermagnetic semiconductor MnTe.

In photoexcited monolayer WSe2, we observe an unconventional 'step-like' electron intervalley scattering dynamics and meanwhile a Rabi oscillation driven by the coherent phonons, as a direct manifestation of the nonadiabatic electron-phonon coupling beyond equilibrium; On the other side, we demonstrate the light-driven coherent phonon can also be utilized to break the crystal symmetry in the altermagnet MnTe. Such symmetry breaking phase holds an extra spin-splitting particularly in the zone center, and thus a strongly enhanced spontaneous anomalous Hall effect.

HL 11.5 Mon 17:00 H14

Semiconductor Bloch Equations and Ehrenfest Dynamics in a Wannier Function Framework: An Integrated Approach to Ultrafast Electron and Ion Dynamics — •Stefano Mocatti, Giovanni Marini, Giulio Volpato, Pierluigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Real-time simulations of photoexcited semiconductors offer valuable insights but are challenged by the complex interplay of interactions and high computational cost. Here, we present an efficient ab initio scheme within the EPIq code, combining semiconductor Bloch equations with Ehrenfest dynamics in the Wannier representation. Electron-phonon and electron-electron interactions follow a Fan-Migdal+GW approximation, while phonon-phonon interactions include non-perturbative quantum anharmonic effects. Through the real-time tracking of the dynamics, we find that electron-electron interaction dominates photocarrier thermalization, yielding a double chemical potential electronic Fermi distribution. Furthermore, atomic forces converge to those calculated within constrained density functional perturbation theory. This work connects out-of-equilibrium and quasi-equilibrium states, advancing the understanding of ultrafast light-driven phenomena.

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15 min. break

HL 11.6 Mon 17:30 H14

Ultrafast Dynamic Coulomb Screening of X-ray Core Excitons in Photoexcited Semiconductors — •Thomas C. Rossi[1], Lu Qiao[2], Conner P. Dykstra[3], Ronaldo Rodrigues Pela[4], Richard Gnewkow[1,5], Rachel Wallick[3], John H. Burke[3], Erin Nicholas[3], Anne-Marie March[6], Gilles Doumy[6], D. Bruce Buchholz[7], Christiane Deparis[8], Jesus Zuñiga-Pérez[8,9], Michael Weise[10], Klaus Ellmer[10], Mattis Fondell[1], Claudia Draxl[2], and Renske M. van der Veen[1,5,11] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Department of Physics and CSMB, Humboldt Universität zu Berlin, Berlin, Germany — [3]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA — [4]Supercomputing Department, Zuse Institute Berlin (ZIB), Berlin, Germany — [5]Institute of Optics and Atomic Physics, Technische Universität Berlin, Berlin, Germany — [6]Chemical Sciences and Engineering Division, Argonne National Laboratories, Lemont, Illinois, USA — [7]Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States — [8]Université Côte d'Azur, CNRS, CRHEA, rue Bernard Gregory, Sophia Antipolis, Valbonne, France — [9]Majulab, International Research Centre Laboratory IRL 3654, Singapore — [10]Optotransmitter-Umweltschutz-Technologie (OUT) e.V., Berlin, Germany — [11]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA

The screening of core excitons is an inherent many-body process that can reveal insight into charge-transfer excitations and electronic correlations. Here we demonstrate the dynamic Coulomb screening induced by photoexcited carriers on core excitons employing X-ray transient absorption (XTA) spectroscopy with picosecond time resolution. Our interpretation is supported by state-of-the-art *ab initio* calculations including many-body perturbation theory. Using ZnO as an archetypal wide band-gap semiconductor, we show that the Coulomb screening modification at the Zn L_3- and K-edge leads to a decrease in the core-exciton binding energy. We also theoretically predict the effect of core-exciton screening on the femtosecond time scale for the case of ZnO, a major step towards hard X-ray excitonics. The results have implications for the interpretation of ultrafast X-ray spectra in general and their use in tracking charge carrier dynamics in complex materials on atomic length scales.

HL 11.7 Mon 17:45 H14

Ultrafast Coherent Dynamics of a Hybrid WS2/Plasmon Structure Probed by Two-Dimensional Electronic Spectroscopy — •Daniel Timmer[1], Moritz Gittinger[1], Daniel C. Lünemann[1], Thomas Quenzel[1], Sven Stephan[1,2], Martin Silies[1,2], Antonietta De Sio[1], and Christoph Lienau[1] — [1]IfP, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]ILO, Hochschule Emden/Leer, Emden, Germany

Transition metal dichalcogenide (TMD) monolayers (1L) have been established as important building blocks for quantum materials. Hybridization between

light and matter states, in particular in plasmonic nanostructures, offers great opportunities to tailor their optical and electronic properties [1]. Here, we investigate such a hybrid plasmonic structure in the intermediate coupling regime comprised of 1L-WS2 [2] placed on a periodic silver nano-slit array using ultrafast two-dimensional electronic spectroscopy (2DES). We observe a 20-fold increase of the optical nonlinearity and ultrafast coherent plexciton dynamics during the dephasing time (~50 fs). We rationalize our observations via a Tavis-Cummings model that gives rise to collective dark states and a Rabi contraction of the 2-quantum states. Using ultrafast 2DES, we obtain access to probe and disentangle the coherent and incoherent dynamics in TMD-based plasmonic systems. [1]: Timmer et al. "Plasmon mediated coherent population oscillations in molecular aggregates." Nat. Commun. 14.1 (2023): 8035. [2]: Timmer et al. "Ultrafast Coherent Exciton Couplings and Many-Body Interactions in Monolayer WS2" Nano Lett. 24.26 (2024): 8117-8125.

HL 11.8 Mon 18:00 H14

Excited-state symmetry breaking and antisymmetric mode brightening in quadrupolar dye — •Somayeh Souri[1], Katrin WInte[1], Daniel Lünemann[1], Fulu Zheng[2], Mohamed Madjet[2], Teresa Kraus[3], Elena Mena-Osteritz[3], Peter Bäuerle[3], Sergei Tretiak[4], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Bremen University, Germany — [3]Ulm University, Germany — [4]Los Alamos National Laboratory, USA

Quadrupolar acceptor-donor-acceptor (A-D-A) dyes are chemically tunable materials displaying a rapid photo-induced charge transfer of interest for applications in solution-processed photovoltaics. The origin of the ultrafast charge transfer is unknown. Using sub-10-fs ultrafast spectroscopy, we investigate the excited-state dynamics of a prototypical A-D-A with comparable electronic and vibronic coupling strengths. Our results reveal that vibronic couplings to high-frequency C-C-stretching vibrations on each arm of the quadrupolar dye induce a double-minimum potential energy surface (PES) in the excited-state S1 driving symmetry breaking along the antisymmetric vibrational coordinate (Q-). Upon excitation, this induces periodic splitting of the optically launched coherent wavepacket along Q- with 20-fs period, rapidly relaxing into local minima of the symmetry-broken PES within less than 100 fs. Our results demonstrate highly nonadiabatic vibronic quantum dynamics, theoretically predicted for this class of dyes [1], and unravel their role for the ultrafast charge transfer in this class of molecules. [1] J. Chem. Phys. 141, 164317 (2014).

HL 11.9 Mon 18:15 H14

Phonon-driven exciton population oscillations in Methylammonium Lead Bromide Perovskites. — •Mohsin Sayar[1], Katrin Winte[1], Daniel Timmer[1], Somayeh Souri[1], Davide Ceratti[2], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Weizmann Institute of Science, Rehovot, Israel

Halide perovskites exhibit unique optoelectronic properties significantly influenced by electron-phonon interactions. Recent work shows that the internal fields induced by coherent lattice motions can transiently control ultrafast excitonic optical response in bulk $CsPbBr_3$[1]. Here, we demonstrate this behaviour also in $CH_3NH_3PbBr_3$ across different crystal phases, using temperature-dependent ultrafast transient reflectivity with 10 fs time resolution. Following resonant exciton excitation reveals coherent low-frequency phonon oscillations at 40cm^{-1} and 67cm^{-1}, corresponding to Pb-Br-Pb bending and stretching modes[2] that most strongly couple to the exciton. Additionally, we observe faster oscillations with dominant period of 105 fs in all crystal phases, arising from coherent exciton population transfer between 1s and 2p excitonic states, off-resonantly driven by the low-frequency phonon fields. We rationalize these results by a phenomenological model accounting for the coupling of excitons to the low frequency phonon modes and coupling of 1s-2p vibronic manifolds via the phonon fields[1]. These results may have important implications for transiently modifying the optoelectronic properties of perovskites.

HL 11.10 Mon 18:30 H14

Coherent suppression of high-harmonic generation in Dirac materials — •Wolfgang Hogger[1], Alexander Riedel[1], Debadrito Roz[2], Angelika Knothe[1], Cosimo Gorini[3], Juan-Diego Urbina[1], and Klaus Richter[1] — [1]Institute for theoretical physics, University of Regensburg, Germany — [2]Indian Institute of Science, Bengaluru 560012, India — [3]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

The study of high-harmonic generation in solids by intense laser pulses provides a fascinating platform for studying ultra-fast electron dynamics and material properties, where the coherent character of the electron dynamics is a central aspect. Starting with the semiconductor Bloch equations, we show the ubiquitous presence of a mechanism suppressing the high harmonic spectrum arising from the coherent superposition of intra- vs inter-band contributions to the total signal [1]. We provide evidence for the generality of this phenomenon by extensive numerical simulations exploring the parameter space of this coherent suppression of high harmonic generation in systems of massive Dirac Fermions (as a prototypical model for topologically non-trivial matter [2]), systems with a pseudo- relativistic dispersion. We supplement our numerical observations with analytical results for a simplified single-mode analysis.

[1] Y. Murakami and M. Sch*uler, Phys. Rev. B 106, 35204 (2022)

[2] C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Physical Review B 82, (2010)

HL 12: Quantum Transport and Quantum Hall Effects (joint session HL/TT)

Time: Monday 16:45–18:15 Location: H15

HL 12.1 Mon 16:45 H15

kdotpy: A Python application for k·p band structure simulations of zincblende semiconductors — •Wouter Beugeling[1,2], Florian Bayer[1,2], Christian Berger[1,2], Jan Böttcher[3], Leonid Bovkun[1,2], Christopher Fuchs[1,2], Maximilian Hofer[1,2], Saquib Shamim[1,2], Moritz Siebert[1,2], Li-Xian Wang[1,2], Ewelina M. Hankiewicz[3], Tobias Kiessling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik (TP4), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The software project kdotpy aims at simulations of electronic band structures of semiconductor devices with k·p theory. The application implements the widely used Kane model, capable of reliable predictions of transport and optical properties for a large variety of topological and non-topological materials with a zincblende crystal structure.

In this presentation, I present the core functionality and features of kdotpy. I will explain how we have implemented principles of modern software engineering and good scientific practice in this project.

HL 12.2 Mon 17:00 H15

End states in zigzag Haldane model nanoribbons — Simone Traverso, Maura Sassetti, and •Niccolò Traverso Ziani — Physics Department, University of Genova, Italy

As topological materials based on the graphene lattice become experimentally realizable in materials such as germanene, the physics of the bound states that characterize them at step edges and in quasi one-dimensional settings becomes relevant.

In this context, the appearance of topological bound states in zigzag Haldane nanoribbons will be addressed [1]. A reentrant topological phase diagram is found. Together with numerical results, a low energy theory extending the Jackiw-Rebbi paradigm will be presented.

[1] S. Traverso, M.Sassetti, N. Traverso Ziani, NPJ Quantum Materials 9, 9 (2024).

HL 12.3 Mon 17:15 H15

Time-reversal invariant Chalker-Coddington model and the real-space renormalisation group — •Syl Shaw and Rudolf A. Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

The Chalker-Coddington model has been utilised to great success in understanding the plateau transitions in the quantum Hall effect. Since the model's inception, it has been extended to a time-reversal invariant symmetry class to describe the quantum-spin Hall effect. Here we adapt a real-space renormalisation group method[1] to respect time-reversal symmetry and use it investigate the phase diagram of the quantum-spin Hall effect. We aim to find distinct phases as a function of both saddle-point height, z and spin-mixing angle ϕ. At the phase boundary between insulator and metal, we compute the value of the critical exponent of the localisation length, ν, with the same real-space renormalisation technique. [1] S. Shaw, R. A. Römer Physica E 165, 116073 (2025)

HL 12.4 Mon 17:30 H15

Utilizing Silicon Qubit Devices for Quantum Electrical Metrology — •Dustin Wittbrodt[1], Johannes Christian Bayer[1], Lars Schreiber[2,3], Janne Lehtinen[4], Marcelo Jaime[1], and Frank Hohls[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Forschungszentrum Juelich, Juelich, Germany — [4]SemiQon Technologies Oy, Espoo, Finland

The 2019 redefinition of the SI system established fixed values for fundamental constants such as the elementary charge (e) and the Planck constant (h), enabling the quantum realization of the units of Ampere, Volt, and Ohm. While the quantum realization of Volt and Ohm is well-established, the realization of the Ampere, whether directly through Single Electron Pumps (SEPs) or indirectly via the Volt and Ohm, has yet to achieve the same level of accuracy. Moreover, further device applications in practical circuits require paralelization approaches to achieve higher current outputs. The international project "Advanced Quantum Technology for Metrology of Electrical Currents" (AQuanTEC) aims to upscale SEPs beyond the 1 nA threshold. To achieve this, AQuanTEC explores several strategies, including the use of silicon devices first designed for spin qubit realization. These devices are highly promising due to their potential scalability, driven by ongoing advancements in integrating large numbers of qubits.

HL 12.5 Mon 17:45 H15

Surface state dominated transport in HgTe topological insulator devices — •Maximilian Hofer[1,2], Christopher Fuchs[1,2], Lena Fürst[1,2], Tobias Kiessling[1,2], Wouter Beugeling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

Recently grown three dimensional topological insulators based on tensile strained HgTe exhibit an exceptionally high mobility and very low intrinsic carrier density. The high quality material has made it possible to study the Landau level dispersion at low magnetic fields and identify four distinct transport regimes. We demonstrate that while a contribution from the topological surface states to transport measurements is expected across the full experimentally accessible density range, there exists only a narrow density regime for which the electronic transport is exclusively carried by the topological surface states. We present the corresponding phase diagram for pure topological surface state transport depending on layer thickness and carrier concentration. For thick HgTe films grown pseudomorphically strained on CdTe, the total carrier density needs to be kept between 1.8×10^{11} cm^{-2} and 2.6×10^{11} cm^{-2} to remain in the pure surface state region and avoid contributions from bulk states. The experimental observations are supported by eight band $\boldsymbol{k} \cdot \boldsymbol{p}$ band structure calculations.

HL 12.6 Mon 18:00 H15

Designing a quantum sorter based on two-dimensional topological insulators — •Amanda Teodora Preda[1,2], Iulia Ghiu[2], Lucian Ion[2], Andrei Manolescu[3], and George Alexandru Nemnes[1,2] — [1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, Magurele- Ilfov, 077125, Romania — [2]University of Bucharest, Faculty of Physics, Atomistilor 405, Magurele-Ilfov, 077125, Romania — [3]Department of Engineering, Reykjavik University, Menntavegur 1, Reykjavik IS-102, Iceland

The idea of a quantum sorter emerged in quantum information, a field that aims to exploit quantum effects and manipulate qubits for information processing. In theory, it was proven that one can propose a universal quantum sorter for any arbitrary observable. To this point, suitable experimental schemes of implementation for this proposal were explored mainly in quantum optics. In our study, we introduce a solid-state version of a quantum sorter, based on a multi-terminal mesoscopic device with multiple output ports, that aims to separate the incoming states by both their spin and transversal mode. In order to maximize the state-separation efficiency of such a device, we chose to exploit the unique transport properties of topological insulators. Employing the tight-binding based simulation package Kwant, we modeled a device that meets the criteria of an irreversible quantum sorter, using the well-established BHZ Hamiltonian to simulate a multi-terminal quantum system made up of both trivial and topological materials.

HL 13: Heterostructures, Interfaces and Surfaces

Time: Monday 16:45–18:30 Location: H17

HL 13.1 Mon 16:45 H17

reducing waste through substrate reuse: a pathway to cost-effective iii-v optoelectronics — •radouane ennadir — 3IT, Sherbrooke University, Sherbrooke, QC, Canada

III-V materials, such as Gallium Arsenide (GaAs), are widely used in optoelectronic devices due to their superior electronic and optical properties. However, the high cost of III-V substrates, primarily made from Ge or other expensive materials, represents a significant barrier to the widespread adoption of these technologies. Our research focuses on reducing waste in the production of III-V optoelectronics through the reuse of Germanium (Ge) substrates. In this study, we propose a novel approach to mitigate substrate waste by reusing Ge substrates in the fabrication of III-V optoelectronics. By carefully optimizing the recycling process, including substrate cleaning, surface treatment, and the integration of new III-V layers, we aim to significantly reduce material costs without compromising device performance. This approach not only enhances the sustainability of optoelectronic manufacturing but also provides a cost-effective pathway to large-scale production of III-V-based devices. The findings of this study contribute to both environmental sustainability and economic viability in the growing field of optoelectronics, opening up new opportunities for the development of advanced, cost-effective optoelectronic devices.

HL 13.2 Mon 17:00 H17

Understanding local charge transfer processes in nanostructured photosystems — •Nina Miller, Sven Doll, Sergej Levashov, Lukas Wolz, Matthias Kuhl, and Johanna Eichhorn — Physics Department, School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical energy conversion offers a promising approach for directly converting solar energy into storable chemical fuels. For scalability, photoelectrodes are often fabricated using thin film technologies yielding material architectures with complex micro- and nanoscale structures. One challenge in this context is that the characteristics of these nanostructured material architectures often deviate from the properties of idealized model systems. To understand energy conversion processes at surfaces and interfaces of nanostructured material systems, novel atomic force microscopy methods have emerged recently, such as AFM-based scanning electrochemical microscopy, to resolve local chemical transformations, charge transport, and material changes under operation conditions. By correlating nanoscale and macroscale properties, we will establish the link between nanoscale processes and macroscopic performance, advancing the design of efficient semiconductor/catalyst systems for PEC applications.

HL 13.3 Mon 17:15 H17

Simulation of charge and excitation dynamics across nanostructured organic-organic interfaces — •Giacomo Cotelli[1,2], Engin Torun[2], Stefano Gottardi[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics (EP II), University of Bayreuth, Bayreuth 95440, Germany — [2]Simbeyond B.V., Eindhoven, The Netherlands

The deposition of organic layers via solution processing may lead to rough interfaces or intermixed regions between layers. To investigate the impact of roughness at organic-organic interfaces on the performances of OLEDs, we performed 3D kinetic Monte Carlo simulations of symmetrical bi- and three-layer devices. Our results reveal that the macroscopic behaviour of a device can be significantly affected by the shape and size of roughness at the organic interfaces, influencing both charge and exciton dynamics.

Namely, we introduced interfaces with periodic corrugation and either triangular or rectangular cross-section. In presence of charge accumulation at an interface with triangular cross-section, bilayer devices exhibit strong inhomogeneity in the spatial distribution of charge carriers, excitons and excitonic losses. Comparison to a flat-interface device reveals an increment in current density by a factor from 2 to 10^3, depending on the height of the energy barrier at the interface. This current density boost was successfully applied to improve charge injection towards a central emissive layer (EML) in simulated three-layer devices; the size and configuration of the interfaces can also be leveraged to fine-tune the recombination zone inside the EML. Nevertheless, we raise our concerns in terms of increased local material degradation.

HL 13.4 Mon 17:30 H17

Strain gradients in bent GaAs nanowires as a new way of engineering electronic transitions — •Francisca Marín[1], Yiannis Hadjimichael[2], Christian Merdon[2], Patricio Farrell[2], Constanza Manganelli[3], Oliver Brandt[1], and Lutz Geelhaar[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V. Berlin, Germany — [2]Weierstraß-Institut für angewandte Analysis und Stochastik. Berlin, Germany — [3]Institut für Halbleiterphysik, Leibniz-Institut für innovative Mikroelektronik. Frankfurt (Oder), Germany

Strain gradients open up a new degree of freedom in strain engineering, enabling polarization in all dielectric materials through the flexoelectric effect. However, flexoelectric coefficients remain unknown for many inorganic semiconductors, including GaAs, leaving this phenomenon unexplored in this material system.

Here, we exploit the pronounced strain gradient in bent GaAs nanowires grown by molecular beam epitaxy to study this effect using photoluminescence spectroscopy. Strain and strain gradients in these nanowires influence the bandgap and generate electric fields from piezoelectric and flexoelectric effects. By combining experiments with a simple one-dimensional model to calculate

the expected shift of the electronic transitions, and finite element simulations of piezoelectricity, we provide new insights into flexoelectricity in GaAs.

HL 13.5 Mon 17:45 H17

Understanding Local Charge Transport Using Advanced Kelvin Probe Force Microscopy — •Sven Erik Doll, Sergej Levashov, Nina Miller, and Johanna Eichhorn — Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.

To this end, we use Kelvin probe force microscopy (KPFM) in a controlled atmosphere to spatially resolve band bending, charge accumulation, and local variations of the generated surface photovoltage. However, analyzing nanostructured materials with complex morphologies is not trivial since topographic crosstalk can dominate the results. To overcome these limitations, we combine a commercial AFM with an external Lock-In amplifier to enable dual-frequency and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventionally frequency-modulated and amplitude-modulated KPFM modes. Here, we compare different KPFM modes and highlight the importance of careful imaging and data analysis to reveal insights into local semiconductor material properties at grain boundaries or different facets.

HL 13.6 Mon 18:00 H17

Topological Phase Diagram of Mercury Cadmium Telluride Quantum Wells — •Leonid Bovkun[1,2], Lena Fürst[1,2], Christopher Fuchs[1,2], Vladimir Marković[1,2], Maximilian Hofer[1,2], Moritz Siebert[1,2], Christian Berger[1,2], Florian Bayer[1,2], Wouter Beugeling[1,2], Steffen Schreyeck[1,2], Hartmut Buhmann[1,2], Laurens W. Molenkamp[1,2], and Tobias Kiessling[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

The key ingredient for the formation of a topological insulator phase in Mercury Cadmium Telluride is the inversion of the energetic positions of the electronic Γ_6 and Γ_8 bulk bands, that can be controlled by alloying with Cd to get within reach of electronic tunability.

We present a systematic experimental study of the topological phase transition in a series of ~ 10 nm thick $Hg_{1-x}Cd_xTe$ quantum wells by tuning the Cd content x. We provide detailed structural and magneto-optical spectroscopic characterization measurements and establish a comprehensive picture of the alloy structural and energetic properties.

Using these as input, we employ $\mathbf{k} \cdot \mathbf{p}$ modeling to establish the topological phase diagram of $Hg_{1-x}Cd_xTe$ in dependence of the Cd content and quantum well thickness for thin films which are pseudomorphically strained to the lattice constant of pure CdTe.

HL 13.7 Mon 18:15 H17

Electrostatic control of the band structure in HgTe heterostructures — •Moritz Siebert[1,2], Maximilian Hofer[1,2], Leonid Bovkun[1,2], Vladimir Marković[1,2], Christian Berger[1,2], Florian Bayer[1,2], Julian Kuther[1,2], Daniel Michel[1,2], Lena Fürst[1,2], Christopher Fuchs[1,2], Wouter Beugeling[1,2], Steffen Schreyeck[1,2], Hartmut Buhmann[1,2], Laurens W. Molenkamp[1,2], and Tobias Kiessling[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

We investigate the band structure of topologically inverted thick HgTe quantum wells employing magneto-optical THz- and IR-spectroscopy. The lithographic fabrication of a semi-transparent gate enables control of the charge carrier density in the quantum well. Our magnetic field dependent self-consistent $\mathbf{k} \cdot \mathbf{p}$ band structure calculations give insights into the physical origin of the observed spectral signatures. In this talk, I present how the electrostatic gating not only sets the number of free charge carriers in the HgTe quantum well - but also modifies the electronic dispersion - and explain the observed features.

HL 14: 2D Materials and their Heterostructures II (joint session DS/HL)

Time: Tuesday 9:30–13:00 Location: H3

See DS 4 for details of this session.

HL 15: Quantum Dots and Wires: Growth and Properties

Time: Tuesday 9:30–11:00 Location: H13

HL 15.1 Tue 9:30 H13

Predictive theory of multi-particle states of GaAs quantum dots — •Petr Klenovsky — Masaryk University, Brno, Czech Republic — Czech Metrology Institute, Brno, Czech Republic

The correlated multi-particle electronic structure of GaAs quantum dots (QDs) in AlGaAs matrix is studied. GaAs QDs have unique physical properties, like an absence of built in strain as well as exhibiting the effects of the weak confinement, leading to the superradiance. GaAs QDs are an almost ideal candidate as a source of single and entangled photons for usage in quantum cryptography and computing. Unfortunately, so far current physics models of their electronic structure were not successful to *quantitatively* reproduce observed experimental results like, e.g., binding energies of trions (X+ and X-) and biexciton (XX) with respect to exciton (X) as well as the radiative emission of those complexes. We endeavored to change that and show in this contribution the results of our improved theory model based on $\mathbf{k} \cdot \mathbf{p}$ approximation and configuration interaction (CI) schemes. Using that we demonstrate computed binding energies of X+, X-, and XX in agreement with experiment which are also *converged* with respect to the size of CI basis, i.e., they include the effects of the Coulomb correlation. While the latter is found to be of a paramount role, surprisingly, we also find that the binding energies strongly depend on the way the electron-electron and hole-hole *exchange* integrals are calculated. Our results show very good agreement with photoluminescence and nuclear spin relaxation experiments on GaAs/AlGaAs QDs.

HL 15.2 Tue 9:45 H13

Electron capture and emission dynamics of self-assembled quantum dots far from equilibrium — •Maximilian Erdmann[1], Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Severin Krüger[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

The subject of the experiment were the electron capture and emission dynamics of Self-Assembled Quantum Dots (SAQD) far away from equilibrium conditions, at a temperature of 77 K. The SAQDs are located in a semiconductor structure that can be regarded as a Schottky diode. For analysing the capture and emission dynamics, the capacitance transients of this sample were investigated using the methods of Deep Level Transient Spectroscopy (DLTS).

HL 15.3 Tue 10:00 H13

Spatial Statistics of InAs Quantum Dots on GaAs(100) — •Normen Auler[1], Viktoryia Zolatanosha[2], and Dirk Reuter[1,2,3] — [1]Department Physik, Universität Paderborn, DE — [2]Institute for Photonic Quantum Systems (PhoQS), Universität Paderborn, DE — [3]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, DE

Self-assembled InAs quantum dots (QDs) on GaAs are potential building blocks for quantum technology applications. One interesting aspect is the spatial arrangement of the QDs.

In this contribution, we investigated the spatial distribution of QDs for samples with different QD densities by analyzing atomic force microscopy images. We evaluated Voronoi cell areas and nearest neighbor configurations. Contrary to the expected random distribution for Stranski-Krastanow-grown QDs, we observe deviations indicating an influence of strain fields and a corresponding effect on inter-island adatom diffusion on the final QD arrangement. We discuss the behavior for different densities in detail.

HL 15.4 Tue 10:15 H13

Epitaxial growth and in-situ integration of high-quality single InGaAs quantum dots on a silicon substrate — •Imad Limame[1], Peter Ludewig[2], Aris Koulas-Simos[1], Chirag C. Palekar[1], Wolfgang Stolz[2], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin — [2]NAsP III/V GmbH, Marburg, Deutschland

For over two decades, the integration of light sources onto the silicon (Si) platform has garnered significant interest in both scientific and industrial commu-

nities. Despite the cost-effectiveness of Si and its extensive use in semiconductor technology, its indirect bandgap limits its potential for optoelectronic applications. The direct growth of III-V materials, which offer excellent optical properties, on Si is appealing but challenging due to factors such as lattice mismatch, differences in thermal expansion coefficients, Si surface reactivity, and dislocation formation. We report on the direct epitaxial growth of InGaAs QDs in both the 940 and 1300 nm ranges with excellent quantum optical properties on a Si substrate. The heteroepitaxy of GaAs heterostructures on Si is achieved using a GaP buffer layer. The resulting QDs exhibit outstanding optical properties, showcasing the significant potential of this approach. Furthermore, using a strain-reducing layer (SRL), we grow single QDs in the telecom O-band, which are then integrated via in-situ electron beam lithography (EBL) into circular Bragg gratings (CBG) to enhance extraction efficiency for quantum communication applications.

Our results represent a significant step toward scalable, cost-effective, and Si-compatible quantum photonics devices.

HL 15.5 Tue 10:30 H13

Electrostatic Inter-Layer Coupling between Self-Assembled Quantum Dots — •Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Charlotte Rothfuchs-Engels[2], Nikolai Bart[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

Electrostatic coupling between Self-Assembled Quantum Dots (SAQDs) in spatially separated layers is studied using transient capacitance spectroscopy. The coupling effect is analysed as a function of temperature, applied bias voltage, and the occupancy of the quantum dot layers. The observed interaction is attributed to the electric field modulation induced by charge redistribution in one layer, influencing the capture and emission dynamics in the other. A rate equation model was developed, incorporating self-consistent band bending calculations, to describe the impact of the inter-layer coupling on the charge transfer processes. The findings indicate that the coupling arises from the electrostatic field generated by the charged quantum dots in the adjacent layer, providing a quantitative explanation for the altered capacitance transients.

HL 15.6 Tue 10:45 H13

Photoluminescence from SiGe and Ge quantum dots on Si nanotips: role of composition and capping — •Diana Ryzhak[1], Johannes Aberl[2], Enrique Prado-Navarrete[2], Lada Vukušić[2], Agnieszka Anna Corley-Wiciak[1], Oliver Skibitzki[1], Marvin Hartwig Zoellner[1], Markus Andreas Schubert[1], Michele Virgilio[3], Moritz Brehm[2], Giovanni Capellini[1,4], and Davide Spirito[1] — [1]IHP Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenberger Strasse 69, 4040, Linz, Austria — [3]Dipartimento di Fisica E. Fermi, Università di Pisa, Largo Pontecorvo 3, 56127, Pisa, Italy — [4]Dipartimento di Scienze, Università Roma Tre, V.le G. Marconi 446, 00146 Roma, Italy

Quantum dots (QDs) have been studied for their unique optical properties, which are essential for LEDs and lasers. The main challenge remains to control the fabrication processes of QDs. Therefore, we have used a nanoheteroepitaxy (NHE) approach and fabricated nearly strain-free SiGe and Ge QDs on Si(001) nanotip (NT) patterned substrates. The QDs were deposited by molecular beam epitaxy at 850°C, yielding defect-free structures selectively on the NTs as observed by transmission electron microscopy. Upon tuning the Si content, the photoluminescence (PL) peak emission shifted from 0.78 to 0.9 eV. The PL emission can be remarkably enhanced by capping the QDs with Al2O3 or Si3N4 for reduction of the surface recombination processes.

HL 16: Organic Semiconductors

Time: Tuesday 9:30–12:00 Location: H14

HL 16.1 Tue 9:30 H14

Modeling charge transport in organic semiconductors: why and when the conventional Miller-Abrahams rate is inappropriate — •Magdalena Dörfler, Heinz Bässler, Andrey Kadashchuk, Harald Oberhofer, and Anna Köhler — Universität Bayreuth, 95447 Bayreuth

A widely applied expression to model charge transport in organic semiconductors is the Miller-Abrahams rate, which describes the probability for charge transfer from one site, e.g. a molecule, to a neighboring site. However, the expression that is conventionally referred to as Miller-Abrahams rate is an approximation of a more general term. This approximation is only valid when energy differences between neighboring sites are large compared to the thermal energy. Here, we show the differences that result when charge transport is modelled by kinetic Monte Carlo simulations (KMC) using either of the two expressions. The widely used, approximate, rate can lead to serious errors in the magnitude and, more importantly, in the trends obtained for the temperature and field dependence of charge transport. The implications for modelling work and the interpretation of experimental data are discussed.

HL 16.2 Tue 9:45 H14

Accurate ab-initio parametrization of electron-phonon coupling models with Gaussian and plane-wave basis sets — •Konrad Merkel[1], Maximilian Dorfner[1], Manuel Engel[2], and Frank Ortmann[1] — [1]TUM School of Natural Sciences, TU Munich, Germany — [2]VASP Software GmbH, Vienna, Austria

For the simultaneous treatment of electronic and vibrational degrees of freedom, the Holstein-Peierls model has become a cornerstone in various scientific communities due to its versatility and remarkable success in the accurate description of materials. To use it, one needs to calculate all model parameters for the electronic structure, phonons and electron-phonon coupling constants. In particular, the calculation of the electron-phonon coupling constants is a challenge as they involve both degrees of freedom. Although various approaches exist, comprehensive benchmarks comparing different methods and basis sets are still rare. In our study, we investigate two different methods to calculate the electron-phonon couplings. The first approach was developed by Engel et al. [1] and is based on the projector-argumented-wave formulation and maximally localized Wannier functions and is implemented in the VASP code. The second approach is based on a real-space description in terms of Gaussian basis functions and is implemented using cp2k. Both approaches use a finite-displacement and finite-difference scheme to calculate the coupling constants. We compare both methods using different molecules and discuss critical points for accurate calculations.

[1] Physical Review B 106, 094316 (2022)

HL 16.3 Tue 10:00 H14

Excitons in organic donor-acceptor cocrystals — •Sebastian Anhäuser[1], Ana Maria Valencia[2], Caterina Cocchi[2], and Gregor Witte[1] — [1]Philipps-Universität Marburg, FB Physik — [2]Carl von Ossietzky Universität Oldenburg, Institut für Physik

Organic donor-acceptor heterostructures have gained significant attention due to their unique properties, such as low-bandgap semiconductivity and ambipolar transport, making them promising candidates for optoelectronic applications like organic photovoltaics. There, the formation of charge-transfer excitons is typically regarded as the precursor state for charge separation. However, the microscopic nature of these excitons is not yet well understood. In the presented study, we perform detailed polarization-resolved optical spectroscopy on high quality acene-perfluoroacene donor-acceptor single crystals in the optical and UV range. This approach allows us to investigate both the excitation energies and the transition dipole moments of various (charge-transfer-)excitons. Using complementary state-of-the-art first principles calculations based on density functional and many-body pertubation theory, we analyse the nature of different classes of excitons within the cocrystalline structure. Our findings provide a refined understanding of charge-transfer excitons in organic materials, paving the way for improved design strategies in organic optoelectronics.

HL 16.4 Tue 10:15 H14

Detecting charge patterns on a novel type of rubrene crystals by time-of-flight photoemission electron microscopy — •Moha Naeimi[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]University of Rostock, Institute of physics, Rostock, Germany — [2]University of Rostock, Department of life, light and matter, Rostock, Germany

Organic molecules are increasingly drawing attention due to their broad applications, not only in organic field effect transistors and organic light emitting diodes [1], but also with respect to the exciton dynamics and charge transfer [2]. To this end, single crystalline domains with compact and stable molecular packing are beneficial. In this work, we focus on charge patterns and its dynamics for a recently discovered type of rubrene single crystals consisting of two distinct types of domains [3]. We show that both domains exhibit different charging properties, and that one of them can be controlled by photon exposure. This charge pattern can be *reset* by a second light source with lower photon energy, essentially neutralizing the charged sections. We tentatively attribute the behavior to the selective photo-injection of mobile excitons, resulting in spatially dependent conductivities.

[1] Wei-Cheng Su et al., Influence of Singlet and Charge-Transfer Excitons on the Open-Circuit Voltage of Rubrene/Fullerene Organic Photovoltaic Device ACS Appl. Mater. Interfaces, 8, 28757-28762 (2016) [2] Drew M. Finton et al., Routes to singlet exciton fission in rubrene crystals and amorphous films

AIP Advances 9, 095027 (2019) [3] Moha Naeimi et al., Characteristics of zone-sectored tabular orthorhombic rubrene microcrystals in preparation.

HL 16.5 Tue 10:30 H14

Toward High Efficiency and Stable Blue OLEDs/Organic Light-Emitting Diodes with Lanthanide-Based Complexes: Host Material Impact — •Mahmoud Soleimani[1,2], Paulius Imbrasas[2], Sebastian Schellhammer[1], Carsten Rothe[2], and Sebastian Reineke[1] — [1]Institute for Applied Physics (IAP), Technische Universität Dresden, Germany — [2]beeOLED GmbH, Dresden, Germany

Lanthanides offer a new approach for achieving blue emission in organic light-emitting diodes (OLEDs). Cerium (III) and Europium (II) complexes emit in the blue range via the 5d-4f transition, potentially enhancing the stability and efficiency of OLEDs, outperforming current emitters. However, precise ligand design around the lanthanide is required for a stable, blue-emissive complex. With the right ligands, emitters with near-unity photoluminescence quantum yield in solution have been demonstrated. In the transition to OLED-compatible thin-films, we found that the host material plays a key role in maintaining this luminescence efficiency and that it can also impair emission through quenching mechanisms caused by unfavorable energy level alignment and coordination of the metal-organic complex by the host. This study investigates the photoluminescence of Cerium (III) tris(pyrazolyl)borate complex blended with four common OLED emission layer hosts. These insights guide the development of efficient blue OLEDs with lanthanide complexes.

HL 16.6 Tue 10:45 H14

Modifying the density of states in dipolar organic semiconductors — •Andrei Stankevich[1], Prakhar Sahay[3], Heinz Bässler[1], Wolfgang Brütting[3], Fabian Eller[2], Eva M. Herzig[2], Andrey Kadashchuk[1], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth — [3]Institute of Physics, University of Augsburg,

Charge transport properties of amorphous organic semiconductors are controlled by energetic disorder. Certain device properties, such as the energies of charge transfer states in organic light-emitting diodes, can be improved by using dipolar molecules as host. Such molecules, however, also introduce interactions between charge carriers and randomly aligned dipoles. A key consequence of this is that increases the energetic disorder, hence causing a broad distribution of localized states, which hinders charge transport. We combined thermally stimulated luminescence studies with grazing incidence wide angle X-ray scattering, to demonstrate how the density of states in dipolar materials can be tailored. We demonstrate that the DOS is highly sensitive to the deposition technique and, consequently, the resulting film morphology. Furthermore, we show that the energetic disorder is not only determined by the static dipole moment, but also by the polarizability of charged molecules. Through this insight we derive design rules for common OLED materials that exhibit a with high dipole moments while maintaining charge transport properties comparable to those of non-polar counterparts.

15 min. break

HL 16.7 Tue 11:15 H14

Electrical and Optical Processes in Blue TADF OLEDs Studied by Temperature-Dependent Spectroscopy — •Ahmed Mohamed, Felix Kübert, Klara-Maria Bögle, Tolga Durmus, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, German

This study explores the electrical and photophysical processes in Thermally-Activated Delayed Fluorescence (TADF) Organic Light- Emitting Diodes (OLEDs) using temperature-dependent spectroscopic techniques. Key aspects such as charge carrier transport, current loss mechanisms and recombination dynamics are examined to pro- vide a comprehensive understanding of device performance. We analyze current density-voltage-luminance (JVL) with respect to leak- age current, efficiency roll-off, and current density at 90% external quantum efficiency *90. Electroluminescence (EL)/photoluminescence (PL) microscopy is employed to analyze the photophysical processes in OLEDs. EL spectra of blue OLEDs with the multi-resonance emitter *-DABNA exhibit remarkable spectral stability at temperatures be- tween 200-300 K. Analysis of transient EL with rate equations yields activation energy and the rates of triplet-singlet transitions in OLEDs, including reverse intersystem crossing (rISC), triplet-triplet annihilation (TTA), and triplet-polaron annihilation (TPA). Understanding the mechanisms of current loss and (non-)radiative transitions is the prerequisite for enhancing the efficiency and stability of blue OLEDs.

HL 16.8 Tue 11:30 H14

Low Invasive Deposition of Metal Films on Carbon Nanotubes — •Martin Ernst[1,2], Martin Hartmann[1,2,3], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nano Technologies, Chemnitz University of Technology, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

Carbon nanotubes (CNTs) are one of the most promising materials for the next generation of electronics. Their unique one-dimensional electronic structure and their remarkable optical, thermal and mechanical properties makes them ideal candidates for different application scenarios. These range from the integration in transistors for analog and digital applications, as well as their usage in CNT-based gas, bio and stress sensors. One of the key challenges is the realization of a proper CNT-metal contact, in order to effectively transport charge carriers trough an electronic device, such as the carbon nanotube field-effect transistor (CNTFET). In this study we investigated the effects of different deposition parameters on the amount of lattice defects in single-walled semiconducting CNTs by Raman spectroscopy. There, a clear dependency between the amount of introduced defects and the deposition parameters, like the kinetic energy of the incident target atoms, was observed. Moreover, these finding were correlated to electrical results of CNTFETs, that were fabricated with the same deposition parameters.

HL 16.9 Tue 11:45 H14

High-Frequency CNT-based FETs for Radio Frequency Communication — •Martin Hartmann[1,2,3], Simon Böttger[1,2,3], Martin Ernst[1,2], and Sascha Hermann[1,2,3,4] — [1]Center for Micro and Nanotechnologies, Chemnitz University of Technology, Germany — [2]Center for Materials Architecture and Integration of Nanomembranes, Chemnitz University of Technology, Germany — [3]Fraunhofer Institute for Electronic Nanosystems ENAS, Chemnitz, Germany — [4]Center for Advancing Electronics Dresden, Dresden University of Technology, Germany

High frequency carbon nanotube-based (CNT) field effect transistors (FETs) are a highly promising candidate for future communication electronics due to their high charge carrier mobility and low intrinsic capacitance. It has already been shown in 2019 that this technology surpassed comparable silicon-based radio frequency FETs e.g. in terms of their extrinsic current gain cut-off frequencies as well as maximum frequencies of oscillation [1]. Moreover, in recent years their performance was further enhanced approaching the THz region [2]. We report on the impact of the device geometry as well as the CNT layer properties of high frequency CNTFETs onto their operating speed, linearity and contact resistance. Therefore, the spacers between the gate and the source electrode and gate to drain electrode were varied resulting in extrinsic current gain cut-off frequencies up to 14 GHz. By manipulating the spacer region, the device electrostatics in the CNT-metal contact area are balanced. This impacts the charge carrier injection and reflection at the Schottky-like barriers.

HL 17: 2D Semiconductors and van der Waals Heterostructures III

The session covers electronic and optoelectronic phenomena in two-dimensional semiconductors and van der Waals heterostructures.

Time: Tuesday 9:30–13:00 Location: H15

HL 17.1 Tue 9:30 H15

Size-Dependent Electrical Transport in Quasi-1D $ZrSe_3$-Stripes — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hannover, Germany

The anisotropy in form of quasi one-dimensional (1D) chains in transition metal trichalcogenides (TMTCs) makes them stand out compared to other more conventional two-dimensional (2D) materials [1]. Building on previous work [2], we investigated the electrical properties of thin stripes of the TMTC $ZrSe_3$ particularly regarding their width and thickness. The bulk material used was fabricated by a chemical vapor transport method and then exfoliated to achieve thin stripes.

We determined band gap energies for samples with varying heights. Those are

shown to increase linearly from 0.37 eV to 0.63 eV as the thickness of the material decreases from 35 nm to 14 nm. Furthermore, we compared narrow samples with wider samples where both have comparably similar length and thickness and found that the conductivity happens dominantly in the outer selenium atoms i.e. across the chains.

[1] J. O. Island et al., 2D Materials 4, 0220033 (2017)
[2] L. Thole et al., ACS Omega 7, 39913-39916 (2022)

HL 17.2 Tue 9:45 H15

MOCVD Growth of two-dimensional, high-mobility InSe — •Robin Günkel[1], Milan Solanki[1], Daniel Anders[2], Markus Stein[2], Badrosadat Ojaghi Dogahe[1], Oliver Massmeyer[1], Max Bergmann[1], Nils Langlotz[1], Jürgen Belz[1], Sangam Chatterjee[2], and Kerstin Volz[1] — [1]Department of Physics and Material Sciences Center, Philipps-University Marburg, Germany — [2]Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus-Liebig-University Giessen, Germany

To advance Moore's Law, transistors must shrink while maintaining performance, but 3D semiconductor-based gates face limitations as their thickness approaches the nanometer scale due to surface scattering effects. 2D materials, such as graphene, offer a promising alternative that combines miniaturization with high field effect mobility. Among these, layered indium selenide (InSe) is a focus for logic devices due to its high mobility. However, the complex phase diagram of InSe poses challenges, often resulting in undesired phases. This study uses metal-organic chemical vapor deposition (MOCVD) to grow homogeneous, single-phase InSe on 2" sapphire by tuning the precursor ratio of DiPSe and TMIn. Growth starts with small nuclei forming a continuous layer, with subsequent layers growing as InSe triangles. Atomic force microscopy, Raman spectroscopy, STEM, and XRD provide insight into the growth behavior and the role of surface chemistry. Terahertz spectroscopy confirms carrier mobilities in the order of 1000 cm^2/(Vs). Ongoing efforts focus on heterostructures with other van der Waals materials to further tailor properties.

HL 17.3 Tue 10:00 H15

Transparent and reproducible contacts to MoS_2 nanotube quantum dots — •Robin T. K. Schock[1], Stefan B. Obloh[1], Korbinian Fink[1], Matthias Kronseder[1], Matjaž Malok[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Jožef Stefan Institute, 1000 Ljubljana, Slovenia

MoS_2, a leading material among transition metal dichalcogenides, exhibits remarkable optical and electronic properties. However, its high effective electron mass necessitates narrow confinement potentials to achieve single quantum level transport.

Nanotubes offer a compelling solution by naturally confining electrons in two dimensions. Our previous work demonstrated single level transport in nanotube QDs confined to the active device area, using the classical Scotch tape method.[1] Despite this, a major challenge remains in fabricating reliable electrical contacts, as devices still exhibit large resistance variations. We attribute this to the curved geometry of the nanotube surface, leading e.g. to nanogaps between the contact material on the tube and the chip surface.[2]

Here we introduce a contact deposition technique that addresses these challenges, achieving highly improved contact yield and reproducibility. This advancement enables the fabrication of more complex device architectures, as e.g., nanotube QDs on top of 2D material heterostacks. - [1] R. T. K. Schock et al., Adv. Mat. 35, 2209333 (2023); [2] R. T. K. Schock et al., PSSb, 2400366 (2024)

HL 17.4 Tue 10:15 H15

Defect engineering in two-dimensional materials for resistive switching — •Manoj Dey, Matthias Scheffler, and Wahib Aggoune — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft, Berlin, Germany

Non-volatile resistive switching (RS) in memristors has attracted significant attention for advancing in-memory technologies. Recently, exceptional RS has been observed in defected two-dimensional (2D) materials, called atomristors. Adsorption/desorption of metal atoms from the electrodes onto vacancy sites is experimentally observed and proposed as its origin [1,2]. Here, we explore the characteristics of defects and demonstrate their relationship with the observed RS. Using hybrid density functional theory with many body van der Waals corrections, we reveal that the defective monolayers are semiconducting (*i.e.*, high resistivity), whereas adsorption of metal atoms leads to a metallic character (*i.e.*, low resistivity). Interestingly, the adsorption energy of metal is found to be exothermic, with magnitude varying depending on the host materials. This indicates the feasible adsorption and switching in experiments. To bridge with experiments we also consider both the effects of the electrode (*e.g.* Au(111)) and finite-temperature vibrations. While vibrational effects are negligible, electrode screening induces band gap renormalization and slightly stabilizes metal adsorption compared to free-standing monolayers. These insights will guide the exploration of novel 2D materials for RS applications.

[1] Ruijing Ge *et al.*, *Adv. Mater.*, **33**, 2007792 (2021).
[2] Saban M. Hus *et al.*, *Nat. Nanotechnol.*, **16**, 58 (2021).

HL 17.5 Tue 10:30 H15

Anisotropic supercurrent suppression and revivals in a graphene-based Josephson junction under in-plane magnetic fields — •Katarina Stanojević[1,5], Philipp Schmidt[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Bernd Beschoten[1], Vincent Mourik[5], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Research Center for Electronic and Optical Materials, National Institute for Materials Science, Japan — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan — [5]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany

Graphene-based Josephson junctions represent a promising platform for hybrid quantum devices due to their unique electronic properties. The absence of Schottky barriers enables highly transparent interfaces, while graphene's ability to host proximity-induced superconductivity make it an interesting candidate for realizing tunable weak links. A key step towards harnessing graphene Josephson junctions for topological quantum applications is understanding the influence of in-plane magnetic fields, which tune the Zeeman energy and might enable the formation of topologically protected states. Here, we report on a tunable bilayer graphene Josephson junction encapsulated in WSe_2. We investigate the behavior of the supercurrent under applied in-plane magnetic fields, revealing a pronounced anisotropy in the magnetic field induced decay and revival of the supercurrent for varying in-plane field angles.

HL 17.6 Tue 10:45 H15

Electric field control of the proximity-induced spin-orbit gap in bilayer graphene/WSe2 quantum dots — •Hubert Dulisch[1,2], David Emmerich[1,2], Eike Icking[1,2], Katrin Hecker[1,2], Samuel Möller[1,2], Leonie Müller[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]2nd Institute of Physics, RWTH Aachen — [2]PGI-9, Forschungszentrum Jülich — [3]Research Center for Functional Materials, NIMS, — [4]International Center for Materials Nanoarchitectonics, NIMS

We investigated induced spin-orbit coupling (SOC) in a bilayer graphene (BLG) quantum dot (QD), which is in proximity to tungsten diselenide (WSe_2). Magneto-transport measurements were performed on the Coulomb-resonance of the first charge carrier to extract the spin-orbit gap Δ_{SO}. In-plane magnetic field measurements indicate an increased SOC-induced energy splitting. Out-of-plane field measurements demonstrate a reduced valley g-factor at larger displacement fields, consistent with weaker lateral confinement of the QD wavefunction. Our measurements reveal an enhanced SOC effect that decreases with the applied displacement field, distinguishing it from the behavior observed in pure BLG. We interpret this as a reduced influence of the WSe_2, which we attribute to the increased displacement field. This causes the QD to become more localized in the lower layer of the bilayer graphene. Being farther from the WSe_2, this layer experiences reduced induced SOC, leading to a diminished spin-orbit gap in the BLG QD.

HL 17.7 Tue 11:00 H15

High-Performance and Energy-Efficient Sub-5nm 2D Double-Gate MOSFETs Based on SiAs Monolayers — •Dogukan Hazar Ozbey and Engin Durgun — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey

As the demand for high-performance, energy-efficient transistors grows, traditional silicon-based MOSFETs face significant scaling limitations. To overcome these challenges and sustain advancements in semiconductor technology, new materials and device architectures are being explored. In this study, sub-5nm double-gate metal-oxide-semiconductor field-effect transistors (MOSFETs) based on 2D SiAs are investigated using first-principles calculations and the Non-equilibrium Green's function (NEGF) formalism to assess their potential as a high-performance alternative. SiAs monolayers exhibit an indirect bandgap of 1.58 eV and demonstrate promising electronic properties. Key performance metrics such as the on/off current ratio, subthreshold swing (SS), gate capacitance (C_g), intrinsic delay time (τ), and power-delay product (PDP) are evaluated. Devices with 1 nm and 2 nm underlap (UL) structures show enhanced performance, achieving on-state current (I_{on}) values up to 1206 $\mu A/\mu m^{-1}$, meeting ITRS-2028 high-performance (HP) standards. The SS ranges from 112 to 142 mV/dec, and minimized delay and power-delay products indicate the suitability of SiAs transistors for ultra-scaled, energy-efficient applications. Results suggest that 2D SiAs transistors offer a promising solution to the scaling challenges of MOSFET technologies.

15 min. break

HL 17.8 Tue 11:30 H15

Resistance standards from artifact wire coils to graphene quantum Hall resistance — •Yefei Yin[1], Mattias Kruskopf[1], Stephan Bauer[1], Teresa Tschirner[1], Klaus Pierz[1], Frank Hohls[1], Rolf J. Haug[2], and Hans W. Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Historically, resistance standards were made by physical artifact wire coils before 1990 and quantum resistors based on GaAs heterostructures after 1990. However, conventional GaAs quantum Hall resistance (QHR) standards with the quantized resistance $R_H = h/2e^2$ are operating under high magnetic flux densities B > 10 T, limited currents I < 50 μA, and low temperatures T < 1.5 K, which significantly hinder the dissemination of primary resistance standards. In this work, we developed practical primary QHR standards based on n- and p-type epitaxial graphene. This study first systematically demonstrated that p-type epitaxial graphene can also be used for primary resistance standards, as accurate (10^{-9} accuracy) as GaAs and n-type graphene counterparts for realizing the SI unit ohm in quantum metrology. [1] The n-type graphene QHR standards achieved the world best performance so far with a 10^{-9} accuracy under relaxed conditions (B = 4.5 T, I = 232.5 μA, T = 4.2 K) simultaneously. [2-3] Our graphene QHR standards have been utilized in the national metrology institutes in European countries. [1] Appl. Phys. Lett., 125, 064001 (2024). [2] Adv. Phys. Res. 1, 2200015 (2022). [3] Phys. Rev. Applied, 2024

HL 17.9 Tue 11:45 H15

1D graphene superlattices and the influence of the potential shape — •Julia Amann[1], Alina Mreńca-Kolasińska[2], Angelika Knothe[1], Ming-Hao Liu[3], Takashi Taniguchi[4], Kenji Watanabe[4], Dieter Weiss[1], and Jonathan Eroms[1] — [1]University of Regensburg, Germany — [2]AGH University, Krakow, Poland — [3]National Cheng Kung University, Tainan, Taiwan — [4]National Institute for Materials Science, Tsukuba, Japan

One-dimensional superlattices (1DSLs) in graphene have been predicted to exhibit intriguing effects such as transport anisotropy, additional Dirac points and hence higher degeneracy, leading to a different quantum Hall plateau sequence compared to pristine graphene. We use a patterned few-layer graphene gate under an encapsulated monolayer graphene to fabricate a 1DSL device. With the combined effect of a global gate and a patterned bottom gate, we are able to control the superlattice potential strength and carrier density independently. We show low-temperature transport measurements on a gate-tunable 1DSL in monolayer graphene with a period of 50 nm in directions parallel and perpendicular to the modulation using an L-shaped Hall bar. We observe anisotropic transport and the appearance of multiple Dirac points and additional Landau fans in the modulation direction. We also see Weiss oscillations, confirming the 1DSL modulation. However, the predicted anomalous quantum Hall sequence was not observed and we looked more closely at the 1DSL potential we were applying. We found an asymmetric potential shape, which strongly influences the change in the band structure and degeneracy.

HL 17.10 Tue 12:00 H15

Ultrafast mid-infrared interferometric photocurrents in graphene-based two-terminal devices for femtosecond autocorrelation — •Sebastian Loy[1,2], Nina Pettinger[1,2], Johannes Schmuck[1,2], Xiaoyi Zhou[1,2], Sergey Zherebtsov[1,2], Christoph Kastl[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center of Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

We present the autocorrelation of femtosecond mid-IR pulses with wavelengths ranging from 5.5 μm to 14 μm and pulse durations of approximately 100 fs on graphene-based two-terminal devices. The results indicate that the interaction between the electric field and optoelectronic dynamics at the metal-graphene interface underlies the principle of ultrafast detection. Our approach stands out due to the ease of nanofabricating graphene two-terminal optoelectronic devices and their inherent robustness [1].

[1] Nina Pettinger et al., accepted (2024).

HL 17.11 Tue 12:15 H15

Enhancement of optoelectronic properties of layered 2D semiconductors — •Borna Radatović[1,2], Onur Çakiroğlu[2], Hao Li[2], Fedor Lipilin[1], Aljoscha Soll[1], Andres Castellanos-Gomez[2], and Zdenek Sofer[1] — [1]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, Prague 6, 166 28 Czech Republic — [2]2D Foundry group. Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), E-28049 Madrid, Spain

Standard semiconductor methods for the enhancement of electronic devices' properties, such as doping via ion implantation and similar approaches, do not apply to 2D materials due to their atomical thickness. However, various alternative methods for customization of optoelectronic properties of 2D devices have been investigated, from electric or magnetic fields to substitutional doping, that were demonstrated for many devices, such as light sources, optical modulators and photodetectors. In our work, we focus on photodetectors based on different 2D semiconductors (i.e. MoS2, ZrSe3, Sb2S2O and CuInP2Se6) in monolayer and few-layer forms. We investigated how external strain can modulate the intrinsic optical and electronic properties of 2D materials and enhance photodetectors' performances. Furthermore, we have demonstrated how 2D heterostructures can offer a practical approach to specific custom optoelectronic properties of 2D devices.

HL 17.12 Tue 12:30 H15

Surface acoustic wave-controlled photocurrent in few-layer TMDCs — •Benjamin Mayer, Felix Ehring, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

Surface acoustic waves (SAWs) provide a versatile platform for integrating GHz-frequency control and sensing schemes at micron-scale wavelengths on a chip. Combining the SAWs dynamic electric field, high-resolution optical spectroscopy, and electrical transport allows a deep insight in the optical properties and carrier transport processes in nanoscale materials, paving the way for innovative acousto-optoelectronic devices [1].

Here, we study the SAW-driven acousto-electric current (AEC) and the underlying charge carrier dynamics in mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials. To this aim, few-layered TMDCs are placed on top of two gold electrodes integrated in hybrid lithium niobate-based SAW-devices with design frequencies of 150-250MHz. The power and directional dependence of the induced AEC offer an initial understanding of the contact barriers forming at the Au-TMDC interface. By locally photodoping our samples, we establish a qualitative model for the formed Schottky and tunneling barriers, enabling the investigation of their influence on the wavelength-dependent SAW-driven charge carrier dynamics [2].

[1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)
[2] Adv. Mater. 2402799 (2024)

HL 17.13 Tue 12:45 H15

Accelerated electron-hole separation at the organic-inorganic anthracene/Janus MoSSe interface — •Hamid Mehdipour[1], Peter Kratzer[2], and Oleg Prezhdo[3] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]University of Duisburg-Essen, Duisburg, Germany — [3]University of Southern California, Los Angeles, United States;

Organic light-absorbing materials with two-dimensional semiconductor layers as contact electrodes are promising for efficient and low-cost energy-harvesting applications. Considering anthracene as an absorber and a MoSSe Janus monolayer, and basing our work on a set of preliminary DFT calculations, we employ non-adiabatic molecular dynamics to show that electron transfer from anthracene to MoSSe is faster on the Se than on the S side. The transfer from anthracene to MoS_2 and $MoSe_2$ monolayers takes intermediate times. As a rule, we find that a shorter adsorption distance produces a stronger donor-acceptor coupling. The smaller distance on the Se side is rationalized by the attractive dipolar interaction between the intrinsic dipole moment of the Janus structure and the dipole induced upon molecule adsorption. Quantum coherence adjusted by the out-of-plane vibrations also has a significant impact on the transfer time. Our study provides detailed insights into adsorption of molecules on Janus structures and the resulting electronic and electron-vibrational interactions. The results suggest that the dipole interaction plays an important role in thermodynamic stability, alignment of electronic levels, and electron-vibrational dynamics.

HL 18: Focus Session: Nanoscale Light-matter Interaction I

The focus session highlights recent breakthroughs in resolving the optoelectronic properties of individual nanostructures down to the atomic scale. Moreover, the session introduces the rich field of surface polaritons, confined electromagnetic modes through which light can be guided on subwavelength scales.

The focus session is organized by Markus Huber (U Regensburg) and Fabian Mooshammer (U. Regensburg).

Time: Tuesday 9:30–13:00 Location: H17

Invited Talk HL 18.1 Tue 9:30 H17

Ultrafast Nano-Spectroscopy of Photo-Induced Dynamics in Low-Dimensional Materials — •Takashi Kumagai — Institute for Molecular Science, Okazaki, Japan

Low-dimensional semiconductors have been extensively studied as platforms for fascinating physics and as potential components for quantum nano-devices. Their low dimensionality leads to unique physical properties, driven by strong quantum confinement and reduced dielectric screening. However, this also renders low-dimensional materials highly sensitive to local structures and interactions with their surroundings. To fully understand their superior properties, it is essential to investigate their local structures and how they correlate with photo-induced dynamics. Recently, ultrafast infrared nano-spectroscopy based on scanning near-field optical microscopy (IR-SNOM) has emerged as a powerful tool to directly visualize local structures and dynamics in real time and space at the nanoscale. I will present our latest research to apply ultrafast IR-SNOM to explore nanoscale photo-induced dynamics in low-dimensional materials [1]. In single-layer transition metal dichalcogenides, we have visualized the local many-body dynamics of high-density electron-hole plasma, uncovering the significance of dynamic heterogeneity linked to the non-uniform optoelectronic properties. Furthermore, we have extended ultrafast IR-SNOM to study local exciton dynamics in single-walled carbon nanotubes (SWCNTs). Within individual, isolated SWCNTs, the non-uniform formation of electron-hole pairs is correlated with local strain. [1] Y. Wang, J. Nishida et al. ACS Photonics, accepted.

Invited Talk HL 18.2 Tue 10:00 H17

Landau level Nanoscopy of charge and heat transport in low-dimensional heterostructures — •Mengkun Liu — Stony Brook University

In contemporary condensed matter physics and photonics, four key length scales play an essential role in shaping the behavior of quantum materials: (1) the polaritonic wavelength, which governs light confinement and light-matter interactions; 2) the magnetic lengths, determined by the magnetic field B, which constrains electron motion; 3) the diffusion length of the hot carriers at interfaces and the edges, which dictates energy relaxation, and 4) the periodicities of superlattices induced by moiré engineering, which defines the energy scale of emerging quantum phases. For instance, the commensurability of the magnetic lengths (~10 nm for graphene at 7T) and superlattice constant (~10 nm for twisted bilayer graphene at "magic" angle) would give rise to exotic fractal quantum states. In this talk, I will present: 1) A cutting-edge optical spectroscopy technique, Landau-level nanoscopy, capable of simultaneously probing all four critical length scales in a single experiment; 2) the discovery of classes of infrared polaritons that can be tuned by magnetic fields, enhancing our ability to manipulate light-matter interactions and probe many-body physics at the nanoscale; 3) nanoscale mapping of thermoelectric properties in the quantum Hall bulk, revealing strong violations of the Wiedemann-Franz law. Our approach establishes Landau-level nanoscopy as a versatile platform for investigating magneto-optical effects and many-body interactions at the nanoscale.

Invited Talk HL 18.3 Tue 10:30 H17

Real space mapping of electrically tunable anisotropic THz plasmon polaritons in hBN encapsulated black phosphorus — •Eva Pogna — Institute of Photonics and Nanotechnology, CNR-IFN, Milan, Italy

Polaritons in two-dimensional layered crystals offer effective means to confine and manipulate terahertz (THz) electromagnetic waves at the nanoscale, a crucial step in advancing photonic technologies.

In this study, we investigate anisotropic plasmon polaritons in black phosphorus nanoflakes at THz frequencies, utilizing near-field photocurrent nanoscopy combined with THz hyperspectral near-field scattering techniques.

Encapsulation with hexagonal boron nitride protects black phosphorus from air-induced degradation, while field-effect transistor (FET) devices enable photo-thermoelectric detection of plasmon polaritons.

Our findings reveal highly confined, gate-tunable plasmon polaritons with subwavelength dispersion ($\sim \lambda/76$ at 2.01 THz).

The dielectric anisotropy of black phosphorus leads to polaritons with elliptic wavefronts at THz frequencies, enabling enhanced confinement and control over THz field propagation. Moreover, electrostatic control of carrier density allows precise tuning of polariton wavelength, highlighting the versatility of this platform for nanoscale THz light manipulation and reconfigurable infrared nanophotonics.

Notably, the four-gate FET architecture introduced here to examine in-plane propagation anisotropy can be readily adapted for the study of other anisotropic conductive materials.

15 min. break

Invited Talk HL 18.4 Tue 11:15 H17

Ultra-confined THz hyperbolic phonon polaritons in a transition metal dichalcogenide — Ryan A. Kowalski[1], Niclas S. Mueller[2], Gonzalo Alvarez-Perez[3], Maximilian Obst[4], Katja D. Granados[1], Giulia Carini[2], Aditha Senarath[1], Saurabh Dixit[1], Richarda Niemann[1,2], Ragu B. Iyer[5], Felix Kaps[4], Jakob Wetzel[4], J. Michael Klopf[6], Ivan I. Kravchenko[7], Deliang Bao[1], Sokrates T. Pantelides[1], Martin Wolf[2], Lukas Eng[4], Pablo Alonso-Gonzalez[3], Susanne Kehr[4], Thomas G. Folland[5], •Alexander Paarmann[2], and Joshua D. Caldwell[1] — [1]Vanderbilt University, Nashville, TS, USA — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [3]University of Oviedo, Oviedo, Spain — [4]TUD Dresden University of Technology, Dresden, Germany — [5]The University of Iowa, Iowa City, IA, USA — [6]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [7]Oak Ridge National Laboratory, TN, USA

Phonon polaritons are hybrid light-matter quasiparticles in polar crystals that enable waveguiding of light on length scales much smaller than the photon wavelength. Here, we introduce $HfSe_2$ as a new van der Waals material that supports phonon polaritons in the terahertz (THz) spectral range. Using THz near-field optical microscopy, we demonstrate extreme confinement of light from 61 μm free-space wavelength to 245 nm. We show that the origin of this record-high confinement is an exceptionally large light-matter coupling of hyperbolic $HfSe_2$.

Invited Talk HL 18.5 Tue 11:45 H17

Programmable polariton nanophotonics using phase-change materials — •Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

Tailoring light-matter interaction is essential to realize nanophotonic components and can be achieved with polaritons, an excitation of photons coupled to charges in metals and semiconductors. Adding a thin layer of Phase-change material (PCM) leads to stronger polariton confinement and enables optical writing of resonator structures based on a change in the refractive index [1]. The recently introduced plasmonic PCM In_3SbTe_2 (IST) can be reversibly switched from an amorphous dielectric to a crystalline metallic state, enabling optically re-writable IR nanoantennas and metasurfaces [2].

Here, we show direct optical writing of resonators for surface phonon polariton (SPhP) by crystallizing IST on top of a SiC crystal and investigate the strongly confined resonance modes with s-SNOM. Reconfiguring the size and shape of the resonators leads to mode confinements of $\lambda/35$ [3]. We also demonstrate the real-space imaging of IR surface plasmon polaritons on bulk doped semiconductors, enabled by the strong polariton confinement induced by the added thin dielectric PCM layer [4]. Our concept allows for the rapid prototyping of reconfigurable structures for polaritonics, especially useful with anisotropic 2d materials.

[1] Li et al., *Nat. Mat.* **15**, 870 (2016) [2] Heßler et al. *Nat. Com.* **12**, 924 (2021) [3] Conrads et al. *Nat. Com.* **15**, 3472 (2024) [4] Conrads et al. *Sci. Adv. under review*

HL 18.6 Tue 12:15 H17

Heralding non-classical light by tailored free-electron interactions with photonic modes — •Armin Feist[1,2], Guanhao Huang[3,4], Germaine Arend[1,2], Yujia Yang[3,4], Jan-Wilke Henke[1,2], Zheru Qiu[3,4], Hao Jeng[1,2], Arslan Sajid Raja[3,4], Rudolf Haindl[1,2], Rui Ning Wang[3,4], Tobias J. Kippenberg[3,4], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, DE — [2]4th Physical Institute, University of Göttingen, DE — [3]Institute of Physics, EPFL, Lausanne, CH — [4]Center for Quantum Science and Engineering, EPFL, Lausanne, CH

Integrated photonics facilitates control over fundamental light-matter interactions in manifold quantum systems. Extending these capabilities to electron beams [1] fosters free-electron quantum optics.

Here, we show the coupling of single electrons and photons at an integrated photonics waveguide [2,3]. Spontaneous scattering of the nanoscale-focused electron beam at empty optical modes creates multi-photon superposition states. Energy-selective and event-based electron detection enables herald-

ing non-classical light, which we characterize by intensity correlations in a Hanbury Brown and Twiss (HBT) setup, showing high-fidelity single-photon generation [3].

This provides a pathway toward novel hybrid quantum technology with entangled electrons and photons, as well as the capability for quantum-enhanced electron imaging and Fock-state photon sources.

[1] J.-W. Henke *et al.*, Nature **600**, 653 (2021). [2] A. Feist *et al.*, Science **377**, 777 (2022). [3] G. Arend *et al.*, arXiv:2409.11300 (2024)

HL 18.7 Tue 12:30 H17

Attosecond electron microscopy using free-electron homodyne detection — •John H. Gaida[1,2], Sergey V. Yalunin[1,2], Hugo Lourenço-Martins[1,2], Murat Sivis[1,2], Thomas Rittmann[1,2], Armin Feist[1,2], F. Javier García de Abajo[3,4], and Claus Ropers[1,2] — [1]MPI for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany — [3]ICFO-Institut de Ciencies Fotoniques, Castelldefels (Barcelona), Spain — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

Advancements in condensed matter science aim to map material structures and dynamics at levels of ångströms and attoseconds. Although X-ray and electron methods offer structural detail, attosecond temporal resolution is progressing through optical spectroscopy techniques. Techniques like PINEM allow nanometric resolution imaging of near-field intensities [1], but to examine the evolution of nanoscale fields and structures within the light cycle, optical phase sensitivity is needed, as provided by phase-contrast Lorentz PINEM [2], interferometric detection [3], or electron pulse bunching [4]. This contribution introduces Free-Electron Homodyne Detection (FREHD), a universally applicable approach for high spatiotemporal resolution imaging of phase-resolved optical responses [3].

[1] B. Barwick *et al.*, Nature **462**, 902–906 (2009). [2] J. H. Gaida *et al.*, Nat. Commun. **14**, 6545 (2023). [3] J. H. Gaida *et al.*, Nat. Photonics **18** 509–515 (2024). [4] K. E. Priebe *et al.*, Nat. Photon. **11**, 793–797 (2017).

HL 18.8 Tue 12:45 H17

Light-matter interaction on subcycle time and atomic length scales — •Tom Siday[1,2], Johannes Hayes[1], Felix Schiegl[1], Fabian Sandner[1], Peter Menden[1], Valentin Bergbauer[1], Martin Zizlsperger[1], Svenja Nerreter[1], Sonja Lingl[1], Jascha Repp[1], Jan Wilhelm[1], Markus A. Huber[1], Yaroslav A. Gerasimenko[1], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham, UK

Near-field microscopy has revolutionized the study of nanoscale light-matter interaction, achieving subcycle temporal and ~10 nm spatial resolution. However, the geometry of the tip apex has so far restricted access to atomic resolution. By harnessing extreme nonlinearities within tip-confined evanescent light fields, we introduce a novel contrast mechanism, advancing all-optical microscopy to the atomic scale while preserving subcycle temporal resolution. This Near-field Optical Tunnelling Emission (NOTE) microscope can resolve nanometer-scale packing defects on a gold surface and trace the subcycle quantum flow of electrons between the scanning tip and a semiconducting van der Waals trilayer in real time. Moreover, NOTE microscopy is compatible with insulating samples, where rectified currents cannot flow, and enables the integration of all-optical subcycle spectroscopy with atomic-scale resolution. Thus, NOTE provides direct access to atomic-scale quantum light-matter interactions and dynamics on their natural spatial and temporal scales.

HL 19: Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)

In recent years, significant progress has been made in realizing and exploring correlated quantum states in multilayer moiré heterostructures of graphene or transition metal dichalcogenides. These achievements have been made possible by the high level of control and tunability of these systems. Striking phenomena have been demonstrated experimentally, including unconventional superconductivity, fractional quantum anomalous Hall states, Mott-Wigner states and density waves, as well as kinetic ferromagnetism. Moreover, recently novel spectroscopic experimental techniques have been developed which allow for new ways to explore the dynamical response of these exotic states. This focus session will discuss recent experimental advancements as well as theoretical developments in the field of strongly correlated moiré heterostructures.

Organizers: Dmitri K. Efetov (LMU München), Michael Knap (TU München)

Time: Tuesday 9:30–13:15 Location: H36

See TT 18 for details of this session.

HL 20: Poster I

The first poster session covers the physics of semiconductor heterostructures, interfaces and surfaces. Moreover, most recent results on oxide semiconductors, as well as perovskite and photovoltaics are presented.

Time: Tuesday 10:00–12:30 Location: P3

HL 20.1 Tue 10:00 P3

Accuracy Requirements for Polarizabilities in MD-based Raman Spectra — •Markus Amaseder[1], Manuel Grumet[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Faculty of Natural Sciences, Comenius University Bratislava — [3]Institute of Inorganic Chemistry, Slovak Academy of Sciences

Raman spectroscopy provides a versatile and accessible method for characterizing atom dynamics in materials. While frozen phonon approaches have proven well for the prediction of Raman spectra in many cases, they do not inherently include anharmonic and temperature-dependent effects. Raman spectra calculated from molecular dynamics (MD) offer an alternative [1] and have received considerable interest. However, they remain computationally challenging as they require many single-point polarizabilities. We have shown previously that machine learning (ML) can aid in the speed-up using a delta learning approach [2]. However, it is still to be fully understood how accurate single-point polarizabilities need to be in order to provide sufficiently correct spectra. We present an evaluation of polarizabilities from density functional theory and ML for MD Raman spectra, investigating the effects of the functional and further parameters. This is relevant both in terms of training data and ML predictions. Since many single-point calculations are needed, the trade-off between accuracy and computational cost is crucial for the practical application of MD-based Raman spectra. [1] Thomas, et al. Phys. Chem. Chem. Phys. 15, 6608-6622 (2013) [2] Grumet, et al. J. Phys. Chem. C 128, 6464-6470 (2024)

HL 20.2 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain

structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility $\mu_h = 25$ $cm^2V^{-1}s^{-1}$ being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measurement, the ionization energy of shallow acceptors $E_{I,S}$ = 137 ± 8 meV and deeper acceptors $E_{I,D}$ = 262 ± 23 meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.3 Tue 10:00 P3

Semiconductor membrane transfer for deterministic Circular Bragg Gratings fabrication — •Juan Nicolas Claro Rodriguez, Dennis Deutsch, Leonie Schubert, Dirk Reuter, and Klaus Joens — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn

Highly indistinguishable single photons and strongly entangled photon-pairs are fundamental for photonic quantum communication [1]. InGaAs quantum dots (QDs) grown on InP substrates using MBE deposition [2] emit in the telecom C-band, making them ideal for long-distance communication, though their brightness is limited. Embedding these QDs in hybrid Circular Bragg Gratings (CBGs) enhances photon collection efficiency and the Purcell factor, supported by a backside mirror and transparent medium configuration [3]. We present a membrane transfer method involving backside mirror growth, press-bonding, and InP substrate removal via HCl etching, enabling emitter localization and CBG integration. PL spectra are used to assess sample quality.

[1] Applied Physics Letters, 118(10), 100502. [2] AIP Advances, 13(5). [3] Journal of the Korean Physical Society, 73(10), 1502*1505.

HL 20.4 Tue 10:00 P3

Comparative Investigations of GaN/p-GaInP and p-GaInP Photocathodes: Stability and Performance in Acidic Electrolytes — •Sahar Shekarabi[1], Mohammad Amin Zare Pour[1], David Osteimer[1], Haoqing Su[2], Wentao Zhang[2], Agnieszka Paszuk[1], Wolfram Jaegermann[3], Shu Hu[2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Yale University, Department of Chemical and Environmental EngineeringNew Haven, USA — [3]Technische Universität Darmstadt, Department of Materials and Earth Sciences, Darmstadt, Germany

GaInP(100) is a widely used photoabsorber in tandem solar cells and photoelectrochemical (PEC) devices. To enhance stability against photo-induced corrosion, GaN passivation layers have been employed. This study evaluates the stability of p-GaInP/GaN and p-GaInP electrodes for solar-driven hydrogen evolution reactions (HER) in 1.0 M HClO4. Faradaic efficiency was monitored via gas chromatography during PEC, while X-ray photoelectron spectroscopy and atomic absorption spectroscopy were used to investigate surface and dissolution process conditions. The large valence band offset of around 2.0 eV at the GaN/p-GaInP interface acts as a hole barrier, reducing recombination, while conduction band alignment facilitates electron transport. The GaN passivation layer enhances stability and achieves a low onset potential of -0.5 V for HER. Surface and electronic structural changes were analyzed to understand corrosion mechanisms.

HL 20.5 Tue 10:00 P3

Characterization of surfaces of mixed semiconductor crystals — •Marsel Karmo[1] and Martin Brehm[2] — [1]Warburger Str. 100 33098 Paderborn — [2]Warburger Str. 100, 33098 Paderborn

Compositionally disordered crystals, also known as mixed-crystals, play a crucial role in semiconductor engineering. They enable the manipulation of material properties such as the band gap, which is important for opto-electronic devices like solar cells. Additionally, these crystals are used as buffer layers to mitigate strain from lattice constant mismatches between different material layers. However, accurately describing mixed crystals theoretically presents significant challenges. Due to the random occupation of atomic sites it is not possible to introduce a unit cell in other words the crystal as a whole is the unit cell. This prohibits also the use of boundary conditions. A commonly used approach to approximate mixed crystals is the Supercell Method (SCM), which employs a large, unit cell with random atomic site occupations. While this method approximates a mixed crystal, it is limited by computational resources. Another approach is the Virtual Crystal Approximation (VCA), which replaces the mixed crystal with an analytically averaged system. This method reduces the computational effort by using a smaller unit cell but may overlook local atomic environments, potentially limiting its ability to capture certain physical properties. In this work, we compare these two methods, VCA and SCM within the Vienna Ab Initio Simulation Package (VASP) to evaluate their performance in calculating the electronic structure and surface formation energy.

HL 20.6 Tue 10:00 P3

Photoelectrochemical characterisation of InGaN/GaN nanowire arrays — •Genrietta Steingelb[1], Hannah Nell[1], Rudolfo Hötzel[1], Ruben Neelissen[1], Stephan Figge[1], Tim Grieb[1], Florian Krause[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them ideal candidates for use as electrochemical biosensors [1]. In this work, we present a detection mechanism that combines simultaneous photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, allowing sensitive and selective detection of redox-active biomolecules. However, the performance of the NW photoelectrode is limited by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly caused by unpassivated surface states. The deposition of ultrathin metal oxide films is a possibility to suppress such effects. The influence of surface coatings on sensor properties was analysed through photoelectrochemical characterisation, with and without metal oxide coatings. This analysis highlights how surface modifications affect sensor performance for the detection of redox-active molecules in complex biochemical environments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003).

HL 20.7 Tue 10:00 P3

Impact of Surface States on the Performance and Stability of AlGaAs/GaAs HEMT Structures — •Vincent Leon Spreter[1,2], Selma Delic[1,2], Xuelin Jin[1,2], Nils von den Driesch[1], Christoph Krause[1], Detlev Grützmacher[1,2], and Beata Kardynal[1,2] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, RWTH, 52074 Aachen, Germany

Electrostatic gating is commonly used to define single-electron quantum dots (QDs) in two-dimensional electron gases, such as those in GaAs/AlGaAs heterostructures. It can also be used to tune the electronic states of epitaxial quantum dots. For the use for quantum information processing applications, gated devices must maintain a stable working point over long time.

In our contribution, we investigate the effect of surface preparation of GaAs/AlGaAs heterostructure on the long-term stability of gates on the example of split-gate devices. In addition, we explore the use of passivation layers to mitigate the effects of dangling bonds associated with surface states. We discuss the processing of devices with AlOx passivation and action of electrostatic gates on device performance, offering insights into its potential for optimizing GaAs-based optoelectronic devices.

HL 20.8 Tue 10:00 P3

Low-temperature RAS of MOVPE-prepared Si(100) surfaces — •Kai Daniel Hanke[1], Max Grossmann[2], Chris Y. Bohlemann[1], Mohammad Amin Zare Pour[1], Paszuk Agnieszka[1], Runge Erich[2], and Hannappel Thomas[1] — [1]1Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]2Technische Universität Ilmenau, Theoretical Physics I, Ilmenau, Germany

Recent studies have shown that As-modified Si(100)-(2 x 1) surfaces prepared in a MOCVD environment exhibit asymmetric hydrogen-passivated Si-As dimers as dominating surface motif, in contrast to the previously assumed symmetric As dimers. Due to the importance of this surface for subsequent nucleation of III-V materials, such as GaP, for high-efficiency solar cell structures, we have performed low-temperature reflection anisotropy spectroscopy measurements, which are extremely surface sensitive, in combination with density functional theory and many-body perturbation theory calculations. We also performed X-ray photoelectron spectroscopy and low-energy electron diffraction measurements for a detailed understanding of the structure and electronic properties of this surface. Our method seeks to improve knowledge of the spectral properties of semiconductor surfaces by combining theoretical understanding with experimental data to understand the complex variables that influence RAS spectra.

HL 20.9 Tue 10:00 P3

Optimization of GaSb(100) Substrate Preparation for MBE Growth of GaSb Layers — •Peter Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany

The preparation of epi-ready substrates for MBE growth typically involves degassing and oxide removal. The latter is often done by thermal processes, resulting in rough interfaces that are associated with pyramidal defects (PDs) in GaSb layers grown on GaSb(100) substrates [1].

This study aims to optimize GaSb substrate preparation and buffer layer growth to reduce PD formation.

We compare standard thermal oxide desorption to methods proposed in the literature, such as Ga-assisted oxide removal [2] and the insertion of an AlAsSb layer into the buffer layer [1].

Using photoluminescence spectroscopy (PL) mapping, we assess quantum well and buffer layer luminescence as indicators of material quality. Additionally, we analyze the surface morphology with atomic force microscopy (AFM), focusing on the properties of pyramidal defects.

[1] Murray, Lee M., et al. *J. Vac. Sci. Technol. B* **31.3** (2013).
[2] Mathews, Sen, et al. *J. Vac. Sci. Technol. B* **35.2** (2017).

HL 20.10 Tue 10:00 P3

Passivation Protection Layers for Highly efficient Multi-Absorber Devices for Photoelectrochemical Solar Fuel Production — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Jennifer Velázquez Rojas[3], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]Paszuk Group, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

In photoelectrochemical cells with the highest solar-to-hydrogen conversion efficiencies, the heterointerface between a III-V top layer and a metal oxide protection layer should be optimized to minimize charge carrier losses. Using photoemission spectroscopy, we study the TiO_2/InP(100) heterointerface as a function of InP surface preparation and Ti precursor.

InP(100) substrates were prepared with either a well-ordered, phosphorus-terminated surface in a metal-organic chemical vapor deposition (MOCVD) reactor or with a thin oxide layer. TiO_2 was deposited via atomic layer deposition (ALD) using either titanium tetrachloride ($TiCl_4$) or titanium isopropoxide (TTIP) as the Ti precursor, along with water as the co-reactant.

Depending on the Ti precursor and the InP surface preparation, we observed either a nucleation delay or acceleration and differences in the band alignment. Layers grown with the TTIP precursor showed the presence of Ti^{3+} states, which may act as trap centers.

HL 20.11 Tue 10:00 P3

Characterization of Arsenic- and Antimony Containing Heterostructures Grown by Molecular Beam Epitaxy — •Max H. W. Ziehfreund[1], Peter F. Zajac[1], Sascha R. Valentin[2], Timo A. Kurschat[1,2], Rainer Krage[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik der Ruhr-Universität Bochum, 44801 Bochum, NRW, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, NRW, Germany

This study focuses on the investigation of the surface morphology of various arsenic- and antimony-containing semiconductor heterostructures grown by molecular beam epitaxy. The objective is to optimize the growth parameters used in fabrication and to gain a better understanding of the underlying growth process. The characterization methods developed and approved for GaAs-based heterostructures are applied to GaSb-heterostructures. The primary methods employed are photoluminescence spectroscopy and atomic force microscopy. It was possible to examine the influence of various parameters, such as the antimony flux used during growth on the epitaxial quality of the grown layers and collect valuable experience for defect-free growth of arsenic- and antimony-containing heterostructures.

HL 20.12 Tue 10:00 P3

High Resolution Temperature Mapping of GaSb Wafers during MBE Growth — •Timo A. Kurschat[1], Sascha R. Valentin[1], Peter Zajac[2], Rainer Krage[1], and Andreas D. Wieck[2] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, D-44143 Dortmund — [2]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44801 Bochum

The substrate temperature is one of the most important parameters during MBE growth. Thermocouples and pyrometers, as well as more advanced techniques, measure only a single spot on the wafer at a time. Knowing the temperature distribution allows to optimize the growth parameters from just a single grown sample.

To obtain high-resolution thermal maps we use a commercial SLR camera with its infrared filter removed. The sensor is sensitive up to a wavelength of about 1000 nm and can therefore be used as a high resolution pyrometer. Without substrate rotation and 10 s exposure time, measurements can be made down to T_S = 400 °C. With rotation enabled and a reduced exposure time of 0.25 s, it is still possible to obtain images at the growth temperature of T_S = 680 °C.

Images of quarter 2-inch GaSb wafers show differences of more than 20 K between the center and the corners. The effect of a washer was investigated with this method, which is a ring placed at the backside of the wafer to improve its temperature uniformity. The temperature differences also effect the photoluminescence intensity of a quantum well grown on the wafer.

HL 20.13 Tue 10:00 P3

Raman spectroscopy on MBE grown III-V semiconductors heterostructures — •Arijit Chakraborty[1], Yiteng Zhang[1], Tom Fandrich[1], Doaa Abdelbarey[1], Tom Rakow[1], Krupali Dobariya[1], Sulabh Shrestha[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover, Institute for Solid State Physics, Hannover, Germany — [2]Leibniz Universität Hannover, Laboratorium for Nano- und Quantum Engineering, Hannover, Germany

We present micro-Raman spectroscopic measurements on molecular beam epitaxy (MBE) grown semiconductors heterostructures, and quantum dots. This technique offers unique insights into the vibrational modes, crystal structure, strain, alloying effects and defects of grown semiconductor structures, making it invaluable for the optimization of MBE processes. The Raman results for the relaxed material have been interpreted in the framework of the modified random element isodisplacement theory considering different vibrational modes of the lattice with changing compositional range. Optical-phonon deformation potentials have been successfully used to fit the different vibrational phonon frequencies in strained layers of semiconductors. Using comparable theoretical models, a substantial compositional dependency with phononic vibrations is found and established. Disordered activated vibrational modes are investigated for layers produced on various substrates. An analogous conclusion with the peak shift in photoluminescence spectra is reached by analyzing the Raman spectra of herostructures grown on InP-based substrates.

HL 20.14 Tue 10:00 P3

Copper tin oxide: an amorphous, bipolar, ternary oxide system with tunable electrical and optical properties — •Arne Jörns, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics

Copper oxide (CuO) is one of the most studied p-type semiconducting metal oxides [1]. Tin oxide (SnO_2) features high transparency in the visible range, high n-type electrical conductivity and non-toxicity [2]. Due to mismatching crystal structures of CuO and SnO_2 (and their other oxidation states) an amorphous alloy, copper tin oxide (CTO), can form when combining these materials. Depending on growth pressure and cation composition the material can be p-type [1] or n-type making it a promising candidate for complementary amorphous devices. In this work, we investigated physical properties of CTO thin films, deposited by combinatorial pulsed laser deposition of segmented CuO and SnO_2 targets at room temperature and in oxygen atmosphere, as a function of cation composition and growth pressure. The resulting samples are X-ray amorphous and n-type semiconducting with mobilities up to 11 cm^2/Vs for Cu/(Cu + Sn) < 0.8. Optical and electrical properties can be tuned by varying composition ratio and oxygen pressure. A temperature-dependent Hall effect analysis has led to the conclusion that the percolation model provides the most accurate description. For Cu/(Cu + Sn) > 0.8, the samples become p-type conducting and feature low mobilities.

[1] Isherwood *et al.*: J. Appl. Phys., 118, 105702, (2015)
[2] Ni *et al.*: Surface and Coating Technology, 206, 4356-4361, (2012)

HL 20.15 Tue 10:00 P3

low-temperature buffer layer-assisted heteroepitaxial growth of γ-CuI thin films by pulsed laser deposition: tailoring electrical properties — •Yang Chen[1], Michael S. Bar[1], Susanne Selle[2], Daniel Splith[1], Michael Lorenz[1], Marius Grundmann[1], and Holger v. Wenckstern[1] — [1]Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, 04103 Leipzig, Germany — [2]Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle, Germany

As the first discovered p-type transparent conductive material, copper(I) iodide (CuI) is considered to be among the most competitive p-type candidate in the field of transparent electronics. Herein, we introduced a low-temperature buffer-layer-assisted strategy to grow γ-CuI on c-plane sapphire by pulsed laser deposition with unprecedented structural quality and electrical transport properties. By adjusting the growth temperature, we can manipulate the rotation domain structure, control the hole concentration in the range from 10^{14} cm^{-3} to 10^{19} cm^{-3} and achieve mobility μ_h = 25 $cm^2V^{-1}s^{-1}$ being similar to that of bulk CuI. Based on the temperature dependent Hall-effect measurement, the ionization energy of shallow acceptors $E_{I,S}$ = 137 ± 8 meV and deeper acceptors $E_{I,D}$ = 262 ± 23 meV were determined. This strategy not only enables high-quality CuI film preparation, but also to tailor their electrical properties for integration with n-type semiconductors in transparent electronic circuits.

HL 20.16 Tue 10:00 P3

Mechanical, electronic and optical properties of $LiNbO_2$ and $NaNbO_2$ from first-principles calculations — •Frederik Schmidt and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

The layered compound $LiNbO_2$ is of interest as a superconductor and possible battery material, but its electronic and optical properties have not yet been extensively analyzed, especially in theoretical simulations. There are even fewer studies of the closely related $NaNbO_2$. In this work, we perform first-principles calculations to investigate the properties of $LiNbO_2$ and $NaNbO_2$. The elastic constants and related parameters, such as elastic moduli, are determined using density-functional theory. We show that even small biaxial strain up to ±5%, which corresponds to common substrates like $MgAl_2O_4$ or SiC, may lead to significant changes in the electronic band structure and to a qualitative transition from a direct to an indirect band gap. Accurate results for the electronic band structure and the optical absorption spectrum are obtained from the *GW* approximation and the Bethe-Salpeter equation. We find that both the quasiparticle corrections and excitonic effects have a significant influence on the dielectric function. Good quantitative agreement with the experimentally measured absorbance and the absorption edge at 2 eV for $LiNbO_2$ is achieved only by a proper inclusion of both factors.

HL 20.17 Tue 10:00 P3

Bismuth oxyselenide (Bi2O2Se): Insights into chemical bonding and structural properties — •Sumayya Sumayya[1], Yuan Yu[1], Carl Friedrich Schon[1], Kim Dasol[1], Yueyang Yang[2], and Matthias Wuttig[1] — [1]RWTH, Aachen, Germany — [2]Tsinghua University, China

The Bismuth Oxychalcogenides (Bi2O2X, X=S, Se, Te) are potential candidates in various fields such as Thermoelectrics, Ferroelectrics, Piezoelectrics, and photodetectors due to their unique 2D layered structure containing a bismuth oxide layer and a chalcogen layer. In this family, Bi2O2Se is considered the 2D rising star for the semiconductor industry because of its high crystallographic symmetry, tunable band gap, ultra-high electron mobility, strong Shubnikov-des Haas quantum oscillations, unique defects, and excellent stability. The relationship between bonding and material properties offers a versatile platform for tailoring electronic and vibrational properties, potentially leading to improved functional characteristics. Recently, many theoretical and experimental bonding descriptors such as electron transferred and shared values, Born effective charge, electrical conductivity, optical dielectric constant, Grüneisen parameter, and Probability of Multiple events in atom probe tomography have been devised. Our study employs a combination of advanced characterization techniques and theoretical calculations to probe the nature of bonding at different length scales, from local atomic level to extended structural motifs. In the future, this model can be used for other layered materials to understand the structure-property relationship via chemical bonding.

HL 20.18 Tue 10:00 P3

Reactive Sputter Deposition and Nitrogen Modification of $CuBi_2O_4$ as Photocathode — •Dominic Rapf[1,2], Tsedenia A. Zewdie[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, D-85748 Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, D-85748 Garching, Germany

Copper bismuthate ($CuBi_2O_4$) is a ternary oxide that is of special interest for photoelectrochemical (PEC) water splitting. Unlike most transition metal oxides, which predominantly exhibit n-type conductivity, copper bismuthate is a native p-type semiconductor. [1] In addition, it has a suitable bandgap for the absorption of visible light, as well as a high photocurrent onset potential > 1 V vs. RHE. [2] These properties make $CuBi_2O_4$ highly desirable as a photocathode. This project focuses on the development of reactive co-sputter recipes to deposit copper bismuthate thin films and their structural, optical, morphological and opto-electronic analysis. In addition, we explore nitrogen incorporation to narrow the band gap of $CuBi_2O_4$ for more efficient light absorption (N:$CuBi_2O_4$). By modifying the nitrogen content in the reactive gas mixture and applying post-annealing treatments, we can tailor the level of nitrogen incorporation. On a library of N:$CuBi_2O_4$ thin films, we investigate the impact of nitrogen incorporation on optical and structural properties and assess their PEC performance.

[1] J. K. Cooper et al., Chem. Mater. 2021, 33, 3, 934–945 [2] D. Kang et al., Chem. Mater. 2016, 28, 12, 4331–4340

HL 20.19 Tue 10:00 P3

The impact of Bi and Na non-stoichiometry on the electrocaloric effect in (Na0.5Bi0.5)TiO3-BaTiO3 ceramics — •Sobhan M. Fathabad, Mohammadamin H. Kashani, Eva Kröll, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisubrg-Essen (CENIDE), University of Duisburg Essen, Essen, Germany

The electrocaloric effect (ECE) is the phenomenon where polar crystals experience a change in isothermal entropy or adiabatic temperature in response to the application or removal of an electric field. In this work, we investigate the influence of Bi and Na non-stoichiometry on the depolarization mechanism and electrocaloric effect in BaTiO3 - (Na0.5Bi0.5)TiO3 compounds at the morphotropic phase boundary. Ceramic samples were prepared using the solid-state synthesis method. The polarization hysteresis loops were measured in the temperature range from -20 °C to 200 °C and subsequently the ECE was indirectly estimated in the framework of the thermodynamic approach based on the Maxwell relation. The depolarization temperature was studied using dielectric permittivity, X-ray diffraction, and pyrocurrent analysis. Direct measurements of the ECE were conducted using a quasi-adiabatic calorimeter. It was shown that the introduced defects reduce the depolarization temperature, consequently shifting the maximum ECE towards room temperature.

HL 20.20 Tue 10:00 P3

Structure and lattice distortions of KTaO3(001) studied by LEED I-V and nc-AFM — Dominik Wrana[1,2], Marek Kuzmiak[1], Michele Reticcioli[3], Tomas Dolak[1], Florian Kraushofer[4], Michele Riva[5], Aji Alexander[1], Llorenc Albons[1], Jesus Redondo[1], Cesare Franchini[3], and •Martin Setvin[1] — [1]Charles University, Prague, Czech Republic — [2]Jagiellonian University, Krakow, Poland — [3]University of Vienna, Vienna, Austria — [4]TU Munich, Germany — [5]TU Wien, Vienna, Austria

Perovskites attract attention in many fields, yet understanding their surface structure represents a challenge. Special emphasis is focused on little lattice distortions associated with ferroelectric properties, often present in this broad class of materials. Hydroxylated KTaO3(001)-(2x1) is used here as a test case to extract the precise positions of lattice atoms by means of low energy electron diffraction (LEED) I-V, obtaining a final Pendry R-factor below 0.17. The main challenge lies in the extreme sensitivity of this surface to damage induced by the electron beam; the progressing damage is visualized at the atomic scale by noncontact atomic force microscopy (nc-AFM). Positions of lattice atoms obtained from LEED I-V analysis are used as a benchmark for a comparison with theoretical calculations performed within 30 different setups. The overall trend is that the closest match with the experiment is obtained for setups without the Hubbard U-term and with the SCAN functional

Work supported by GACR 20-21727X and MSMT LL2324.

HL 20.21 Tue 10:00 P3

Photoluminescence and photophysical properties of halide perovskite MAPbBr3 single crystal — •Liangling Wang[1,2], Francesco Vitale[2], Edwin Eobaldt[2], Thomas Alexander Zaunick[2], and Carsten Ronning[2] — [1]School of Physics and Technology, University of Jinan, Jinan 250022, P. R. China — [2]Institute of Solid State Physics, Friedrich-Schiller University Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The remarkable optoelectronic properties of halide perovskite MAPbBr3 (MA=methylammonium), including near-unity photoluminescence quantum yield (PL QY), small full width at half-maximum (FWHM), tunable bandgap by mixing halide and defect tolerance, make it a compelling candidate material in solar cell, light emitting diodes (LED), photodetectors, X-ray imaging, and so on. The PL spectrum of MAPbBr3 at room temperature can be deconvoluted into two emission peaks. The major peak at 545 nm arises from band-to-band transition, while the lower energy peak at 560 nm is associated with recombination in trap states (Br vacancies) below the optical gap. Interestingly, PL enhancement of MAPbBr3 is found under certain laser irradiation, indicating that the surface defects are benefit charge carrier trapping and recombination. In order to verify the origin of the emission centers, power dependent PL, including both power increase and decrease processes, will be analyzed. Furthermore, thermal activation and excitonic effects of PL under different temperature from cryogenic temperature of liquid Helium to room temperature will be investigated.

HL 20.22 Tue 10:00 P3

Resolving temporal signatures of optical excitations in semiconductor nanostructures — •Lion Krüger, Fabian Brütting, Moritz B. Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Characteristic ultrafast signatures in the photo-induced response of nanostructured materials encode the class of optical excitations and characterize the performance for opto-electronic applications. Time-resolved visible transient absorption (TA) spectroscopy and optical pump THz probe (OPTP) spectroscopy are well-established methods for contact-free probing of ultrafast dynamics. Here, we present correlated TA-OPTP measurements performed in a setup that combines multiple probing modalities under identical excitation conditions. In particular, we present different strategies to enhance detection speed and sensitivity, enabling the disentanglement of free carrier and excitonic signatures in semiconductor nanostructures of varying dimensionality and quantum-confinement [1].

[1] Motti, Silvia G., et al. "Exciton Formation Dynamics and Band-Like Free Charge-Carrier Transport in 2D Metal Halide Perovskite Semiconductors". Advanced Functional Materials 33 (2023)

HL 20.23 Tue 10:00 P3

Characterization of the electrical properties of Bismuth doped Methylbenzylamine Lead Iodide 2D Perovskites using impedance spectroscopy — •Keito Mizukami[1,2,3], Hannes Hergert[1,3], Tim Schneider[3,4], Jan Heinrich Littmann[1,3], Satoko Fukumori[2], Philip Klement[1,3], Derck Schlettwein[3,4], Hirokazu Tada[2], Sangam Chatterjee[1,3], and Matthias T. Elm[1,3] — [1]Institute of Experimental Physics I, JLU Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan — [3]Center for Materials Research, JLU Giessen, Giessen, Germany — [4]Institute of Applied Physics, JLU Giessen, Giessen, Germany

Low-dimensional organic-inorganic perovskites offer largely tunable materials properties such as the crystal structure or the electronic band gap due to the flexibility of the incorporated building blocks. Perovskites with incorporated chiral organic molecules as the cation attract a lot of attention as they exhibit chiral properties such as chirality-induced spin selectivity or spin-polarized electron current. However, the typically low electrical conductivity hinders applications and requires appropriate doping schemes to improve the device performance. In this study, we investigate the impact of Bi substitution for Pb in methylbenzylamine bismuth lead iodide single crystals and thin films on the electric properties using impedance spectroscopy. Our objective is to get a fundamental understanding of the charge transportation and relaxation mechanism in these mixed conductors.

HL 20.24 Tue 10:00 P3

Hysteretic Piezochromism in a two-dimensional perovskite — •Paul Steeger[1], Mohammad Adnan[1], Thorsten Deilmann[2], Xiang Li[3,4], Susanne Müller[4], Katarzyna Skrzynska[5], Michael Hanfland[4], Efim Kolesnikov[3], Jutta Kösters[6], Theresa Block[6], Robert Schmidt[1], Ilya Kupenko[3,4], Carmen Sanchez-Valle[3], Vijaya Prakash[7], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Physikalisches Institut Universität Münster — [2]Institut für Festkörpertheorie Universität Münster — [3]Institute für Mineralogie Universität Münster — [4]Europäischer Synchrotron ESRF Grenoble — [5]Institute of Earth Sciences University of Silesia — [6]Institut für Anorganische und Analytische Chemie Universität Münster — [7]Department of Physics IIT Dehli

Two-dimensional inorganic-organic hybrid perovskites hold potential for application in the field of optoelectronics. One representative of this class of materials is cyclohexenyl-eythylammonium lead-iodide (CHPI). Here, we present pressure-dependent optical absorption and emission spectra of CHPI. We find a strong change of the band gap when exerting pressure on the crystal using a diamond anvil cell. In contrast to other 2D perovskites the bandgap of CHPI undergoes a full hysteresis loop under pressure. To reveal the origin of the observed phenomena, we combine our optical experiments with DFT calculations as well as X-ray diffraction measurements under high pressure. Reference: Steeger et al., Hysteretic Piezochromism in a Lead Iodide-Based Two-Dimensional Inorganic-Organic Hybrid Perovskite. JACS 146, 23205 (2024)

HL 20.25 Tue 10:00 P3

Electron and Hole polaron Formation in lead-free CsGeX3 (X=Cl,Br,I) perovskites — •Mehmet Baskurt — Chalmers University of Technology

The unique electronic properties of CsGeX3 (X = Cl, Br, I) perovskites make them promising candidates for nonlinear optical applications. The nature of charge localization must be understood to explain their physical and electronic behaviors. Here, we carry out a theoretical investigation on electron and hole polaron formation in CsGeX3. We carry out density functional theory calculations in the hybrid function level. Our results show that there is a trend in the polaron formation energies, CsGeCl3 > CsGeBr3 > CsGeI3. In particular, single electron polarons form highly favorably in all three materials, whereas single hole polarons can only be formed in CsGeCl3. Moreover, double electron polarons form energetically favorably across the series. These findings constitute a basis for understanding polaronic effects on the electronic properties of CsGeX3 perovskites and open up access to their optimization in nonlinear optical applications.

HL 21: Graphene: Electronic Structure and Excitations (joint session O/HL)

Time: Tuesday 10:30–12:15 Location: H6

See O 28 for details of this session.

HL 22: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

See O 29 for details of this session.

HL 23: Quantum Dots and Wires: Transport (joint session HL/TT)

Time: Tuesday 11:15–13:00 Location: H13

HL 23.1 Tue 11:15 H13

Transport properties of quantum dots for single-electron pumps — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Frank Hohls, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, 31668 Braunschweig, Germany

A single-electron pump (SEP) is a device emitting a well-defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e, this results in a current of $I = nef$. Since the revision of the SI system, the elementary charge e hereby is an exact value, so that SEPs provide a suitable basis for a quantum current standard. The accuracy of this current is directly related to erroneous cycles, where the emitted number of electrons deviates from n. Our SEP devices are based on electrostatically defined quantum dots in GaAs/AlGaAs two-dimensional electron gases. In such devices, the tunnel barriers as well as the energy levels are controllable via gate voltages. Based on multiple quantum dot devices we here investigate relations between transport properties and SEP operation characteristics.

HL 23.2 Tue 11:30 H13

Non-Markovian higher-order electron pump: improvement of efficiency — •Lukas Litzba, Jürgen König, and Nikodem Szpak — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany

We consider an electron pump that consists of a non–interacting quantum dot and electron baths. Our pumping setup utilizes only higher–order tunneling processes, which are purely quantum mechanical and have no classical analog. In order to study higher order tunneling–mechanism and non–Markovian effects, we extend the exact Heisenberg equation and the Laplace transform technique to time–dependent Hamiltonians and apply this technique to our model. Thereby, we identify parameter ranges which lead to a significant increase of the current flowing through the quantum dot and an improvement of the energetic efficiency of these processes.

HL 23.3 Tue 11:45 H13

Fast Machine-Learning assisted characterisation of current quantisation — •Wang Ngai Wong[1], Yannic Rath[1], Nikolaos Schoinas[1], Shota Norimoto[1], Masaya Kataoka[1], Alessandro Rossi[1,2], and Ivan Runnger[1,3] — [1]National Physical Laboratory, Teddington, TW11 0LW, UK — [2]Department of Physics, SUPA, University of Strathclyde, Glasgow G4 0NG, UK — [3]Department of Computer Science, Royal Holloway, University of London, Egham, TW20 0EX, UK

Characterisation of single-electron pumps (SEPs) has long been bottlenecked by the process of fine-tuning measurement parameters to study their novel properties. This limits potential experimental parameters to those that can remain static throughout the fine-tuning process. We demonstrate a novel method assisted by machine learning which has led to an eightfold speedup in the measurement process (see Appl. Phys. Lett. 125, 124001 (2024)), and in so doing opens the door to further characterisation experiments which are impossible using conventional methods. Our method is based around an active learning cycle to navigate the information landscape of the gate voltage parameter space, while also significantly reducing the number of measurement points required. This is paired with a post-processing approach which allows us to accurately predict and characterise the small operational regimes significantly more efficiently than conventional sweeps across the parameter space. We exploit the framework to characterise the behaviour of multiplexed GaAs multi-pump devices across a range of magnetic fields.

HL 23.4 Tue 12:00 H13

Novel Mixed-Dimensional Reconfigurable Field Effect Transistors — •Sayantan Ghosh[1,2], Muhammad Bilal Khan[1], Phanish Chava[1], Kenji Watanabe[3], Takashi Taniguchi[3], Slawomir Prucnal[1], René Hübner[1], Thomas Mikolajick[2], Artur Erbe[1,2], and Yordan M Georgiev[1,4] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]National institute for Material Science, Tsukuba, Japan — [4]Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria

The limitations of CMOS downscaling drive the exploration of alternative device concepts like reconfigurable FETs (RFETs), which can dynamically switch between n- and p-polarity through electrostatic gating. This work introduces a novel mixed-dimensional RFET utilizing 1D silicon (Si) nanowires combined with 2D hexagonal boron nitride (hBN) as a dielectric and encapsulating layer. hBN*s insulating properties, chemical stability, and absence of dangling bonds make it ideal for its use as a dielectric in 1D electronics. The RFET fabrication employs electron beam lithography, reactive ion etching, and flash lamp annealing for precise silicide formation. Mechanically exfoliated hBN flakes (5-10 nm) were integrated using dry stamping transfer, with thickness characterized by

microscopy techniques. Device characterization reveals improved subthreshold swing, on-current, and ION/IOFF ratio due to hBN*s 2D passivation, highlighting its potential for advanced nanowire-based RFET architectures.

HL 23.5 Tue 12:15 H13

Kondo effect for half-filling of the third shell of a quantum dot — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]1Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]2Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany

In this work, we investigate the electrical transport in the third shell [1] of a gate-defined GaAs quantum dot. The exact number of electrons in the quantum dot (N_e) is determined using a quantum point contact as a sensitive charge detector, detecting single-electrons tunneling through the system [2]. N_e is varied by changing the applied gate voltage.

The addition energy E_c for N_e = 7 - 11 shows a triangular behavior with a maximum at half-filling of the shell. This observed behavior is described analytically with Hund's rule exchange interaction. Besides, for successive numbers of electrons occupying the quantum dot N_e = 7 to 11, a Zero-bias anomaly (ZBA) characteristic for the Kondo effect is observed [3]. The width of the ZBA exhibits a triangular behavior, with a maximum at N_e = 9, similar to E_c. The broadening of the ZBA is attributed to the contribution of the Kondo resonance as well as Hund's satellite peaks, originating from the degenerate orbitals observed in the spectral function.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64, 701-736 (2001).
[2] T. Wagner, et. al., Nat. Phys.15, 330-334 (2019).
[3] J. Schmid, et. al., Phys. Rev. Lett. 84, 5824 (2000).

HL 23.6 Tue 12:30 H13

Beyond full counting statistics and Langevin theory: The quantum polyspectra approach to multi-detector measurements — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, Germany

The quantum polyspectra approach to quantum measurements has recently been shown to cover the full range between weak and strong quantum measurements [1 - 3]. It provides thus a more general approach to quantum measurements than the full counting statistics used in nano-electronics or the Langevin-approach used in spin noise spectroscopy. This approach draws its strength from comparing higher order spectra of the measurement record with model spectra calculated from quantum expressions that are calculated on the level of a Lindblad master equation. Here, we generalize the polyspectra approach to include the case of the simultaneous measurements of more than one quantity of a quantum system. The approach regards measurement induced damping, measurement backaction, and the quantum Zeno effect. We give a few examples of multi-detector polyspectra that were calculated by a multi-detector extension of our SignalSnap and QuantumCatch library [4, 5].

[1] Hägele et al., PRB 98, 205143 (2018)
[2] Sifft et al., PRR 3, 033123 (2021)
[3] Sifft et al., PRA 109, 062210 (2024)
[4] https://github.com/MarkusSifft/SignalSnap
[5] https://github.com/MarkusSifft/QuantumCatch

HL 23.7 Tue 12:45 H13

Revealing Hidden States in Quantum Dot Array Dynamics: Quantum Polyspectra Versus Waiting Time Analysis — •Markus Sifft[1], Johannes C. Bayer[2], Daniel Hägele[1], and Rolf J. Haug[2] — [1]Faculty of Physics and Astronomy, Ruhr University Bochum, GER — [2]Institute of Solid State Physics, Leibniz Universität Hannover, GER

We show how by virtue of the recently introduced quantum polyspectral analysis of transport measurements [1,2], the complex transport measurements of multi-electron QD systems can be analyzed. This method directly relates higher-order temporal correlations of a raw quantum point contact (QPC) current measurement to the Liouvillian of the measured quantum system. By applying this method to a two-electron double QD system, we uncover dynamics between singlet and triplet states, indistinguishable in the QPC current, without requiring the identification of quantum jumps or prior assumptions about the number of quantum states involved. Our findings demonstrate that system models in such cases of hidden dynamics are inherently non-unique. Furthermore, we compare our method to a traditional analysis via the waiting-time distribution. Our method achieves parameter estimates with up to 50% lower errors, while also being applicable in scenarios with low signal-to-noise, where traditional counting methods falter. Our approach challenges previous assumptions and models, offering a more nuanced understanding of QD dynamics and paving the way for the optimization of quantum devices.

[1] Hägele et al., PRB 98, 205143 (2018)
[2] Sifft et al., PRR 3, 033123 (2021)

HL 24: Thermal Properties

Time: Tuesday 12:15–13:00 Location: H14

HL 24.1 Tue 12:15 H14

Combined optical and thermal characterization of III-nitride membranes by microphotoluminescence and Raman thermometry — •Gordon Callsen[1], Mahmoud Elhajhasan[1], Julian Themann[1], Katharina Dudde[1], Guillaume Würsch[1], Jean-François Carlin[2], Raphaël Butté[2], Nicolas Grandjean[2], Nakib Haider Protik[3], and Giuseppe Romano[4] — [1]Universität Bremen, Germany — [2]EPFL, Lausanne, Switzerland — [3]HU Berlin, Germany — [4]MIT-IBM Watson AI Lab, Cambridge, USA

We present the optical and thermal analysis of photonic III-nitride membranes, which provides novel insights into the physics of thermal transport on the micrometer scale [1]. By combining Raman thermometry (RT) with μPL spectroscopy, we demonstrate a non-invasive approach to extract the thermal conductivity κ. This analysis shows that even at 295 K one can still observe quasi-ballistic phonon transport in GaN, which challenges commonly applied models building on purely diffusive transport. Our membranes are made from c-plane GaN and comprise $In_xGa_{1-x}N$ (e.g., x = 0.15) quantum wells that already served as an active medium in various nanolasers [2]. The material is either grown on silicon or sapphire and is subsequently underetched, yielding freestanding structures. On such samples we perform μ-RT, either based on one-laser RT or spatially resolved two-laser RT. The latter is key to our thermal imaging, representing a significant step towards non-invasive and quantitative thermometry on photonic membranes.

[1] M. Elhajhasan et al., PRB 108, 235313 (2023)
[2] S. T. Jagsch et al., Nat. Commun. 9, 564 (2018)

HL 24.2 Tue 12:30 H14

Impact of AlGaAs interlayers on the thermal conductivity of GaAs micropillars — •Guillaume Würsch[1], Ching-Wen Shih[2], Mahmoud Elhajhasan[1], Katharina Dudde[1], Imad Limame[2], Stefan Reitzenstein[2], and Gordon Callsen[1] — [1]Institut für Festkörperphysik, Universität Bremen, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany

First measurements of coherent heat conduction in semiconductor superlattices (SL) were reported over a decade ago. Interestingly, such an effect that is based on phonon interference can already be observed at room temperature, which sparks interest in measuring and controlling most fundamental phonon parameters like their mean free path l_{mfp} and wavelength λ_{therm}.Observing the effects of phonon interference in SLs can be challenging, because material stacks with superb crystalline quality and interfaces is required. In this work, we follow a step-by-step approach, meaning that we analyse GaAs micropillars (diameter: 0.5 - 2 μm) with a rising number (0 - 7) of $Al_{0.8}Ga_{0.2}As$ interlayers. A thin layer of gold on top of these structures enables the measurement of the thermal conductivity κ via the frequency-domain thermal reflection (FDTR) technique, which is complementary to the Raman thermometry that we apply.Our study on first samples with a small numbers of interlayers provides not only insight into the thermal impact of each individual interface, but highlights the impact of the micropillar diameter. Building on such knowledge will allow us in future studies on larger SLs to disentangle phonon interference effects and phonon scattering phenomena.

HL 24.3 Tue 12:45 H14

Signature of thermal phonon mean free paths monitored by Raman thermometry — •Katharina Dudde[1], Mahmoud Elhajhasan[1], Guillaume Würsch[1], Julian Themann[1], Nakib Protik[2], Dwaipayan Paul[2], Giuseppe Romano[3], and Gordon Callsen[1] — [1]Institut für Festkörperphysik, Universität Bremen, Germany — [2]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [3]MIT-IMB Watson AI Lab, IBM Research, Cambridge, MA, USA

For an understanding of thermal phonon interference effects, one requires knowledge about the related phonon mean free paths l_{mfp}. In the recent past, spectroscopy methods were developed to determine l_{mfp} based on this idea: One performs thermal transport measurements under the variation of a characteristic experimental length scale L aiming to extract effective thermal properties such as the effective thermal conductivity $\kappa_{eff}(L)$. In this contribution, we analyze how non-invasive one-laser Raman thermometry (1LRT) can pose a novel option to perform thermal phonon l_{mfp} spectroscopy. Therefore, we first analyze bulk silicon at 293 K, while varying the laser focus spot radius (w_e). Here, we find a strong dependence of κ_{eff} on w_e. This dependence is more pronounced at 200 K, because l_{mfp} is increased. The second variable length scale for 1LRT

is the light penetration depth (h_α), which is varied in a set of measurements for silicon membranes at 293 K. Again, a dependence of κ_{eff} on h_α is observed. Finally, our variation of w_e or h_α during 1LRT provides first insight into the impact of different thermal phonon l_{mfp} ranges on κ_{eff}.

HL 25: Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

See O 36 for details of this session.

HL 26: Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

See O 37 for details of this session.

HL 27: Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

See O 38 for details of this session.

HL 28: Topological Insulators (joint session MA/HL)

Time: Tuesday 14:00–15:15 Location: H16

See MA 16 for details of this session.

HL 29: Poster II

The second poster session on the physics of semiconductors covers topics from 2D semiconductors and van der Waals heterostructures, the physics of the van der Waals magnetic semiconductor CrSBr, materials and devices for quantum technology, quantum dots and wires, transport properties, to ultra-fast phenomena in semiconductors.

Time: Tuesday 18:00–20:00 Location: P1

HL 29.1 Tue 18:00 P1

Electrical Field Effect and Schottky Barriers in $FePSe_3$ Thin Films — •Paul Perl[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Transition metal selenophosphates (MTPs) are a group of promising 2D materials for applications like transistors and photodetectors [1,2]. Among MTPs, iron selenophosphate ($FePSe_3$) has one of the lowest band gap energies at 1.3 eV [2]. The goal of this work is to examine the influence of the electric field effect on electrical transport and to study the Schottky barriers formed at metal contacts. Moreover, the temperature dependence of the investigated effects is analyzed.

In order to investigate the electrical properties of $FePSe_3$ in thin films below 30 nm, layers are mechanically exfoliated onto a Si/SiO_2 substrate. Electrical contacts for the exfoliated flakes are fabricated via electron beam lithography and physical vapor deposition. $FePSe_3$ exhibits a hysteresis in its transport characteristics when the applied backgate voltage is altered, indicating favorable characteristics for memory devices. Furthermore, differences in Schottky barriers for various contact material compositions become apparent, showing their influence on electric transport properties.

[1] T. Xu et al., Advanced Electronic Materials, 7, 2100207 (2021)
[2] M. A. Susner et al., Advanced Materials, 29, 1602852 (2017)

HL 29.2 Tue 18:00 P1

Fabricating MoS_2 nanotube quantum dots on 2D heterostructures — •Korbinian Fink[1], Robin T. K. Schock[1], Stefan B. Obloh[1], Matthias Kronseder[1], Matjaž Malok[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg — [2]Solid State Physics Department, Jožef Stefan Institute, Ljubljana, Slovenia

MoS_2, a transitional metal dichalcogenide (TMDC) with interesting optical and electronic properties, e.g., broken inversion symmetry and strong spin-orbit coupling leading to spin split bands, is at the center of manifold research efforts. Building a MoS_2 based QD remains challenging: the spatial quantization depends on the effective electron mass, which is high in MoS_2, and minuscule devices sizes are required.

In order to reduce the lithographic constraints we utilize nanotubes, as these confine charges in an additional dimension. However, these QDs are still limited by the disorder from the SiO_2 surface. This can be resolved by fabricating the devices on top of 2D heterostacks consisting of hBN and few layer graphite.[1]

The major challenge for creating such devices is reproducible contacts to the nanotubes, as nanogaps between the contact on the chip and the metal on top of the tube lead to high resistance variations. This can be solved by variation of the incident angle and heating during metalisation as well as fixing the tubes on the chip by cross linked resist. - [1] R. T. K. Schock et al., PSSb, 2400366 (2024)

HL 29.3 Tue 18:00 P1

Preparation of folded graphene heterostructures via dry transfer — •Hannes Kakuschke[1], Dustin Wittbrodt[2], Lina Bockhorn[1], and Rolf Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Mono- and bilayer systems of graphene have been extensively researched due to their unique magnetic and electronic transport properties. In more recent work, folded graphene [1, 2] heterostructures exhibit fascinating phenomena. This is due to the topology of the folded region, causing effects such as snake states and zero line modes. However, in transport measurements of self-assembled, folded graphene [3], multiple effects occur simultaneously. This drastically complicates the analysis of individual contributions. To solve this problem, we use the dry transfer method to fold graphene around hBN, decoupling the overlapping graphene regions.

To simulate the behaviour of such samples, Tight-Binding model calculations [4], considering strain effects [5] at the folded edge have been carried out.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).
[4] M. Koshino & T. Ando, Solid State Commun. 149, 1123-1127 (2009).
[5] A. R. Botello-Méndez et al., JPC C. 122 (27), 15753-15760 (2018).

HL 29.4 Tue 18:00 P1

Ferroelectric Potential Investigations of 3R MoS_2 through fast Optical Measurements — •Jan-Niklas Heidkamp[1], Swarup Deb[1,2], Takashi Taniguchi[3], Kenji Watanabe[3], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]National Institute for Material Science, Tsukuba, Japan

In recent years, sliding ferroelectricity has emerged as a topic of significant interest due to its possible application in nonvolatile random-access memory. This phenomenon is unique to two-dimensional van der Waals materials, where vertical polarization switching is induced by in-plane sliding of the constituent layers. The resulting polarization is influenced by the intrinsic stacking order, creating distinct polarization regions separated by domain walls. These regions, along with the domain walls, can be manipulated using an external vertical electric field, enabling a switchable system that retains the environmental robustness of van der Waals materials under ambient conditions.

In this study, we investigate 3R-MoS_2 using various optical measurement techniques at room temperature. The spatially resolved measurements reveal clear signal changes corresponding to different ferroelectric stacking orders and variations in layer count. Our findings demonstrate that fast optical mapping at room temperature is a reliable method for probing ferroelectric potential steps in 3R-stacked samples. This approach does not require a conductive substrate or backing, making it more versatile than traditional Kelvin Probe Force Microscopy (KPFM) techniques.

HL 29.5 Tue 18:00 P1

Probing TMD-nanowire hybrid structures with second harmonic generation. — •Benedikt Mathes, Maximilian Tomoscheit, Edwin Eobaldt, Alexander Zaunick, Carsten Ronning, and Giancarlo Soavi — Institut of Solid State Physics, University of Jena

Hybrid nanostructures have been drawing attention in fundamental science, since they allow to control and engineer the electronic and optical properties of samples. Transition metal dichalcogenide(TMD)-nanowire(NW) hybrid structures could have interesting applications beyond fundamental science, since they allow to tune the lasing properties of NW lasers. To understand the photophysical response of the hybrid system, it is helpful to measure the optical and electronic response of each of its individual constituent. However, this is in general difficult to achieve. In this work, we solve this problem by showing that polarization-dependent second harmonic generation(SHG) can selectively probe each constituent of a WSe_2-ZnO NW hybrid, provided that the subsystems are properly and deterministically aligned. TMDs exhibit a threefold symmetry with two main axes, armchair(AC) and zigzag(ZZ). When excited along the ZZ axis, the SH is emitted along the AC axis, whereas the SH of the NW is always emitted parallel to its long axis. Hence, by aligning the NW along the ZZ axis one can differentiate the emission from NW and TMD with a polarizer in detection aligned along the ZZ or AC axis, respectively. This way, the subsystems of the hybrid structure can be investigated individually, offering new insights into their contribution to the hybrid system.

HL 29.6 Tue 18:00 P1

Raman and photoluminescence spectroscopy on differently synthesised $MoSe_2$ — •Lara Blinov[1], Hendrik Lambers[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

There are various synthesis methods for the widely researched transition metal dichalcogenides (TMDCs). We examine optical responses of $MoSe_2$ synthesised by chemical vapor transport (CVT) with different halogen contributions in the transport gas. Therefore, mono- and bilayers of those differently grown parental crystals are mechanically exfoliated and investigated by Raman and photoluminescence (PL) spectroscopy at room temperature as well as in temperature-dependent PL measurements.

We analyse and compare the energies and intensities corresponding to the neutral A and B excitons as well as a prominent A^- trion in the PL spectra and the frequency of the first order Raman modes. We conclude that the CVT synthesised crystals seem to have an inhomogeneous distribution of charge carrier densities or defects and that the defect density seems to be larger than in conventionally synthesised $MoSe_2$.

HL 29.7 Tue 18:00 P1

Optical Properties of Janus Transition Metal Dichalcogenides — •Sai Shradha[1], Julian Picker[2], Nicole Engel[1], Lukas Krelle[1], Daria Markina[1], Roberto Rosati[3], Ermin Malic[3], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Institute for Physical Chemistry, Friedrich Schiller University, Jena, Germany — [3]Department of Physics, Philipps-Universität Marburg, Marburg, Germany

Janus transition metal dichalcogenides (JTMDs) have a crystal structure of X-M-Y where X and Y are chalcogens and M is a transition metal. Their asymmetric structure, with chalcogen atoms of different electronegativity above and below the transition metal, leads to an intrinsic out-of-plane electric dipole. This out-of-plane symmetry breaking in JTMDs causes Rashba splitting, vertical piezoelectricity and enhanced exciton-phonon coupling. Due to a reduced overlap of the electron and hole wave functions, excitons in JTMDs are predicted to have lower binding energies and longer lifetimes. This makes them promising candidates for photovoltaic devices. Via chemical vapour deposition (CVD), high-quality Janus monolayers have been synthesised [1]. This work investigates the optical properties of CVD-grown monolayer Janus MoSSe and WSSe. Photoluminescence, Raman and differential reflectivity spectroscopy performed at room temperature and 4K are used as the key techniques to identify and further analyse excitons and exciton-phonon coupling in such systems.

[1] Z. Gan et. al., Adv. Mater., 34, 2205226 (2022)

HL 29.8 Tue 18:00 P1

Microscopic, Optical, and Electrical Characterization of Spray-Coated Graphene Dispersions on Sapphire Substrates — •Yasaman Jarrahi Zadeh[1], Lars Grebener[2], Muhammad Ali[3], Felix Schaumburg[1], Mohaned Hammad[2], Günther Prinz[1], Martin Geller[1], Hartmut Wiggers[3], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics, and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Energy and Materials Processes, and CENIDE, University of Duisburg-Essen, Germany — [3]Institute for Combustion and Gas Dynamics, and CENIDE, University of Duisburg-Essen, Germany

Processing graphene into thin films is crucial for its potential in cutting-edge applications. Here, we report on different characterization techniques to analyze the dispersion and coating performance of spray-coated graphene films on sapphire substrates. The deposited films were characterized using optical and scanning electron microscopy to evaluate coating morphology. Raman Spectroscopy and electrical characterization were used to assess the structural integrity and functional performance of the constituent graphene sheets. The deposited films fabricated from graphene sheets dispersed in water with carboxymethyl cellulose (CMC) exhibited uniform surface morphology compared to deposition with ethanol dispersion. Raman spectroscopy and electrical characterization confirmed the quality and structural integrity of the water-CMC dispersion. This study highlights key process-structure relationships for optimizing dry-synthesized graphene films for advanced technologies.

HL 29.9 Tue 18:00 P1

Vibrational fingerprint of 2D transition-metal dichalcogenide WSe_2 — •Kanivar Türk, Bastian Thomssen, Gerhard Berth, and Klaus Jöns — PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany

Thin-layered transition-metal dichalcogenides (TMDC) are on high demand in the material science community [1]. The advantages of monolayer configurations of these TMDCs include the transition from indirect to direct band gap, which leads to way superior properties when compared to bulk, like optical, electrical, magnetic, thermal and mechanical improvements [2].

In this work, exfoliated 2D flakes of WSe_2 have been produced and analysed in terms of their vibrational properties via Raman spectroscopy. Beside a comprehensive phonon mode assignment, a layer number specific analysis has been performed and compared to results from photoluminescence measurements.

[1] Saju Joseph et al.; Materials Chemistry and Physics 297: A review of the synthesis, properties, and applications of 2D transition metal dichalcogenides and their heterostructures (2023)

[2] Mingxiao Ye et al.; Photonics, 2: Recent Advancement on the Optical Properties of Two-Dimensional Molybdenum Disulfide (MoS_2) Thin Films (2015)

HL 29.10 Tue 18:00 P1

Tuning of excitonic emission of 2D-TMDs by hybridization with phase change materials — •Jakob Cornelius Wurschi, Martin Hafermann, Edwin Eobaldt, and Carsten Ronning — Institut für Festkörperphysik FSU Jena

Transition metal dichalcogenides (TMDs) are a subject of growing interest, given their wide range of potential applications, such as transistors or biosensors. Especially in the context of optoelectronic devices a precise tuning of the emission behaviour can be a powerful tool for the realisation of advanced technologies. To gain insight into potential tuning mechanisms of the excitonic emission of TMD monolayers, we investigate the hybridization of 2D MoS_2 and WS_2 flakes with germanium-antimony-telluride (GST). This compound system is capable of undergoing a phase transition between an amorphous and two crystalline states accompanied with drastic changes in the electrical and optical properties. Thermal heating triggers the phase transitions of GST, which we monitor by measuring the reflectivity of the GST thin films on silicon. After 2D-TMD flake exfoliation, in-situ measurements of the TMD photoluminescence spectra were obtained during or after the phase transitions of the GST substrate. With our approach, we observe a significant spectral shift of the excitonic emission of MoS_2 on GST/Si by precisely tuning the phase of the underlying GST. Further, for WS_2

flakes on gold substrates we observed a GST layer thickness dependent spectral shift for the excitonic emission of WS_2.

HL 29.11 Tue 18:00 P1

Gate defined exciton confinement in $MoSe^2$. — •Moritz Scharfstädt[1], Abdul R. Kanikode[1], Lasse Ebeling[2], Max Wegerhoff[1], Michael Köhl[1], Stefan Linden[1], Bernd Beschoten[2], Christoph Stampfer[2], Lutz Waldecker[2], and Andrea Bergschneider[1] — [1]Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany — [2]II. Physikalisches Institut, RWTH Aachen University, 52074 Aachen, Germany

Excitons in transition metal dichalcogenides (TMDs) are ideal candidates for strong light-matter interactions due to their high oscillator strength. This has been demonstrated in numerous experiments where 2D semiconductors were embedded in photonic cavities. However, these systems lack strong nonlinearity, necessitating further efforts to realize applications such as single-photon sources. One possible approach could be the spacial confinement of excitons using an in-plane inhomogeneous electric field, as first demonstrated by [1].

We present measurements on a similar system that achieves 1D confinement of excitons along the edge of a few-layer graphene gate. While the excitons are polarized perpendicular to the edge, we observe two orthogonal linear polarization axes of the confined states. This raises questions about the selection rules in such a system.

Furthermore, we show our approach to shape the confinement into a 0D configuration to enhance exciton-exciton interactions and, presumably, the system's nonlinearity.

HL 29.12 Tue 18:00 P1

PROBING INTERLAYER EXCITONS IN PARALLEL STACKED FERROELECTRIC MOS2 — •Johannes Krause[1], Jan-Niklas Heidkamp[1], Swarup Deb[3], Kenji Watanabe[2], Takashi Taniguchi[2], Rico Schwartz[1], and Tobias Korn[1] — [1]University of Rostock, Insitute of Physics, Germany — [2]International Center for Materials Nanoarchitectonics, National Institute for MAterials Science, Tsukuba — [3]Saha Institute of Nuclear Physics, Kolkata, India

2D Transtion Metal Dichalcogenides (TMDCs) garnered significant scientific interest, due to their unique optical properties. Interestingly, 3R-stacked TMDCs exhibit sliding ferroelectricity, which opens up new platforms for nanoelectronic and memory devices. Here, we investigate the photoluminescene (PL) associated with a 3R-stacked molybdenum disulfide homobilayer, particularly the signals attributed to the interlayer exciton. Additionally, electric fields are applied to control the characteristic properties of the stack. We employ mechanical exfoliation of bulk 3R-grown MoS2-crystals and the deterministic transfer technique to fabricate and transfer the homobilayers onto SiO2 wafers with pre-patterned electrical contacts. We utilize PL measurements to characterize the relevant optical signals. By applying gate voltages across the homobilayer, we explore the optical behavior of the homobilayer stack, enabling precise modulation of exciton properties by controlling charge carrier density and Stark effect.

HL 29.13 Tue 18:00 P1

Moiré superlattice effects in $MoSe_2$-WS_2 heterobilayers — •P. Parzefall[1], N. Paulik[1], M. Lorenz[1], C. Serati de Brito[1,2], J. Göser[3], J. Trapp[3], T. Taniguchi[4], K. Watanabe[4], A. Högele[3], Y. Galvão Gobato[2], and C. Schüller[1] — [1]Institut für Exp. und Angewandte Physik, Uni Regensburg (UR), Germany — [2]Physics Department, Federal University of São Carlos, Brazil — [3]Faculty of Physics, Munich Quantum Center and Center for NanoScience, LMU Munich, Germany — [4]NIMS, Tsukuba Ibaraki, Japan

We report about optical studies on type-I $MoSe_2$-WS_2 heterostructures at cryogenic temperatures. We confirm the influence of the moiré superlattice on excitonic features of angle aligned R- and H-type structures in photoluminescence spectroscopy. The moiré-exciton and moiré-trion features are further studied by resonant low-frequency Raman spectroscopy. Here, we tune a Ti:Sapphire laser into close resonance to the $MoSe_2$ intralayer excitonic transitions. We detect an efficient pumping of the moiré trion when exciting resonantly to the moiré exciton, as the binding energy is equivalent to a phonon energy.

In time-resolved measurements using a Streak camera, we measure the lifetimes of both H-type and R-type moiré-excitonic species. The detected short excitonic lifetimes in the R-type sample is indicative of a type-I band alignment and the longer moiré-exciton lifetimes in the H-type samples might be due to a hybridization in the conduction bands [1, 2]. [1] B. Polovnikov et al., Phys. Rev. Lett. 132, 076902 (2024), [2] Y. Galãvo Gobato et al., Nano Lett. 22, 8641 (2022)

HL 29.14 Tue 18:00 P1

Acousto-optic characterization of van der Waals systems — •Felix Ehring, Benjamin Mayer, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

With wavelengths in the micrometer range at GHz frequencies, surface acoustic waves (SAWs) are a versatile tool for radio frequency control and probing of charge carrier dynamics in novel semiconductor nanostructures. They are generated on a piezoelectric chip and routed over long distances to couple either mechanically or electrically with almost any nanosystem [1]. In our experiments, we fabricated hybrid lithium niobate SAW-devices including SAW delay lines with design frequencies of 150-250MHz, on which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials can be placed. The dynamic strain and electric field of the SAW induce a band modulation in the TMDC structure. The focus of the experiments was the investigation of MoSe2-WSe2 heterostructures and their interlayer excitons. For the characterization, the influence of the SAW fields on the recombination time and energy was investigated. Since interlayer excitons provide a much longer lifetime than intralayer excitons, transport along the propagation direction of the wave should be possible and will be part of future experiments. [1] J. Phys. D:Appl. Phys. 52(35):353001 (2019)

HL 29.15 Tue 18:00 P1

Influence of interface dielectric disorder on interlayer excitons in mixed binary/ternary TMD heterostructures — •Mohammed Adel Aly[1,2], Emmanuel Oghenevo Enakerakpor[2], Hilary Masenda[2], and Martin Koch[2] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [2]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

The unique properties of transition metal dichalcogenide (TMD) monolayers and their heterostructures offer exceptional tunability. In these heterostructures, interlayer excitonic emission can be tailored based on the selection of the monolayer materials. In this study, we fabricated heterostructures based on binary-ternary monolayers, which offer enhanced tunability of the interlayer exciton emission. To understand the physics behind the interlayer excitons and their photoluminescence linewidths, we measured the photoluminescence of excitons in two TMD heterostructures, MoSe2/Mo0.5W0.5Se2 and WSe2/Mo0.5W0.5Se2, at different temperatures ranging from 10 K - 300 K. Besides neutral excitons and trions, we found that the linewidths of interlayer excitons are significantly broadened due to dielectric disorder caused by the spatial inhomogeneity at the interfaces of the heterostructures. These are important for our understanding of the nature of the interlayer excitons and their tunability for future optoelectronic devices.

HL 29.16 Tue 18:00 P1

High-Pressure Optical Spectroscopy of Intralayer and Interlayer Excitons in 2H-MoS_2 Bilayers — •Vedhanth Senthiappan Vellaiappan Uthayasurian, Paul Steeger, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Molybdenum disulfide (MoS_2) is a van der Waals material from the class of Transition Metal Dichalcogenides (TMDCs). In 2H-MoS_2 homo-bilayers, interlayer excitons, where the electron and hole are located in different layers, are observed with a large oscillator strength and distinct energy separation from intralayer excitons. We investigate these inter- and intralayer excitons in 2H-MoS_2 homobilayers under applied pressure using a diamond anvil cell [1]. Optical transmission spectra reveal that increasing pressure reduces the energy splitting between the A exciton and the interlayer exciton. Ab initio calculations, combined with our experimental observations, indicate that this behavior cannot be attributed to conventional hydrostatic compression. Instead, it results from the MoS_2 bilayer adhering to the diamond surface, which limits in-plane compression. Furthermore, we show that the unique real-space distributions and the associated contributions from the valence band are responsible for the differing pressure responses of the inter- and intralayer excitons in compressed MoS_2 bilayers. References : [1] P. Steeger et al, Nano Lett., 23, 8947 (2023)

HL 29.17 Tue 18:00 P1

Magneto-Optical Spectroscopy of van der Waals CrSBr — •Lukas Krelle[1], Ryan Tan Qai Shen[1], Daria Markina[1], Priyanka Mondal[1], Kseniia Mosina[2], Kevin Hagmann[1], Regine von Klitzing[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

The layered antiferromagnet CrSBr is a promising Van der Waals material due to its quasi 1D nature and the strong coupling between excitons, phonons and magnons. In particular, the strong coupling of excitons to the magnetic order of the crystal opens new avenues for the study of correlated magnetic phases in optical spectroscopy. In this work, we perform magneto-optical spectroscopy on multilayer CrSBr. We use Photoluminescence and Reflectivity measurements to identify the different magnetic phases present in the sample. We report drastic changes of the emission and absorption depending on the magnetic phase of the material, which we control through the application of magnetic fields along specific directions.

HL 29.18 Tue 18:00 P1

Raman investigation of the 2D magnetic semiconductor $MnPS_3$ — •Thomas Kliewer[1], Pierre-Maurice Piel[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

The van-der-Waals (vdW) material $MnPS_3$ is a member of the group of metal phosphorus trichalcogenides (MPX_3; X=S, Se) which experiences rising interest due to its rich physical, chemical and structural properties. $MnPS_3$ is a 2D magnetic semiconductor with an electronic bandgap of 2,79 eV[1]. Below the Néel-Temperature of 78 K, it exhibits an antiferromagnetic order within the layers and a ferromagnetic coupling between adjacent layers[2]. These properties are interesting for fundamental studies on magnetism in the 2D limit, the investigation of coupling between spin, lattice and charge degrees of freedom and for possible applications in spintronics. $MnPS_3$ flakes of various thicknesses have been studied by temperature dependent Raman spectroscopy to uncover the coupling of lattice and spin degree of freedom. The Raman-spectra of $MnPS_3$ show several phonon modes in accordance with the crystal structure. The intensity of the modes varies with the thickness of the crystal. Besides the expected hardening of the modes, the temperature-dependent measurements imply possible influence of the magnetic ordering on the observed modes. [1] Grasso et al. Physical Review B 44.20 (1991), p. 11060 [2] Wildes et al. Journal of Physics: Condensed Matter 6.24 (1994), p. L335

HL 29.19 Tue 18:00 P1

Polarisation dependant reflectance measurements of CrSBr — •Manuel Terbeck, Aleksandra Lopion, Pierre-Maurice Piel, and Ursula Wurstbauer — Institute of Physics, University of Muenster, Germany

The van der Waals layered material CrSBr has multiple interesting characteristics. It is an air-stable, optically active magnetic semiconductor. Magnetically, CrSBr exhibits ferromagnetic ordering in-plane and antiferromagnetic ordering between adjacent layers, with the easy axis being in-plane [1]. In this material the coupling between magnetic and optical properties is strong allowing us to study magnetic properties by measuring interband emissions and absorption spectra. The electronic structure is often described as quasi-1D due to the highly anisotropic properties [1]. Thus the polarisation of light is important when measuring CrSBr optically. With Raman scattering, we checked the symmetry of the crystal. Considering those axes, we measured reflectance from thin CrSBr flakes using different polarisation of light to get information about the excitonic states in this material. Unlike emission, reflectance measurements enables additional access to higher electronic states. [1] J. Klein, et al. ACS Nano, 17, 5316-5328 (2023)

HL 29.20 Tue 18:00 P1

Semiconductor-Metal Interfaces in 2D TMDCs for High-Efficiency Optoelectronic Devices — •Linus Schneider[1], Ariane Ufer[1], Elena Vinnemeier[1], Rebecca Saive[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]MESA+ Institute for Nanotechnology University of Twente, Enschede, Netherlands

Efficient solar energy conversion requires new materials and technologies that enhance solar cell performance while minimizing material usage. Two-dimensional (2D) materials, specifically transition metal dichalcogenides (TMDCs) like molybdenum disulfide (MoS_2), exhibit strong exciton-mediated light-matter interactions, making them ideal for optoelectronic devices and solar energy conversion. A critical challenge for implementation is effective charge carrier extraction at the metal-semiconductor interface. We prepare TMDC flakes using mechanical exfoliation and fabricate semiconductor-metal junctions by transferring these layers onto metallic contacts using a dry viscoelastic stamping technique. The structural and optical properties of these samples are characterized using photoluminescence (PL) and Raman spectroscopy. The charge transfer behavior at the 2D semiconductor-metal interface is probed by localized laser beam-induced current measurements and the local potential change across the junction regions by kelvin probe force microscopy (KPFM).

HL 29.21 Tue 18:00 P1

Advancing 2D Materials for Optoelectronic and Photonic Devices: Insights from WSe_2 — •Bastian Thomssen, Ioannis Caltzidis, and Klaus D. Jöns — PhoQS Institute, CeOPP and Department of Physics, Paderborn University, Paderborn, Germany

Two-dimensional (2D) materials have garnered significant attention due to their unique structural, electronic, and optical properties, which make them ideal candidates for next-generation optoelectronic and photonic devices. [1] Transition metal dichalcogenides (TMDs), such as tungsten diselenide (WSe_2), exhibit remarkable characteristics: in monolayer form, WSe_2 transitions from an indirect to a direct bandgap semiconductor, enhancing light-matter interactions. This property positions WSe_2 as a promising material for applications in light-emitting diodes, lasers, and quantum emitters. [1] The layer-dependent properties of WSe_2, including the transition from an indirect to a direct bandgap, can be effectively characterized using photoluminescence measurements. These allow for precise determination of the layer number, providing valuable insights into the electronic and optical behavior of the material. Such measurements are essential for tailoring the material's properties for specific optoelectronic and photonic applications.

[1] Maja Groll et al. https://doi.org/10.1002/smll.202311635

HL 29.22 Tue 18:00 P1

Having a Good Vibe: Electron-Phonon Coupling in 1L-TMDCs Measured by Transient Absorption Spectroscopy — Tim Völzer[1,2], •Julian Schröer[1,2], Marvin Krupp[1,2], Annika Bergmann[1,2], Tobias Korn[1,2], and Stefan Lochbrunner[1,2] — [1]University of Rostock, Institute of Physics — [2]Department "Life, Light & Matter, University of Rostock

The optoelectronic properties of monolayer transition metal dichalcogenides (1L-TMDCs) are strongly determined by their electronic dynamics after light excitation. In this work, we present insights on the ultrafast dynamics of three different 1L-TMDCs by employing transient absorption (TA) spectroscopy. Our findings show that the basic processes after optical excitation can be divided into cooling of the electronic and phononic system and the subsequent recombination of the excited species. We reveal the importance of the differing coupling strengths to high- versus low-energy phonons. Due to the ultrashort pump pulse excitation, we are also able to trigger the displacive excitation of coherent phonons, which we assign to the A'_1 Raman mode of the system. Our results demonstrate the strong coupling between the electronic and phononic systems and lead to better understanding of excited state carrier dynamics in 1L-TMDC materials.

HL 29.23 Tue 18:00 P1

Probing time-reversal symmetry breaking in graphene — •Konrad Krieghoff[1], Nele Tornow[1], Omid Ghaebi[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

In graphene, space inversion symmetry (SIS) and time-reversal symmetry (TRS) combined with a hexagonal lattice give rise to a linear band dispersion at the +/−K points of the Brillouin zone. Breaking TRS can result in exotic phenomena, such as the realization of the Haldane model and the photoinduced anomalous quantum Hall effect. Thanks to its high sensitivity to changes in the crystal symmetry, nonlinear optical spectroscopy provides an excellent tool to study these effects.

In our work, we use an elliptically polarized laser beam to excite monolayer graphene, where the circular polarization component breaks TRS. This symmetry breaking induces new nonzero elements in the third-order nonlinear susceptibility tensor, which are then probed by the linear component of the excitation beam. The combination of the already existing and the light induced tensor elements results in a rotation of the emitted third harmonic signal. Preliminary experimental results further indicate an impact of both excitation power and doping of the sample. Since SIS is still intact, our approach offers a new method for exploring broken TRS and topology in centrosymmetric materials.

HL 29.24 Tue 18:00 P1

Optical Probing of the K-Point Band Structure in Monolayer TMDs *via* SHG — •Jonas Margraf[1], Paul Herrmann[1], Sebastian Klimmer[1,2], Shridhar Sanjay Shanbhag[3], Jan Wilhelm[3], and Giancarlo Soavi[1,4] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]ARC Centre of Excellence for Transformative Meta-Optical Systems, Department of Electronic Materials Engineering, Research School of Physics, The Australian National University, Canberra, Australia — [3]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — [4]Abbe Center of Photonics, Institute of Applied Physics, University of Jena, Germany.

Crystal properties are ultimately defined by their band structure and dispersion relation, which are typically measured *via* angle-resolved photoemission spectroscopy. Recently, all-optical approaches based on non-perturbative nonlinear optics (NLO) have been proposed as a promising alternative. While optical probing of the band structure requires non-perturbative measurements of the entire Brillouin zone, it is often sufficient to probe the dispersion relation in the vicinity of optical resonances. In this work, we aim to measure the dispersion relation of a transition metal dichalcogenide monolayer at the ±K valleys using perturbative NLO. We investigate a modulation of the total second harmonic (SH) intensity as a function of the fundamental polarization angle upon two-photon resonant SHG. We assign this modulation of the SH intensity to the specific dispersion relation of the ±K valleys induced by trigonal warping.

HL 29.25 Tue 18:00 P1

Optical properties of transition metal dichalcogenides under high pressure — •Paul Luca Grosserhode, Paul Steeger, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDCs), such as MoS_2 or WS_2, have received growing attention during the last years. Using micromechanical exfoliation, sin-

gle semiconducting layers can be readily prepared. Furthermore, multi-layered artificial crystals can be fabricated with single layer precision. In this study, we use a diamond anvil cell to apply pressures in the gigapascal range on such samples and observe how their optical properties change due to the induced deformation.

HL 29.26 Tue 18:00 P1

Analytical Theory Of Third Harmonic Generation In Two-Dimensional Materials — •Shridhar Sanjay Shanbhag[1], Florentine Friedrich[2], Paul Herrmann[2], Giancarlo Soavi[2,3], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany

Valleytronics explores the valley degree of freedom in materials like transition metal dichalcogenides, using electrons in *K valleys as binary states for information encoding. In valleytronics, efficient valley readout is crucial, and third harmonic generation (THG) could provide an ultrafast solution to valley readout for any material, regardless of inversion symmetry.

We derived an analytical expression for THG by solving the semiconductor Bloch equations perturbatively to obtain an expression for the polarization state of the outgoing third harmonic. Our compact expression reveals how material parameters influence the polarization and attributes polarization rotation to valley-dependent optical Stark and Bloch-Siegert shifts. Our theoretical predictions closely align with experiments, providing the microscopic mechanism and thus helping to advancing valleytronic readout mechanisms.

HL 29.27 Tue 18:00 P1

Plasma-Induced Defect Emission in Hexagonal Boron Nitride — •Felix Schaumburg, •David Plitt, Timo Wagner, Nicolas Wöhrl, Martin Geller, Günther Prinz, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Hexagonal boron nitride (hBN) has been the subject of numerous research efforts in the last decade. Of particular interest is the creation of single emitters in hBN because of their easy integration, e.g. in van-der-Waals heterostructures, and their room temperature photon emission. Many methods to create single emitters in hBN are still under investigation. We present our approach to create single quantum emitters in hBN using a remote plasma with different plasma species. We have used argon, nitrogen, and oxygen plasmas and present statistics on the emitters, produced by the different gas species, and their optical properties. In particular, we examine the emission of the exfoliated flakes before the plasma processes *without* an annealing step to avoid creating emitters that are not caused by the plasma exposure. Our findings suggest that the purely physical argon plasma treatment is the most promising route for creating optically active single emitters in hBN by plasma exposure.

HL 29.28 Tue 18:00 P1

Single-photon emission in the van der Waals material hBN — •Akhilesh Dubey, Janne Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Single-photon sources are crucial components for quantum networks and communications. Recently, single-photon sources in 2D materials have emerged as robust solid-state light emitters. Promising materials include transition metal dichalcogenides, such as WSe_2, transition metal monochalcogenides (e.g. GaSe), and also hexagonal boron nitride (hBN). Here, we investigate the light emission from single-photon emitters in hBN. We measure photoluminescence spectra of individual centers in hBN nanocrystals and analyze their prominent phonon sidebands. Time-resolved photoluminescence measurements reveal typical lifetimes. Our results are important for devising novel nanoscale devices based on these robust quantum light emitters.

HL 29.29 Tue 18:00 P1

Spectroscopic investigation of defects in strained WSe_2 van-der-Waals heterostructures — •F. Stechemesser[1], F. Schaumburg[1], J. König[2], C. Dietrich[2], C. Steiner[3], P. Pesch[3], G. Prinz[1], M. Geller[1], and A. Kurzmann[2] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]University of Cologne, Physics Institute II, Germany — [3]2nd Institute of Physics, RWTH Aachen University, Germany

Van-der-Waals heterostructures offer a versatile platform for tailoring material properties through diverse layer compositions, making them suitable for a wide range of applications. We investigated the single photon emitting behavior of the Van-der-Waals heterostructure, that is composed of stacked layers containing graphene as a front and back gate, hexagonal boron nitride as dielectric layers and the transition metal dichalcogenide tungsten diselenide (WSe_2) as the host of optical emitters. The WSe_2 heterostructure was biaxially strained by nanopillars on the silicon wafer, which was used as substrate. By irradiating the points of large strain with an electron beam, point defects in the lattice structure of WSe_2 were created. The point defects, in the strained area, act as artificial atoms in the structure and can show single photon emission. We studied the samples using spacially resolved photoluminescence spectroscopy using a He-Ne laser. Applying this method, it is possible to localize an emitter and perform temperature, time and power dependent measurements. Finally, to prove the single photon characteristic of the emitter sites, we conducted second order correlation ($g^2(0) = 0.323$) measurements.

HL 29.30 Tue 18:00 P1

Tailoring Quantum Emission in Bilayer WSe2 via Strain Engineering — •Jasleen Kaur Jagde[1], Palwinder Singh[1], Grant Wilbur[1], Megha Jain[1], Edith Yeung[2], David Northeast[2], Seid Mohammad[2], Jean Lapointe[2], Dan Dalacu[2], and Kimberley Hall[1] — [1]Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Nova Scotia B3H 4R2, Canada — [2]National Research Council Canada, Ottawa, Ontario K1A 0R6, Canada

Two-dimensional semiconductors subjected to strain have shown exceptional promise as single-photon emitters, due to their direct bandgap and an ease of integration with photonic structures. Emitters have been observed in a host of monolayer (ML) materials including MoS2, WSe2, WS2, MoTe2 and hBN. Quantum emitters have also recently been discovered in bilayers of TMDs, however their optical properties are less well understood. In this study, we demonstrate site-selective quantum emission in bilayer (BL) WSe2 using strain localized by engineered dielectric nanopillars of varying diameters. Through a systematic investigation of the dependence of quantum emitter properties on strain, we determine the optimum conditions for the observation of bright and narrow photoluminescence emission peaks. We observe a strain-driven blue shift in the emission wavelength that is controllable by the characteristics of the nanopillar. A strong antibunching (g (2)(0) = 0.139) is observed, confirming single photon emission behavior. These results highlight strain engineering of 2D materials as a scalable strategy for on-demand quantum light sources.

HL 29.31 Tue 18:00 P1

Electrical impact of He ion broad beam irradiation on multi-layer WSe2 — •Madhuri Chennur[1,2], Zahra Fekri[1,2], Ulrich Kentsch[1], Gregor Hlawacek[1], Jens Zscharschuch[1,2], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328Dresden, Germany — [2]TUD Dresden University of Technology, 01062 Dresden, Germany

Nanoelectronics enables the development of innovative, cost-effective, miniaturized, and versatile materials. Among these, 2D materials hold immense potential for tailoring nanoscale functionalities. Structural defects in such materials play a significant role. By analyzing defect types, densities, and distributions, it is possible to unlock insights and exploit them for various applications, such as doping, tuning band gaps, or enhancing catalytic activity.

In this work, the impact of defects in multi-layer WSe2 is explored under the influence of Si/SiO2 and hBN substrates, introduced via a single broad-beam Helium ion irradiation at 7.5 keV. Electrical contacts are patterned using electron beam lithography (EBL), and all measurements are conducted under ambient conditions to assess changes in defect states post-irradiation.

The evolution of defects is monitored over time, with observations made one and two weeks following irradiation. Initially, the devices demonstrate degraded performance but later, their current exceeds pre-irradiation levels. Raman spectroscopy before and after irradiation provides deeper insights into the material's behavior. Additionally, the findings reveal the role of defects in influencing gas-sensing capabilities.

HL 29.32 Tue 18:00 P1

Probing the Band Splitting near the Γ Point in the van der Waals Magnetic Semiconductor CrSBr — •Kaiman Lin[1,2], Yi Li[1,3], Mahdi Ghorbani-Asl[1], Zdenek Sofer[4], Stephan Winnerl[1], Artur Erbe[1,3], Arkady V. Krasheninnikov[1], Manfred Helm[1,3], Shengqiang Zhou[1], Yaping Dan[2], and Slawomir Prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Shanghai Jiaotong University, Shanghai, China — [3]TU- Dresden, Germany — [4]University of Chemistry and Technology Prague, Czech Republic

As a van der Waals magnetic semiconductor, CrSBr has a direct bandgap of approximately 1.5 eV and undergoes an antiferromagnetic transition around 131 K [1]. In this study, the electronic band structure of CrSBr is investigated through comprehensive photoluminescence (PL) characterization [2]. We distinctly identify low-temperature optical transitions between two closely adjacent conduction-band states and two different valence-band states. The analysis of the PL data robustly reveals energy splittings, bandgaps, and excitonic transitions across different CrSBr thicknesses, ranging from monolayer to bulk. Temperature-dependent PL measurements shed light on the stability of band splitting below the Néel temperature, suggesting that magnons coupled with excitons are responsible for the symmetry breaking and the brightening of transitions from the secondary conduction band minimum (CBM2) to the global valence band maximum (VBM1). [1] N. P. Wilson, K. Lee, J. Cenker et al., Nat. Mater. 20, 1657 (2021). [2] K. Lin, et al. J. Phys. Chem. Lett. 15, 6010-6016 (2024).

HL 29.33 Tue 18:00 P1

Tuning of non-radiative decay channels in CrSBr by a magnetic phase transition — •Fabian Glatz[1], Minjiang Dan[1,2], Till Weickhardt[1], Zdeněk Sofer[3], Marie-Christin Heissenbüttel[4], Julian Klein[5], and Giancarlo Soavi[1,6] — [1]Friedrich Schiller University Jena, Germany — [2]Southwest University of Science and Technology, Mianyang, China — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Westfälische Wilhelms-Universität Münster, Germany — [5]Massachusetts Institute of Technology, USA — [6]Abbe Center of Photonics, Jena, Germany

CrSBr is a layered magnetic semiconductor with a direct bandgap [1]. Magnetic measurements have shown that below the Néel temperature (132 K) the spins within a single layer arrange ferromagnetically, while multiple layers couple antiferromagnetically (AFM) [2]. Here, we investigate the evolution of CrSBr under a magnetic phase transition by using nonlinear optics. In agreement with existing literature, second harmonic generation (SHG) becomes allowed due to the symmetry-breaking by AFM ordering at low temperatures [3]. Additionally, this phase change from paramagnetic (PM) to AFM leads to a change in the band structure that enhances third harmonic generation (THG) at the lowest energy optical resonance while quenching the photoluminescence quantum yield. This indicates the opening of a phonon mediated non-radiative decay channel upon transition from PM to AFM phase.

[1] Wang et al., Nat. Commun. 14, 5966 (2023). [2] Telford et al., Adv. Mater. 32, 2003240 (2020). [3] Lee et al., Nano Lett. 21, 3511-3517 (2021).

HL 29.34 Tue 18:00 P1

Defect induced magnetic phase transition in CrSBr — •Fangchao Long[1,2], Mahdi Ghorbani-Asl[1], Kseniia Mosina[3], Joachim Thomsen[4], René Hübner[1], Zdenek Sofer[3], Florian Dirnberger[5], Arkady V. Krasheninnikov[1], Slawomir Prucnal[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Forschungszentrum Jülich, Germany — [5]Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

As an air-stable van der Waals magnetic semiconductor, CrSBr is receiving great research attention due to its exceptional properties. Below the Néel temperature of 132 K, CrSBr exhibits a typical A-type antiferromagnetic order comprised of antiferromagnetically coupled ferromagnetic monolayers. This special structure makes it susceptible to external stimuli, such as ion irradiation. In this work, we present the magnetic phase transition from antiferromagnetic to ferromagnetic in CrSBr crystals irradiated by non-magnetic ions. We observe the rise and fall of the ferromagnetic phase in antiferromagnetic CrSBr with increasing the irradiation fluence. Raman spectroscopy reveals phonon softening, suggesting the formation of defects. Structure analysis of the irradiated crystals in conjunction with density functional theory calculations suggest that the displacement of constituent atoms due to collisions with ions and the formation of interstitials favor a ferromagnetic order between the layers.

HL 29.35 Tue 18:00 P1

Self-Driven Photodetectors Based on Intercalated CrSBr — •Aljoscha Söll[1], Kseniia Mosina[1], Martin Vesely[1], Jiří Šturala[1], Florian Dirnberger[2], and Zdeněk Sofer[1] — [1]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic. — [2]Department of Physics, Technical University of Munich, 85748 Munich, Germany.

The intercalation of lithium ions into layered materials has been an important field of research, leading not only to the development of lithium-ion batteries but also to countless insights in solid-state physics. Recently, it was shown that the intercalation of the quasi-1D semiconductor CrSBr can drastically alter its electronic structure, enhancing conductivity and potentially causing a transition from semiconductor to metal. Since the location and degree of intercalation can be precisely controlled, it allows us to fabricate devices using partially or fully intercalated CrSBr, harnessing properties of both the pristine and intercalated phases. Here we present a self-driven photodetector based on intercalated CrSBr, demonstrating high photoresponsivity across the entire NUV to NIR range with a response time in the millisecond range. Our findings not only deepen the understanding of intercalation effects in low-dimensional materials but also pave the way for the development of advanced optoelectronic devices using intercalated CrSBr.

HL 29.36 Tue 18:00 P1

Strong coupling of metal nanoparticles and 2d semiconductors: Physics behind a minimal model — •Lara Greten and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Transition metal dichalcogenide monolayers (TMDCs) feature strong light-matter interaction, governd by tightly bound, 2d-delocalized excitons. Metal nanostructures exhibit localized plasmons allowing for extreme electric field enhancements on the nanoscale. Hybrids of TMDCs and metal nanoparticles combine excitons and plasmons and may reach strong coupling as shown in numerous experiments. These experimental results are typically quantified via the coupled oscillator model (COM) employing a phenomenological coupling constant as a fitting parameter. To provide physical background to this model, we develop an analytical theory based on a microscopic perspective of the material dynamics and Maxwell's equations [1]. The emergent minimal model [2] provides a clear physical interpretation that highlights the importance of the spatial dispersion of 2d excitons. Depending on geometry and material properties we derive analytic expressions for all coupling and dephasing constants in a COM combining three oscillators: plasmons, bright and momentum-dark excitons. Strong coupling, that manifests as a peak splitting in optical spectra, is observed between momentum-dark excitons and plasmons, while the weakly coupled bright exciton yields a distinct third peak.

[1] L. Greten et al., ACS photonics 11.4, 1396-1411 (2024)
[2] L. Greten et al., arXiv preprint arXiv:2410.16796 (2024)

HL 29.37 Tue 18:00 P1

Non-Local Effects in Landau Quantized Two-Dimensional Electron Gases — •Sabrina Meyer[1], Andreas Knorr[1], Stephen Hughes[2], and Lara Greten[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

Landau levels are the quantum analogon of the cyclotron motion under a strong magnetic field in two-dimensional electron gases, as present in high quality GaAs films. Even though recent experimental work examines nanopatterning - introducing metal gaps to localize and amplify electric fields on the nanoscale - current theoretical descriptions still rely on a local susceptibility for excitation with large wavelengths. This study includes non-local effects in a microscopic theory for the electron dynamics: We find modified selection rules beyond the dipole approximation that allow for the direct excitation of ground state electrons to higher Landau levels, that are forbidden in a local description. These modifications become especially important when the electric field varies significantly within the spatial extend of the Landau level wave function ($\propto$ 100 nm). This applies for nanopatterned devices as well as for light scattering with wavelength on the order of the Landau level radius.

HL 29.38 Tue 18:00 P1

Visualizing Atomic-Scale Charge Fluctuations in Real-Space Dielectric Response — •Bernadette Christ and Claudia Rödl — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The wave-vector and frequency-dependent dielectric function contains a plethora of information on the response of a given material to external perturbing electromagnetic fields that is rarely fully exploited. Its off-diagonal elements are known as local-field effects and encode the atomic-scale charge fluctuations that occur due to light-matter interaction or screening within the material.

We aim for developing a tool to visualize the impact of such an external perturbation on the electron density in the material in real space. In a first step, we calculate the independent-particle dielectric response function from first principles using density-functional theory. In this mean-field approach, we expect to see how interband transitions excite individual orbitals and how collective excitations such as plasmon waves propagate in the material. Later on, we will also consider inclusion of many-body effects in the evaluation of the response function to visualize the formation of excitons. This will help us to better understand the intricate interplay between the numerous electronic degrees of freedom and contribute to the analysis of spectroscopic experiments. As first benchmarks, we will study bulk semiconductors heading for more complex, technologically relevant materials systems afterwards.

HL 29.39 Tue 18:00 P1

Assessing Wafer Growth Success in Quantum Dot Photonic Device Fabrication — •Severin Krüger[1,2], Elias Kersting[1], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Sparrow Quantum Aps, Copenhagen, Denmark

Molecular beam epitaxy (MBE) is crucial for fabricating photonic devices, including commercially viable single photon sources (SPS) based on quantum dots (QDs) [1]. Precise control of QD properties and surrounding layer design is essential for optimal device performance. We employ bandstructure and photonic simulations to design heterostructures, followed by comprehensive optical characterization of reference samples using photoluminescence (PL) mapping, Hall measurements, and surface analysis. This efficient characterization cycle allows rapid optimization of growth parameters on full 3" wafers, significantly reducing development time compared to direct SPS fabrication and testing. However, distributed Bragg reflectors in SPS wafers introduce PL signal artifacts due to reflectivity oscillations and stop bands, which significantly modulate the collectable photon yield across different wavelengths, alternately enhancing and suppressing the signal. We present our reference sample approach, characterization methods, and techniques to correct for optical stack-induced PL artifacts, enabling accurate assessment of MBE-grown structures for SPS applications.

[1] R. Uppu et al., Nature Technology 16, 1308-1317, (2022) [2] H.G. Babin et al., Nanomaterials 11, 2703, (2021)

HL 29.40 Tue 18:00 P1

Effect of TiO_2 thin films on the charge state of shallow NV centers in diamond. — •Arthur Witte, Tobias Lühmann, Peter Schlupp, Dominic Reinhardt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute for Solid State Physics, Germany

The nitrogen vacancy (NV) center is a color center in diamond. In its negative charge state, it has a relatively long spin coherence time at room temperature and a spin-dependent photoluminescence that enables optical spin polarization. Because of these properties, the NV center was proposed as a platform for room-temperature quantum computing. For this application the NV centers must be located close to the diamond surface. This can present new challenges due to surface effects resulting in, e.g. charge state instabilities of the shallow NV centers. Various surface treatments can be used to mitigate these effects, such as thermal oxidation, plasma surface treatments or the deposition of a thin passivation layer on the diamond surface.

We present a titanium dioxide thin film as the passivation layer. Titanium dioxide is a wide-bandgap semiconductor with a high refractive index of 2.5. In a first step, we investigate the growth of titanium dioxide layers by pulsed laser deposition and long-throw sputtering under different conditions. We then study the effect of optimized titanium dioxide layers on the luminescence properties of NV centers at implantation depths between 7 nm and 67 nm. Through spectroscopic analysis, we observe a significant increase in charge stabilization of shallow NV centers.

HL 29.41 Tue 18:00 P1

Secondary electron spectrometer for deterministic single ion implantation — •Priyal Dadhich, Nico Klingner, and Gregor Hlawacek — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf(HZDR), Dresden, Germany

The deterministic placement of single ions is essential for programmable quantum computers based on the nuclear spin of the donor atom to serve as a spin qubit.

Spatially revolved single ion implantation requires the reliable detection of implantation events. Our approach utilizes SEs generated during ion impact. To optimize the detection we use a windowless silicon drift detector (SDD) biased up to +10 kV. The SDD measures the electron energy through electron-hole pair generation, enabling quantifying the number of electrons by counting pile-up pulses [1]. Given the low average SE yield per single-ion impact, optimizing the extraction geometry is crucial for achieving the maximum possible success rate.

We use the open-source three-dimensional ion optical C++ library, IBSIMU[2], to simulate a realistic extraction design for efficient SE collection on the detector's active area. For the highest detection efficiency, we must also consider the unlikely event of backscattering of the electrons from the SDD. The extraction geometry is designed to recapture these electrons and re-accelerate them into the detector's active area.

[1] F. Aumayr et. al., Applied Surface science,47(2):139*147, 1991.

[2] Taneli Kalvas et. al., Review of Scientific Instruments, 81(2), 2010.

HL 29.42 Tue 18:00 P1

Emission properties of electron irradiated hBN — •Annkathrin Köhler, Jan Böhmer, Christian T. Plass, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Defect centers in solid state materials have emerged as promising candidates for quantum emitters. In particular, hexagonal boron nitride (hBN) has attracted significant attention due to its ability to host single-photon emitters (SPEs) at room temperature. Here, we systematically examined the luminescence properties of exfoliated hBN flakes as well as hBN nano-powders dispersed in various solutions and drop-casted onto a substrate. The effects of local electron irradiation and thermal annealing on the hBN samples were analyzed, providing insights into the conditions necessary for tuning their emission characteristics. Photoluminescence (PL) spectra were recorded using a micro-PL setup to compare the spectral distribution of the emission under different treatments. To further understand the quantum nature of the emitters, we conducted second-order correlation measurements as a function of the preparation parameters.

HL 29.43 Tue 18:00 P1

Germanium MOSFETs for Quantum Computation — •Thembelihle Dlamini and Mónica Benito — Institute of Physics, University of Augsburg

The project focuses on studying hole dynamics and spin properties in Germanium (Ge) metal-oxide-semiconductor (MOS) nanostructures to achieve high-fidelity single-qubit operations. Leveraging MOSFETs superior compatibility with industrial manufacturing techniques, holes' unique properties such as strong spin-orbit coupling, and Ge advantages over Si, GeMOS hole-spin qubits addresses some of the limitations of state-of-the-art spin quantum processors. The device-design phases will be assisted by three-dimensional structural simulations of the device. Moreover we will develop custom analytical models for holes in low-dimensional GeMOS geometries and the Ge/oxide interface by using symmetry analysis and $k \cdot p$ theory. Finally, we will investigate the effect of the multiband character of holes and their spin-orbit coupling in the effective spin representation of systems with a few holes in realistic quantum-dot potentials.

HL 29.44 Tue 18:00 P1

Crystal Growth and Influence of Fe^{3+} Doping on the Structural, Optical, and Magnetic Properties of Lead-Free Double Perovskites — •Volodymyr Vasylkovskyi[1,2], Anastasiia Kultaeva[1], Olga Trukhina[1], Patrick Dörflinger[1], Daniele Ludwig[1], Mykola Slipchenko[1,2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Institute for Scintillation Materials, NAS of Ukraine, 61072 Kharkiv, Ukraine

Semiconducting perovskite materials have attracted significant attention for their photovoltaic and light-emitting applications, yet their magnetic properties are largely unexplored. Doping perovskites with transition metal ions, such as Fe^{3+}, introduces novel properties, broadening their potential for spintronic and quantum applications.

In this study, Fe-doped $Cs_2AgBiBr_6$ and $Cs_2AgBiCl_6$ single crystals were synthesized using a controlled cooling crystallization technique with varying Fe^{3+} doping concentrations. Despite low Fe^{3+} incorporation (<0.01%), doping significantly affected defect density, optical properties, and magnetic behavior. Electron paramagnetic resonance revealed complex spin properties of the intrinsic spin centers and their interactions, which depend on both temperature and the orientation of single crystals with respect to the magnetic field.

Our findings highlight Fe-doped lead-free perovskites as promising materials for spintronic applications, emphasizing the importance of precise doping and defect manipulation to optimize their performance.

HL 29.45 Tue 18:00 P1

Multi-Frequency ODMR applied to Boron Vacancy Spin Defects of hBN — •Lucas Schreiber, Selin Steinicke, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Spin defects in hexagonal boron nitride (hBN) present a multitude of potential applications in the fields of quantum sensing and quantum information technology. Especially, the negatively charged boron vacancy defect can interact with the nuclear spins of its surrounding nitrogen atoms, thereby giving rise to hyperfine interactions. In this study, the spin defect was analyzed using optically detected magnetic resonance (ODMR) spectroscopy, wherein the spin sublevels are controlled by microwave pulses. In contrast to previous studies, the coherent microwave pulses employed in this work simultaneously utilize the multiple resonance frequencies of the hyperfine splitting. We therefore implement a multi-resonance technique for enhanced contrast and exploitation of the spin system. For an accurate and quantitative comparison with conventional ODMR, we derived a value for the contrast, allowing for a direct comparison of the hyperfine interaction on the spin defect. This approach aims at enhancing the optical detection of resonant excitation of the spin defect and facilitating coherent control experiments in future studies.

HL 29.46 Tue 18:00 P1

Temperature-dependent Studies of Boron-Vacancy Spin Defects in hexagonal Boron Nitride — •Selin Steinicke, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Optically addressable spin-carrying defects in solid-state materials are promising candidates in the field of quantum information technology and sensing applications. The recently discovered negatively charged Boron vacancies (V_B^-) in hexagonal Boron Nitride (hBN) raised the prospect of quantum sensing in a two-dimensional material. Although numerous studies on hBN emerged in the last years, the optical pump cycle has not yet been fully researched. Temperature-dependent spectroscopy on V_B^- ensembles shows broad photoluminescence around 850 nm and an increase in intensity at cryogenic temperatures. Using temperature-dependent transient photoluminescence measurements, we investigate the non-radiative relaxation path from the triplet excited state into the triplet ground state via the metastable intermediate state. The dependence of the intermediate state's lifetime on temperature is examined. These results shed light into the dark processes of V_B^- and can be used to optimize coherent control of V_B^-, which leads to a higher sensitivity in quantum sensing.

HL 29.47 Tue 18:00 P1

Investigating the optical pumping of silicon vacancies in 4H-SiC to increase the maser output — •Emilian Eisermann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

A major breakthrough in the realization of a continuous-wave maser at room temperature was achieved with the utilization of nitrogen vacancies in diamond. However, diamond is a comparatively expensive material. For this reason, silicon carbide (SiC), a material used commercially in electrical systems, has received attention in recent years. Only recently, our group has demonstrated the first room temperature continuous-wave SiC maser. Despite innovative microwave feedback loop engineering, only a low output could be achieved. In an effort to boost the maser output, we investigate the fundamental pumping behavior of

silicon vacancy defects in SiC in dependence of the optical pump wavelength, the temperature and their density. Using electron paramagnetic resonance spectroscopy, we resolve microwave absorption and emission signals due to the optical polarisation of Zeeman-split states. By analyzing these features, we calculate the population inversion in the gain material. This crucial parameter allows us to quantitatively evaluate the pump efficiency. It turns out that an excitation with an energy of the zero-phonon line of the silicon vacancy is particularly efficient. Furthermore, we examine to what extent excitation with an energy lower than that of the zero-phonon line is possible if thermally driven phonons are used to compensate the missing energy. First results are presented on the poster, which we are discussing here.

HL 29.48 Tue 18:00 P1

UV Photolithographic Fabrication of Photonic Structures on Diamond — •Nidhin Varghese, Oleg Peter, and Wolfgang Harneit — Institute of Physics,University of Osnabrück,Germany

The NV center in diamond is a point defect with promising quantum applications at room temperature, combining long spin relaxation times with optical excitation and state readout. Photonic structures such as micron-sized pillars help to increase the photon collection efficiency, improving the SNR ratio and enhancing sensitivity. NV centers in photonic structures can also be used to read out and control other spins, e.g., molecular qubits The top-down approach to fabricating photonic structures is straightforward and based on reactive ion etching of diamond. The process first requires a patterned etching mask, which is usually defined using electron beam lithography (EBL). Although EBL allows to make very small patterns, it is quite expensive and time-consuming. Using photolithographic processes could enhance industry adoption and increase accessibility to diamond quantum technology for research labs that do not have access to EBL. Here, we present a novel approach to nano-pillar fabrication based on direct (UV) laser writing lithography. An easy-to-use epoxy stage was developed for spin coating of photoresists on very small substrates, which largely supresses the formation of edge beads. The photonic pillar structures were fabricated by lithography and ion etching, and characterized. Confocal fluorescence scans demonstrated the increased photon output performance. CW-ODMR measurements confirmed the presence and accessibility of NV centers.

HL 29.49 Tue 18:00 P1

Birefringence effects in crystalline AlGaAs/GaAs mirror coatings from 4 K to room temperature — •Mona Kempkes, Chun Yu Ma, Thomas Legero, Uwe Sterr, and Daniele Nicolodi — Physikalisch-Technische Bundesanstalt, Braunschweig

Coating thermal noise limits the performance of high precision interferometry experiments, including ultra-stable optical oscillators used for interrogating atomic clocks and gravitational wave detectors. Due to their low mechanical losses, Bragg-reflectors from crystalline $Al_{0.92}Ga_{0.08}As$/GaAs heterostructures emerged as a lower thermal noise alternative to traditional dielectric mirror coatings. Mirrors realized with this material exhibit still poorly understood birefringence that can be modified by temperature and incident optical power. Furthermore, experiments at 4 K, 16 K and 124 K revealed spontaneous fluctuations of the birefringence, as well as an additional and yet unidentified noise source that limits the performance well above the expected thermal noise floor [J. Yu et al., Phys. Rev. X 13, 041002 (2023)]. Reconciling these observations from different samples is challenging and hinders a common interpretation. Thus we have set up one system where the temperature can be swept continuously across a wide range. We will present our setup based on a low-vibration closed-cycle cryostat, and measurements of the birefringence of crystalline AlGaAs/GaAs mirror coatings from 4 K to room temperature and as function of optical power.

HL 29.50 Tue 18:00 P1

Stark Effect of color centers studied from a- and m-face 4H-SiC — •Fabio Candolfi, Johannes A. F. Lehmeyer, Michael Krieger, and Heiko B. Weber — Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Angewandte Physik, Staudtstr. 7 91058 Erlangen, Germany

Color centers in silicon carbide (SiC) can operate as single photon sources and are well suited for photonic quantum technology. As compared to the intensively studied diamond platform, SiC provides both mature semiconductor functionality and process technology.

We investigated the Stark effect response of two different color centers in 4H-SiC; the established silicon vacancy defect and the less known TS defect. Both were studied from the c-face, but the photon emission occurs predominantly in the basal plane. This is why in this work low-temperature photoluminescence across the a- and m-faces were studied with Stark effect along three principal crystallographic axes. From the emission polarization of shifted and split photoluminescence lines we obtain the orientation of the dipole moment.

HL 29.51 Tue 18:00 P1

InGaAs quantum dots grown by local droplet etching — •Selma Delić[1,2], Xuelin Jin[1,2], Nils von den Driesch[1], Elias Kersting[3], Arne Ludwig[3], Alexander Pawlis[1], Detlev Grützmacher[1,2], and Beata Kardynał[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, RWTH, 52074 Aachen, Germany — [3]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Gallium arsenide quantum dots (QDs) grown using local droplet etching epitaxy (LDE) have been shown to be excellent single photon emitters. Integrated into GaAs heterostructures with two-dimensional electron gases (2DEG), the LDE QDs could facilitate spin-photon interface to spin-qubits in gated QDs, provided that photon absorption in the 2DEG in eliminated.

In this contribution, we demonstrate that the wavelength of LDE quantum dots can be effectively tuned by filling the holes edged in Al0.33Ga0.67As with InxGa1-xAs with x=10-20%. At such compositions, two-dimensional growth is expected and quantum dot formation should follow the same mechanism as that of GaAs QDs. We characterise the QDs using atomic force microscopy, low-temperature photoluminescence (PL), and microPL and analyse the effects of the growth temperature, etching step parameters, and filling material on the wavelength of QD emission. Furthermore, we show how the wetting layer emission wavelength can be used to evaluate the thickness and composition of the deposited InxGa1-xAs.

HL 29.52 Tue 18:00 P1

Tuning InGaAs quantum dots for quantum interface for heterogeneous quantum network — •Xuelin Jin[1,2], Selma Delic[1,2], Zheng Zeng[1,2], Nils von den Driesch[1,3], Alexander Pawlis[1,3], Detlev Grützmacher[1,2,3], and Beata Kardynal[1,2] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen, 52074 Aachen, Germany — [3]Peter Grünberg Institute 10, Forschungszentrum Jülich, 52425 Jülich, Germany

Abstract. Connecting different spin qubits using photonic qubits could facilitate building networks that would benefit from the inherent advantage of the individual subsystems. An efficient transfer of a qubit from a photon to the spin qubit requires matching of the energies and the bandwidths of the photon wave packet and the spin qubit optical transitions.

We discuss the design of an epitaxial quantum dot device that aim to use electrostatic gates to manipulate the bandwidth of the photons emitted from InAs QDs to improve the match to the spin qubits realized in trapped ions. We show that application of electrostatic fields can change the overlap of the e-h wavefunctions. We will discuss the conditions that the heterostructure has to fulfill for the device operation and will show the status of fabrication, which has centered on optimizing the epitaxial growth of the material. Finally, we will show the results of its characterisation aiming to show how the electronic states in these quantum dots evolve with voltages applied to the surface gates.

HL 29.53 Tue 18:00 P1

Spin-Dependent Processes Involving Defects Caused by Lithography — •Henry Stock[1,3], Michael Göldl[1,3], Niklas Bruckmoser[2,3], Leon Koch[2,3], Stefan Filipp[2,3], and Martin S. Brandt[1,3] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Straße 8, 85748 Garching, Germany — [3]School of Natural Sciences, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany

A precise knowledge of the paramagnetic defects present in quantum devices and their contribution to magnetic noise can be crucial for the optimization of such devices. However, conventional electron spin resonance experiments are often not sensitive enough to observe the defects. Using spin selection rules governing, e.g., recombination, the sensitivity of magnetic resonance experiments can be improved significantly. In its pulsed form, this so-called electrically detected magnetic resonance (EDMR) even enables the time-resolved study of the spin dynamics of the defects, allowing for measurements of the formation and recombination of spin pairs, as well as of the spin relaxation times T_1 and spin decoherence times T_2. Here, we present a study where we investigate paramagnetic P_{b0} defects and lithographically induced fluorine defects in Si substrates used for the manufacturing of superconducting transmon qubits. Our results are important to illuminate the role these defects play in flux noise and their influence on qubit coherence.

HL 29.54 Tue 18:00 P1

Progress on fully gate-defined optical interfaces to spin qubits — •Maxim Reznikov[1], Sebastian Kindel[1], Kui Wu[2], Nikolai Spitzer[3], Andreas D. Wieck[3], Arne Ludwig[3], Jeremy Witzens[2], and Hendrik Bluhm[1] — [1]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Germany — [2]Institute of Integrated Photonics, RWTH Aachen University, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Advancing quantum networks beyond proof-of-concept applications requires an approach for fabricating quantum repeater nodes with multiple qubits and optical interfaces in a controlled manner. Semiconductor spin qubits in gate-defined quantum dots address these needs in terms of established high-fidelity qubit operations and compatibility with industrial semiconductor technology. By employing electrostatic gating on either side of a submicron-thick heterostructure, excitons can be precisely localized at deterministic positions, thus also realizing an optical interface. These exciton trapping devices overcome the fabrication randomness associated with self-assembled quantum dots and enabling fine-tuning of operational wavelengths.

In this work, we demonstrate the successful integration of exciton trapping devices based on GaAs quantum wells into photonic crystal cavities. Additionally, we show the same confinement mechanism can be transferred to the Ge/SiGe platform, which is more compatible with industrial processing and telecom wavelength.

HL 29.55 Tue 18:00 P1

RPCVD growth of nuclear spin-free 70Ge/28Si70Ge heterostructures on industrial SiGe wafers — •Patrick Daoust, Simone Assali, Anis Attiaoui, Gérard Daligou, Patrick Del Vecchio, Sebastian Koelling, Lu Luo, Nicolas Rotaru, Oussama Moutanabbir, and Éloise Rahier — Department of Engineering Physics, École Polytechnique de Montréal, C.P. 6079, Succ. Centre-Ville, Montréal, Québec, Canada H3C 3A7

The coherence and operation of hole spin qubits in planar Ge heterostructures are both very sensitive to the nuclear spin bath. Therefore, developing nuclear spin-depleted materials is critical to control the performance of these quits. To this end, it is important to eliminate the nuclear spin-full 29Si and 73Ge in the epitaxial Ge/SiGe heterostructures. Our group has recently demonstrated highly crystalline, defect free, isotopically purified (>99.9 at.% 70Ge) nuclear spin-depleted 70Ge quantum well (QW) heterostructures grown in a reduced pressure CVD using purified precursors (>99.9 at.% 70GeH4 and >99.99 at.% 28SiH4) on in situ grown reversed graded SiGe buffers [1]. However, this growth protocol is not efficient and consumes significantly these purified precursors. Herein, we show that the growth of 70Ge QW can be achieved on industrial SiGe wafers thus optimizing the usage of precursors, preventing any background contamination from natural precursors, and yielding highly purified 70Ge/28Si70Ge heterostructures.

HL 29.56 Tue 18:00 P1

Time resolved electron imaging of a high-Q nonlinear nanomechanical oscillator — •Kai Nettersheim[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

While micro-electromechanical systems are well adapted for probing nonlinear dynamics in nanomechanical systems, they are often limited in their spatial resolution. Recent advances in ultrafast electron microscopy (UTEM) [1] enable the highly localized probing of nanoscale oscillator dynamics as well as their atomic structure and material defects.

Here, we present the characterization of non-linear free-standing silicon membranes by UTEM imaging techniques using an event-based electron detector with nanosecond temporal resolution. By exiting the sample with a modulated continuous wave laser the sample is driven into the nonlinear regime, resulting in Duffing resonances with high quality factors of up to 10^5. We experimentally characterized the temperature and fluence dependencies of the resonance as well as the mode shapes involved and compare these to finite-element simulations.

[1] A. Schröder et al., arXiv:2410.23961v1 (2024)

HL 29.57 Tue 18:00 P1

Quantum Particles on Strongly Bent Curves — •Tim Bergmann, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

Quantum systems under geometrical restrictions appear both in research and applied fields such as materials design, for example in the context of quantum wires. In the case of a curve these lead to a one-dimensional Schrödinger equation with its curvature appearing as a potential like term. Up to this point, there existed no ansatz for the treatment of singulary bent curves because the curvature diverges. We provide a solution to this problem for a subclass of such curves, employing a useful mathematical tool for the convergence of eigenvalue equations. This desingularization renders the approximation of the eigenspectrum and corresponding wave functions of systems with singular Hamilton operators possible.

HL 29.58 Tue 18:00 P1

Shutter synchronized deposition in molecular epitaxy for wafer scale homogeneous quantum emitter growth — •Elias Kersting, Hans Georg Babin, Nikolai Spitzer, Andreas Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

Most quantum dot (QD) based single photon emitters today are based on random position nucleated QDs with spectrally broad emission properties. Deterministic QD growth in position and emitter wavelength would be highly appreciated for large-scale and good turnabout chip manufacturing. Local droplet etching during molecular beam epitaxy is an all-in-situ method to predetermine the nucleation site of quantum dots. As recently demonstrated, this method can produce strain-free GaAs QDs with excellent photonic and spin properties. We use random position droplet nucleation and hole filling demonstrating enhanced emitter wavelength homogeneity on a wafer scale. By shutter synchronized rotation and ideal growth parameters, we grow QDs with a peak emission wavelength spread of no more than 2 nm on a full 2" diameter area with a narrow inhomogeneous ensemble broadening. While the emission wavelength of these QDs is < 800 nm, we can use this random local droplet nucleation, nanohole drilling and InAs infilling to produce QDs emitting in the telecom optical fibre transparency window around 1.3 μm, the so-called O-band. For this approach, we demonstrate 2" wafer scale control of the emission wavelength and excellent uniformity. We discuss our methodology, structural and optical properties.

HL 29.59 Tue 18:00 P1

Integration of quantum dot-based single-photon sources onto silicon photonic platform using micro-transfer printing — •Simon Oberle, Ponraj Vijayan, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Germany

Silicon photonics for telecommunications applications has garnered much attention recently. The optical transparency and the large refractive index contrast of silicon in the telecommunication wavelengths allow the implementation of high-density photonic integrated circuits. One disadvantage of silicon photonics is the lack of a native light source due to the indirect band-gap nature of silicon. One potential solution is the integration of III-V material, which offers outstanding optical emission properties, on a silicon platform. The direct growth of III-V materials on silicon is economically favourable and therefore the most desired approach. However, it is challenging because of the large lattice mismatch between the III-V materials and silicon. An alternate approach for large-scale integration is through hybrid integration of III-V structures using micro-transfer printing. Our group has previously developed In(Ga)As quantum dots on GaAs emitting in the telecom C-band. Here, we report our approach to designing and fabricating structures for the hybrid integration of these QDs onto a silicon platform using micro-transfer printing.

HL 29.60 Tue 18:00 P1

enhancing the emission Intensity of Mn2+ by doping with Ln3+ ions in ZnSe QDs and heavy metal ions detection — •Iram Gul[1], Zahid U. Khan[2], Latif U. Khan[3], Hermi F. Brito[4], and Muhammad Abdullah Khan[5] — [1]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan — [2]Research Centre for Greenhouse Gas Innovation, University of Sao Paulo (USP), 05508-030, São Paulo * SP, Brazil — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan — [4]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [5]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan

This study enhances the photoluminescence of ZnSe:Mn2+ quantum dots (QDs) by doping with Ln3+ ions (Sm3+, Gd3+, La3+, Y3+, Nd3+, Yb3+, Tm3+, Lu3+). Sm3+ and Gd** exhibited the strongest emissions due to efficient energy transfer to Mn2+, while other ions showed quenching at higher concentrations. These QDs, with uniform morphology, were applied to detect heavy metals (Pb2+, Cr3+, Hg2+, Cu2+, Fe2+), which quenched photoluminescence. Pb2+ showed the highest sensitivity (LoD: 4.648.10-3 mol/L), and Fe2+ the lowest (LoD: 5.257.10 -3 mol/L). ZnSe:Ln3+,Mn2+ QDs demonstrate potential for advanced photoluminescent applications and environmental monitoring of pollutants

HL 29.61 Tue 18:00 P1

enhancing the emission Intensity of Mn2+ by doping with Ln3+ ions in ZnSe QDs and heavy metal ions detection — •Iram Gul[1], Zahid U. Khan[2], Latif U. Khan[3], Hermi F. Brito[4], and Muhammad Abdullah Khan[5] — [1]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan — [2]Research Centre for Greenhouse Gas Innovation, University of Sao Paulo (USP), 05508-030, São Paulo SP, Brazil — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan — [4]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [5]Department of Environmental Sciences, Quaid-i-Azam University (QAU), 15320, Islamabad, Pakistan

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Pb2+ showed the highest sensitivity (LoD: 4.648.10-3 mol/L), and Fe2+ the lowest (LoD: 5.257.10-3 mol/L). ZnSe:Ln3+,Mn3+ QDs demonstrate potential for advanced photoluminescent applications and environmental monitoring of pollutants.

HL 29.62 Tue 18:00 P1

Towards Efficient Entangled Photon Pair Sources by Semiconductor Quantum Dots in Planar Cavities — •Aditi Javali[1], Raphael Joos[1], Ponraj Vijayan[1], Lena Engel[1], Tobias Huber-Loyola[2], Sven Höfling[2], Michael Jetter[1], Simone Luca Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Lehrstuhl für Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Since the EPR violation, entangled photons have become key protagonists in quantum technology, serving as communication carriers via polarization qubits. Photon pairs entangled in telecom C-band are particularly advantageous, as this wavelength range minimizes dispersion and loss in standard optical fibers, enabling long-distance communication with reduced signal degradation. In this work, we demonstrate the generation of entangled photon pairs in the telecom C-band using InAs quantum dots integrated with a planar photonic cavity. The cavity enhances photon emission rates and collection efficiency with high entanglement fidelity. The biexciton state, emitting the entangled pair, is prepared using a two-photon excitation scheme. The entanglement is verified through state tomography, confirming the strong quantum correlations between the photons. This work highlights telecom C-band quantum dots' potential as efficient entangled-photon sources for high-performance quantum communication.

HL 29.63 Tue 18:00 P1

Influence of Short-Wavelength Irradiation on Self-Assembled Quantum Dots — •Julia Avdeev[1], Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Thomas Heinzel[1], Charlotte Rothfuchs-Engels[2], Sven Scholz[2], Arne Ludwig[2], and Andreas Wieck[2] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

Using Deep Level Transient Spectroscopy (DLTS) the charge transfer to and from Self-Assembled Quantum Dots (SAQDs) at large distance from the reservoir can be observed. Measurements are performed at a temperature of 77 K studying the influence of short-wavelength infrared irradiation. With wavelengths larger than 1.5 μm photons are not capable to induce charge emission from neutral Quantum Dots in ground state but can cause free charge carriers from electronic states in SAQDs.

HL 29.64 Tue 18:00 P1

Quantum Mechanics on Periodically Deformed Manifolds — •Theresa Appel, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Deutschland

Quantum systems confined to low-dimensional geometries exhibit unique physical behavior due to curvature-induced potentials. The poster presents results on the dynamics of particles confined to periodically curved manifolds, which we term "deformation crystals". The periodic spatial deformations directly influence the particle dynamics resulting in a band structure similar to other crystalline systems. We examine the transition from a free electron gas to a one-dimensional deformation crystal while analyzing the energy dispersion relation and symmetry-breaking effects. Furthermore, the behavior of different deformations is compared. The results reveal that the specific geometric deformations significantly influence the effective potential landscape and the band structure, thus opening up new opportunities for applications via deformation modulation of the underlying space.

HL 29.65 Tue 18:00 P1

Single-electron charging events on quantum dots in InSb nanowires — •Marcus Liebmann[1], Kanji Furuta[1], Sasa Gazibegovic[2], Diana Car[2], Erik Bakkers[2], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Dept. of Appl. Phys., Eindhoven Univ., The Netherlands

As a first step to realize a single-electron counting tip for a scanning tunneling microscope, we investigate the charge state of a quantum dot (QD) by recording the current through a floating-gate-coupled sensor dot. InSb nanowires are placed mechanically onto bottom gates with hexagonal boron nitride (h-BN) as a dielectric to define two quantum dots capacitively coupled via a floating gate. At zero source-drain voltage and high barriers, charge stability diagrams are acquired, and time series of the QD charge state reveal single-electron charging events. These are analyzed with respect to full counting statistics. The Fano factor and factorial cumulants [1] are extracted to search for correlation effects.

[1] P. Stegmann *et al.*, Phys. Rev. B **92**, 155413 (2015).

HL 29.66 Tue 18:00 P1

Spin relaxation dynamics of the excited triplet state in self-assembeld quantum dots — •Carl Nelson Creutzburg[1], Jens Kerski[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The two-electron triplet state in a self-assembled quantum dot (QD) can pair with the singlet ground state to form a spin qubit. This state is electrically addressable, making it a promising candidate for quantum information processing. Achieving this requires a long coherence time (T_2), which is limited by the spin relaxation time (T_1). While T_1 has been previously studied using optical techniques, we employ an all-electrical measurement approach. The dots are embedded in an inverted high electron mobility transistor (HEMT) to selectively charge and discharge their many-particle states with electrons from a tunnel-coupled electron reservoir (2DEG). The 2DEG also acts as a sensitive detector for the charge in the QD layer. By employing time-resolved transconductance spectroscopy [1] and varying the charging intervals, we observe the relaxation process from the excited triplet state to the singlet ground state. Using a rate equation model, we extract the spin relaxation time T_1. While there are already first results for T_1 [2], an improved temporal resolution provides new insights that could help to refine assumptions in previous studies.

[1] B. Marquardt. et al., Nature Commun. 2, 209 (2011)
[2] K. Eltrudis. et al., Appl. Phys. Lett. 111, 092103 (2017)

HL 29.67 Tue 18:00 P1

Multiphoton Emission of Quantum Dots with Different Excitation Schemes — •Patricia Kallert, Nicolás Claro-Rodríguez, Francesco Salusti, Sonja Barkhofen, Santiago Bermúdez Feijóo, Lukas Hanschke, Normen Auler, Dirk Reuter, and Klaus D. Jöns — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany

High efficiency, single-photon purity, high indistinguishability, and good qualities as entangled-photon pair emitters are key properties of ideal sources for photon-based quantum technologies. Accordingly, semiconductor quantum dots (QDs) are promising candidates. If a multi-level system is excited coherently with optical pulses of different pulse areas, such as 1π, 2π and higher, the system experiences Rabi rotations of the according rotation and the respective population inversions. For each pulse area, the probability of emitting different photon numbers for different pulse areas varies, which is recognizable in the second correlation function. [1] Since various excitation schemes are interesting for different qualities of QDs, we analyze the multiphoton emission characteristics with different excitation schemes. We anticipate that this gives a deeper insight into the structure of the emitted states and possible applications to generate customised quantum light states and required modifications to generate them.

[1] Fischer, K., Hanschke, et al. Signatures of two-photon pulses from a quantum two-level system. Nature Phys 13, 649-654 (2017).

HL 29.68 Tue 18:00 P1

Investigating Photo-Physical Properties of Ag-In-S Core and Core-shell Quantum Dots — •Johannes Kunze, Julian Mann, Sushant Ghimire, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

Non-toxic I-III-VI quantum dots (QDs) are promising candidates for next-generation light-emitting and energy-harvesting devices. However, the optical properties in these QDs are governed by subgap defects which limit their applications. Here, we synthesize AgInS2 QDs, and study them using various steady-state and time-resolved spectroscopy. Photoluminescence spectroscopy reveals that these QDs exhibit a narrow free-exciton emission and a more dominant, broad, red-shifted emission. The observed dominance arises from defects in the QDs, which introduce donor and acceptor states within the bandgap, effectively trapping electrons and holes from the band edge. A femtosecond differential transmission spectroscopy reveals an ultrafast carrier trapping time in these QDs. Additionally, a broad absorption onset with a defect-related Urbach tail is observed. We coated AgInS2 QDs with gallium sulfide, forming core/shell QDs, which significantly enhanced the intensity of the narrow free-exciton emission, reduced defect emissions, and sharpened the absorption onset by lowering the Urbach energy. These results show that the defects in these QDs are located on their surface, and Ga-S coating effectively passivates them, improving the excitonic characteristics.

HL 29.69 Tue 18:00 P1

Effects of vacancies in a bilayer graphene quantum dot — •Ivan Verstraeten, Robin Smeyers, François Peeters, and Lucian Covaci — University of Antwerp, Antwerp, Belgium

Confining the motion of an electron to the nanoscale in all three dimensions, i.e. a quantum dot (QD), sees the emergence of interesting physics and useful applications, such as single electron control or qubits. Bilayer graphene in particular, is a suitable and promising material for quantum dots owing to the many exotic properties of graphene, as well as the possibility to create and tune electronic

confinement simply by applying a (position dependent) perpendicular electric field. In this work, the electronic spectrum of an electrostatically defined QD in a finite bilayer graphene flake is numerically calculated using the tight-binding model, which is compared to existing results in the literature where a low-energy continuum theory was used. The tight-binding approach allows for a straightforward implementation of vacancies in the lattice, of which the effects on the spectrum and its valley character are studied. The results show a generally good agreement between the continuum and tight-binding theory, with some interesting discrepancies. We find that vacancies enhance the inter-valley scattering, as in the magnetic field dependence of the spectrum we observe a widening of the avoided crossings between energy levels of a different valley character. Furthermore, vacancies are found to be able to significantly shift energy levels, alter the shape of the wavefunction density and make a state retain its valley mixed character even in the presence of perpendicular magnetic field

HL 29.70 Tue 18:00 P1

Towards scalable quantum circuits based on microlaser-pumped quantum emitters — •Maximilian Klonz, Aris Koulas-Simos, Léo Roche, Imad Limame, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We report on activities towards the development of a scalable technology platform for integrated quantum photonic circuits (IQPCs) based on semiconductor quantum dots, which are deterministically integrated into photonic waveguides by in-situ electron beam lithography [1], acting as single-photon emitters. Photons, generated by these on-demand quantum emitters, serve as flying qubits in quantum communication systems and as input states for photonic quantum computing [2, 3]. Here, we present innovative technological approaches for a two-step epitaxial growth method to achieve areas with low and high density of quantum dots to further fabricate lasers and single-photon sources monolithically integrated on the same wafer. We show simulations towards a scheme for optical on-chip pumping of these single-photon emitters and first experimental results.

[1] P. Schnauber et al., Nano Letters 18, 2336 (2019)
[2] T. Heindel et al., Advances in Optics and Photonics 15, 613 (2023)
[3] S. Rodt and S. Reitzenstein., APL Photonics 6, 010901 (2021)

HL 29.71 Tue 18:00 P1

Duration of scattering processes on curved quantum wires — •Adrian Henrik Starke, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik

Over the last decade, the duration of quantum processes has become experimentally accessible via measurement of e.g. the Wigner time delay [1]. However, these measurements have so far only been performed in flat space. This study extends the concept of scattering time to curved, one-dimensional quantum wires. Wigner time delay and other parameters are examined for plane waves as well as wave packets constraint to propagate through these structures. The results demonstrate that the geometry-induced potentials significantly affect the scattering time, particularly at low energies, with the classical behavior emerging at higher energies. These findings offer insights into the interplay between curvature and quantum dynamics, paving the way for further analysis of scattering phenomena in complex geometries.

[1] Schulze et al., 'Delay in Photoemission'. In: Science 328 (2010), DOI: 10.1126/science.1189401

HL 29.72 Tue 18:00 P1

Towards a Quantitative Framework for Capacitance-Voltage Spectroscopy in Quantum Dot Ensembles — •Phil Julien Badura[1], Nico Frédéric Brosda[1], Ismail Bölükbaşı[1], Ibrahim Engin[1], Patrick Lindner[1], Sascha René Valentin[1], Andreas Dirk Wieck[1], Björn Sothmann[2], and Arne Ludwig[1] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47048 Duisburg, Germany

This study investigates an inhomogeneous ensemble of quantum dots coupled to a charge reservoir using capacitance-voltage spectroscopy. Experimental measurements reveal shifts in capacitance peak positions influenced by AC frequency and temperature, with frequency-dependent shifts remaining unexplained by existing models. To address this, we develop a master equation-based theoretical model incorporating energy-dependent tunneling effects, which successfully reproduces the experimental data. Our findings emphasize the role of energy-dependent tunneling in distinct regimes: at low temperatures, energy level dispersion dominates, while at high temperatures and frequencies, shifts arise from optimized sequences of in- and out-tunneling events.

HL 29.73 Tue 18:00 P1

Experimental time-bin encoding quantum key distribution with telecom semiconductor quantum dot — •Jipeng Wang[1], Jingzhong Yang[1], Joscha Hanel[1], Zenghui Jiang[1], Vincent Rehlinger[1], Raphael Joos[2], Stephanie Bauer[2], Sascha Kolatschek[2], Eddy Rugeramigabo[1], Michael Jetter[2], Simone Portalupi[2], Michael Zopf[1,3], Peter Michler[2], and Fei Ding[1,3] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany. — [3]Laboratorium für Nano-und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Quantum Key Distribution (QKD) enables secure data transmission via quantum-generated secret keys. Semiconductor quantum dots (QDs) are promising light sources for high-speed quantum networks due to their deterministic single-photon emission. However, polarisation stability in fibre networks is often disrupted by environmental factors. Here, we demonstrate a stable QKD scheme using time-bin qubits derived from polarised photons emitted by a QD in the telecommunication C-band. A 16-bit pseudo-random sequence is encoded via a Sagnac-loop interferometer and decoded using an unbalanced Mach-Zehnder interferometer after transmission through 80 km of fibre. This study highlights QDs' potential for scalable, robust quantum networks.

HL 29.74 Tue 18:00 P1

Experimental time-bin encoding quantum key distribution with telecom semiconductor quantum dot — •Jipeng Wang[1], Jingzhong Yang[1], Joscha Hanel[1], Zenghui Jiang[1], Vincent Rehlinger[1], Raphael Joos[2], Stephanie Bauer[2], Sascha Kolatschek[2], Eddy Rugeramigabo[1], Michael Jetter[2], Simone Portalupi[2], Michael Zopf[1,3], Peter Michler[2], and Fei Ding[1,3] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany. — [3]Laboratorium für Nano-und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Quantum Key Distribution (QKD) enables secure data transmission via quantum-generated secret keys. Semiconductor quantum dots (QDs) are promising light sources for high-speed quantum networks due to their deterministic single-photon emission. However, polarisation stability in fibre networks is often disrupted by environmental factors. Here, we demonstrate a QKD experiment using time-bin qubits derived from polarised photons emitted by a QD in the telecommunication C-band. A 16-bit pseudo-random sequence is encoded via a Sagnac-loop interferometer and decoded using an unbalanced Mach-Zehnder interferometer after transmission through 80 km of fibre. This study highlights QDs' potential for scalable, robust quantum networks.

HL 29.75 Tue 18:00 P1

Cyclic Growth of InAs Quantum Dots: Exploring Structure- Property Relations for Telecom O-Band Applications — •Lennart Anderson[1,2], Danial Kohminaei[1], Severin Krüger[1,3], Marcel Schmidt[1], Nikolai Spitzer[1], Peter Zajac[1,4], Andreas Wieck[1], and Arne Ludwig[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]ICAMS, Ruhr-Universität Bochum — [3]Sparrow Quantum ApS, Copenhagen — [4]Gesellschaft für Gerätebau mbH, Dortmund

Quantum dots (QDs) are promising single-photon emitters that could transform long-range quantum communication within telecom optical fiber transparency windows. In this study, we grow self-assembled InAs QDs using the Stranski-Krastanov growth mode, enhanced by a strain reduction layer to achieve emission at 1.3 μm in the telecom O-band. By employing cyclic sub-monolayer deposition, we observe periodic modulations in QD density, emission wavelength, and geometric properties, driven by nucleation waves, i.e. a new generation of QDs is formed each time a critical material amount for nucleation is reached. We explore the correlations between the structural characteristics and opto-electronic properties by atomic force microscopy and photoluminescence as well as capacitance-voltage spectroscopy. Our results identify optimal regions for QD density and emission wavelength across 3-inch wafers and propose a modified deposition scheme to enhance the usable area of the wafers.

HL 29.76 Tue 18:00 P1

Statistical spectroscopy of perovskite quantum dots — •Christopher Borchers[1], Frederik Benthin[1], Tom Rakow[1], Pengji Li[1], Maximilian Heller[1], Chenglian Zhu[2,3], Ihor Cherniukh[2,3], Gabriele Rainò[2,3], Maksym Kovalenko[2,3], Michael Zopf[1,4], and Fei Ding[1,4] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics, Empa - Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland — [4]Laboratory of Nano and Quantum Engineering, Leibniz University Hannover, Schneiderberg 39, D-30167 Hannover, Germany

The ability to perform fast and automated photoluminescence (PL) spectroscopy measurements greatly improves the efficient development of quantum light emitters and their optimization in quantum technologies.

We adopt and semi-automate standard low temperature optical characterization measurements for lead halide perovskite colloidal quantum dots. Here, PL spectroscopy on CsPbBr3 samples is used to characterize the emission spectrum, polarization properties, and fine structure, and to perform corresponding automated statistical analyses of these measurements. For these analyses, we have developed a program that processes PL spectral data, automatically detecting and fitting emission peaks for subsequent evaluation.

HL 29.77 Tue 18:00 P1

SUPER drived quantum dot at telecom wavelength — •Zenghui Jiang[1], Vikas Remesh[2], Frederik Benthin[1], Michael Zopf[1], and Fei Ding[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Department of Experimental Physics University of Innsbruck Technikerstr. 25d, Office 01/503 6020 Innsbruck, Austria

To obtain the best photon properties from quantum dots (QDs),a direct drive between the S-shell and ground state (resonance excitation) is required. However, since the excitation laser and the emitted wavelength are very close to each other, filtering out the laser becomes highly challenging. A theoretical study conducted in 2021 by Prof. Doris Reiter's group predicted that with two relatively detuned laser pulses, full population inversion can still be achieved without interacting with other energy levels. Consequently, photon properties comparable to those achieved through resonance excitation can be expected.

To efficiently drive QDs, two temporally overlapping laser pulses with different frequencies are needed. Compared to using two separate lasers for "SUPER" excitation, employing a single laser with a pulse shaper eliminates the need for synchronization between two lasers. However, until now, no experiment using a single laser with a pulse shaper has been performed on telecom-wavelength QDs. In our work, we constructed a pulse shaper using a spatial light modulator to generate two sharply defined laser pulses from a single broadband laser pulse,and successfully *SUPER* excited QD at telecom wavelength.

HL 29.78 Tue 18:00 P1

Fabrication of Ohmic contact for Electrical tuning of GaAs quantum dots — •Krupali Dobariya[1], Tom Fandrich[1], Yiteng Zhang[1], Johann Dzeik[1], Arijit Chakraborty[1], Tom Rakow[1], Sulabh Shrestha[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover, Institut for Solid State Physics, Hannover, Germany — [2]Leibniz Universität Hannover, Laboratorium for Nano and Quantum Engineering, Hannover, Germany

Semiconductor quantum dots have shown unique properties as deterministic single photon and entangled photon pair sources. Their outstanding optical properties have the potential for use in quantum applications like quantum communication, quantum key distribution and quantum computing. Nevertheless, due to the stochastic nature of the self-assembly growth process, quantum dots typically emit photons with a broad wavelength distribution across the entire chip, posing challenges for applications requiring specific wavelengths. To address this issue, various tuning techniques have been developed. Electrical tuning, in particular, has emerged as an effective method for adjusting the wavelength and mitigating charge noise in semiconductor quantum dots. Our research focuses on the impact of contact fabrication on the emission properties of GaAs quantum dots. We aim to optimize the process of forming ohmic contacts to n- and p-doped GaAs, placing special emphasis on the selection of materials and the reduction of contact resistance. The quality and performance of the electrical contacts are evaluated through the photoluminescence characterization.

HL 29.79 Tue 18:00 P1

Marker-based deterministic EBL integration of GaAs quantum dots (QDs) into electrically tunable Circular Bragg Gratings (eCBGs) at a wavelength of 780 nm — •Dinara Basharova[1], Mudi Priyabrata[1], Avijit Barua[1], Setthanat Wijitpatima[1], Andreas D. Wieck[2], Sven Rodt[1], Arne Ludwig[2], Richard Warburton[3], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, DE-44780 Bochum, Germany — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Integration of high-quality quantum emitters with photonic structures is essential for advancing quantum information technologies. We present a marker-based deterministic electron beam lithography (EBL) technique to integrate Gallium Arsenide (GaAs) quantum dots (QDs) into electrically contacted Circular Bragg Gratings (eCBGs) at an emission wavelength of 780 nm, combined with a PIN-diode structure. eCBG devices not only enhance the photon extraction efficiency through a circularly symmetric cavity design but also provide precise electrical control over the QD emission. This enables fine-tuning of the wavelength, addressing spectral mismatches, and stabilizing the charge environment around the QD, critical for high-performance quantum light sources. Therefore, combining the eCBG design with deterministic fabrication techniques ensures that the QDs are precisely positioned at the cavity center, maximizing light-matter interaction.

HL 29.80 Tue 18:00 P1

Laboratory management software: Plexy : Python Library for EXperimental Physics — •Frederik Benthin, Christopher Borchers, Nico Eggeling, Tom Fandrich, Dolores García de Viedma, Joscha Hanel, Maximilian Heller, Martin Hesse, Kai Hühn, Johannes Knollmann, Marcel Pölking, Tom Rakow, Eduard Sauter, Pavel Sterin, Fei Ding, Jens Hübner, and Michael Zopf — Leibniz Universität Hannover, Institute of Solid-State Physics, Appelstraße 2, 30167 Hannover

Measurements often involve complex protocols requiring the coordination of many different devices. Laboratory management or measurement software such as Qudi and NOMAD-CAMELS assist in performing these tasks. It provides a framework for easier collaboration and sharing of resources. It often includes a standalone graphical user interface (GUI). This GUI controls new compound instruments consisting of several devices and can be used to coordinate the measurement. Different projects often improve an additional aspect, such as NOMAD-CAMELS with metadata collection or MAHOS with messaging between distributed devices. Here we present Python Library for EXperimental Physics (Plexy), which is a highly modular repository of Python modules. Among the main design goals are automatic metadata recording, distributed device coordination, modular and flexible but standardized code organization as well as independent and common GUIs. An analyzer GUI performs common analyses specific to photoluminescence spectroscopy and time-correlated single-photon counting of quantum dot single-photon sources.

HL 29.81 Tue 18:00 P1

Signatures of the quantum skyrmion Hall effect in the Bernevig-Hughes-Zhang model — •Reyhan Ay, Adipta Pal, and Ashley M. Cook — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Given the recent discovery of the quantum skyrmion Hall effect (QSkHE) revealing that the 2+1 D SU(2) gauge theory should be generalized to include terms from an underlying 4+1 D SU(2) gauge theory subjected to generalized fuzzification, we re-examine the canonical Bernevig-Hughes-Zhang (BHZ) model for the quantum spin Hall insulator (QSHI). Considering that the isospin degrees of freedom in the tight-binding model Hamiltonian effectively encode two additional spatial dimensions, we identify signatures of topological states within the QSkHE framework related to intrinsically 4+1 D topological phases revealed by breaking time-reversal symmetry through a weak Zeeman field. We identify distinctive real-space boundary orbital angular momentum textures due to the QSkHE, as well as gapless boundary modes that are robust against magnetic disorder, which is unexpected for a QSHI but predictable for compactified boundary 3D Weyl nodes in a topological skyrmion phase. Revisiting experimental work on robust edge conduction in HgTe quantum wells under Zeeman and orbital magnetic fields, we find these results consistent with theoretical predictions of compactified boundary 3D Weyl nodes to such external fields. These experiments are thus potentially the first-known experimental observation of the quantum skyrmion Hall effect.

HL 29.82 Tue 18:00 P1

Side-contacted narrow superconducting finger on quantum anomalous Hall insulator — •Bibek Bhujel, Anjana Uday, Gertjan Lippertz, Alexey A. Taskin, and Yoichi Ando — Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany

Recently, the evidence for superconducting pair correlation is obtained in the chiral edge states of a vanadium-doped $(Bi_xSb_{1-x})_2Te_3$ thin film, tuned to the quantum anomalous Hall insulator phase by observing the negative nonlocal resistance downstream from a narrow superconducting (grounded) Nb finger electrode fabricated on the top [1]. This negative downstream resistance is due to the crossed Andreev reflection (CAR) process, which creates superconducting correlations in the chiral edge. To investigate this observation further, we are currently fabricating side-contacted Al and Nb finger electrodes on the etched QAHI. One of the main advantages of fabricating the side-contacted electrodes is their low contact resistance, which has high reproducibility. We will report on our progress on this project so far.

[1] Uday, A., Lippertz, G., Moors, K. et al. Induced superconducting correlations in a quantum anomalous Hall insulator. Nat. Phys. 20, 1589*1595 (2024). https://doi.org/10.1038/s41567-024-02574-1

HL 29.83 Tue 18:00 P1

Anomalous Hall effect in a two-dimensional disordered Lorentz gas — •Frederik Bartels[1], Zakaria Harroud[1], Beate Horn-Cosfeld[1], Mihai Cerchez[1], Jürgen Horbach[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Theoretical Physics II: Soft Matter, Heinrich Heine University, Düsseldorf, Germany

Using a combination of experiment and simulation, it was studied the magnetotransport in a two-dimensional disordered Lorentz gas with cross-shaped ob-

stacles. Our focus is on the investigation of the Hall effect for obstacle densities beyond the low-density limit. From previous studies, we know that for lower obstacle densities, the magnetotransport properties, as obtained from the simulation and the experiment of a pristine sample, can be well described in terms of the Drude-Boltzmann model. At higher obstacle densities, deviations from the normal Hall effect are observed, depending on both obstacle density and magnetic field. These results extend previous studies on circular obstacles, where similar deviations were observed and the Hall coefficient does not accurately reflect the electron density because of the presence of memory effects. [1]

[1] B. Sanvee *et al.* Phys. Rev. B **108**, 035301 (2023)

HL 29.84 Tue 18:00 P1

Accelerated Electrical Transport Predictions of the Non-Perturbative ab initio Kubo-Greenwood Method via a Deep-learned Hamiltonian technique: Strongly Anharmonic Material Cases — •Juan Zhang, Jingkai Quan, Matthias Scheffler, and Kisung Kang — The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany

High-performance thermoelectric materials are characterized by low thermal and high electrical conductivities. Thermal insulators with ultra-low thermal conductivity feature strong anharmonicity, also significantly affecting electronic transport [1]. Strong anharmonicity impedes the application of perturbative methods due to the breakdown of the quasi-particle picture. This challenge can be overcome by the non- perturbative ab initio Kubo-Greenwood approach (aiKG)[1]. However, the aiKG method requires substantial computational cost due to its extensive supercell electronic structure evaluations at each step during ab initio Molecular Dynamics (aiMD). A recent deep neural network technique to train and predict the Kohn-Sham Hamiltonian, implemented by DeepH[2], can provide an efficient bypass to extract the electronic structure of each MD step with nearing ab initio accuracy. This work introduces an AI-assisted aiKG formalism with accelerated carrier mobility evaluations, exemplified by its application to strongly anharmonic materials. We thoroughly examine DeepH's capability for electronic property predictions with its spatial scalability.

[1] J. Quan et al., Phys. Rev. B, accepted (arXiv:2408.12908).

[2] X. Gong, et al., Nat Commun. 14, 2848 (2023).

HL 29.85 Tue 18:00 P1

Magnetotransport in the correlated metal $CaVO_3$ — •Olivio Chiatti[1], Mahni Müller[1], Maria Espinosa[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and Saskia F. Fischer[1,4] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Transparent conductive materials are in great demand in the optoelectronic industry for their high-performance and cost-effectiveness. Enhancing the carrier effective mass through strong electron-electron interactions in correlated metals is a promising approach to achieve both high-optical transparency and high-electrical conductivity [1].

Here, we study the electric transport properties of thin $CaVO_3$ films grown on $LaAlO_3$ substrates by hybrid molecular beam epitaxy, with residual resistivity ratio (RRR) up to 98 [2]. Magnetoresistance and Hall measurements were performed between 50 mK and 300 K. Films with high RRR show nonlinear Hall resistivities and linear magnetoresistance below 40 K. Shubnikov-de Haas oscillations are also observed for magnetic fields above 6 T. The application of a multi-carrier model and the complex Fermi surface of $CaVO_3$ are discussed.

[1] Zhang *et al.*, Nature Materials **15**, 204 (2016)

[2] Kuznetsova *et al.*, APL Materials **11**, 041120 (2023)

HL 29.86 Tue 18:00 P1

Selenium, Silicon and SiC power diodes as temperature sensors, operated in different voltage regimes and under extreme conditions — •Heinz-Christoph Neitzert, Arpana Singh, and Vincenzo Carrano — Dept. of Industrial Engineering (DIIn), Salerno University, Via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy

Commercial semiconductor temperature sensors are nowadays mostly based on silicon diodes and transistors, operated under constant forward current conditions. We compared the temperature sensing capabilities of a series of different power diodes from different materials not only in the forward, but also in the reverse bias and in one example also in the breakdown voltage regime. All investigated devices, including the historical Se rectifiers, showed stable temperature sensing capabilities in the forward bias regime under moderate temperature changes. Some of them have been tested under extreme conditions like extreme temperatures and particle irradiation. In particular it is shown in the case of the SiC Schottky diodes, that the excellent temperature sensing properties are also maintained after irradiation with high energy ions. In the case of Silicon pn diodes the sensitivity as sensor in the forward voltage and avalanche breakdown regime has been determined. In both regimes the sensors showed very good linear characteristics, when biased under constant current conditions. For Silicon diodes, also the temperature limit, where no irreversible device changes are observed has been determined and the defect creation for higher temperatures has been monitored.

HL 29.87 Tue 18:00 P1

Structural Dynamics of Excimer Formation in single crystalline α-Perylene — •Helena Hollstein[1], Simon Versmissen[2], Bram Spijkerman[2], Heinrich Schwoerer[2], and Sebastian Hammer[1] — [1]University of Würzburg, 97074 Würzburg, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany

In the field of organic semiconductors an exact understanding of the formation of multi-molecular excited states, such as excimers, and geometric intermolecular changes caused thereby, is crucial but challenging. Quantum chemical methods are in principle able to capture all structural changes during excimer formation but are hardly feasible due to the complexity of organic crystals. Experimentally on the other hand, the molecular motion can be detected by ultra-fast electron diffraction (UED) on a femtosecond timescale [1], and by using structural modeling the molecular movement can be reconstructed from changes in the diffraction pattern [2].

In this contribution we examine the structural reorganization during the formation of the low lying excimer state in single crystalline perylene in its crystallographic α-phase by means of UED. We are able to reveal the pathways of the geometric relaxation during the excimer formation on a fs timescale and find that the formation happens on a 5 ps timescale.

HL 29.88 Tue 18:00 P1

All-optical spin injection in silicon investigated by element-specific time-resolved Kerr effect — Simone Laterza[1,2], Antonio Caretta[1], •Richa Bhardwaj[1,3], Roberto Flammini[4], Paolo Moras[5], Matteo Jugovac[5], Piu Rajak[6], Mahabul Islam[6], Regina Ciancio[6], Valentina Bonanni[1], Barbara Casarin[2], Alberto Simoncig[1], Marco Zangrando[1,6], Primož R. Ribič[1], Giuseppe Penco[1], Giovanni De Ninno[1], Luca Giannessi[1], Alexander Demidovich[1], Miltcho Danailov[1], Fulvio Parmigiani[1], and Marco Malvestuto[1,6] — [1]Elettra Sincrotrone Trieste, Italy — [2]University of Trieste, Italy — [3]Institute of Physics and Center for Nanotechnology (CeNTech), University of Münster, 48149 Münster, Germany — [4]Istituto di Struttura della Materia-CNR (ISM-CNR), Roma, Italy — [5]Istituto di Struttura della Materia-CNR (ISM-CNR), Trieste, Italy — [6]Istituto Officina dei Materiali (CNR-IOM), Trieste, Italy

Understanding how a spin current flows across metal-semiconductor interfaces at pico- and femtosecond time scales is of paramount importance for ultrafast spintronics, storage applications etc. However, the possibility to directly access the propagation of spin currents, within such time scales, has been hampered by the simultaneous lack of both ultrafast element-specific magnetic sensitive probes and tailored well-built and characterized metal-semiconductor interfaces. Here, by means of a novel free-electron laser-based element-sensitive ultrafast time-resolved Kerr spectroscopy, we reveal different magnetodynamics for the Ni $M_{2,3}$ and Si $L_{2,3}$ absorption edges.

HL 29.89 Tue 18:00 P1

Implementation and operation of a fiber-coupled CMOS detector for time-resolved photoemission electron microscopy — •Philipp Kessler[1], Johanna Kinder[1], Victor Lisinetskii[1], Torsten Franz[2], Florian Schütz[2], Matthias Hensen[1], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]ELMITEC Elektronenmikroskopie GmbH, 38678 Clausthal-Zellerfeld

Since their invention, low-energy electron microscopy (LEEM) and photoemission electron microscopy (PEEM) have predominantly relied on microchannel plates for electron detection and image generation. Recent developments in detector technology allow the LEEM-PEEM community to use pixel- [1] and fiber-based [2] detectors that have a small detection pixel size, avoid blooming effects, and have an extended dynamic range. These advancements are particularly beneficial for ultrafast time-resolved experiments with weak signals. Here, we present the integration of the fiber-coupled CMOS detector XF416 (TVIPS GmbH, Germany) into an Elmitec AC-LEEM III system. This includes a structural solution to address the detector's inability to undergo bake-out, a critical step for achieving ultrahigh vacuum conditions. The first-time operation of the new detector unit is demonstrated through time- and energy-resolved PEEM measurements on terrylene bisimide-based molecular thin films, enabling the study of exciton dynamics at the nanoscale.

[1] G. Tinti et al., J. Synchrotron Rad. 24, 963 (2017).

[2] D. Janoschka et al., Ultramicroscopy 221, 113180 (2021).

HL 29.90 Tue 18:00 P1

Experimental scheme for high-order fluorescence-detected pump–probe micro-spectroscopy on monolayer MoS_2 — •Ruidan Zhu, Patrick Grenzer, Simon Büttner, Matthias Hensen, Tobias Hertel, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Monolayers of transition metal dichalcogenides (TMDCs) are two-dimensional (2D) semiconductors with fascinating optoelectronic properties. However,

exciton–exciton interaction (EEI) sets a fundamental limit to optimizing the quantum efficiency of 2D materials under high exciton densities. In particular, EEI processes are frequently mixed with single-exciton dynamics, thereby complicating the elucidation of their underlying mechanisms. Here, we apply fluorescence-detected pump–probe spectroscopy [1] in a cryomicroscope to detect the exciton dynamics of monolayer MoS_2. By incorporating the high-order separation methods that we recently developed [2], we aim to isolate EEI dynamics from the single-exciton dynamics, other higher-order signal contributions, and non-resonant substrate responses. We present the fundamental concept, the experimental setup, and the first data.

[1] P. Malý and T. Brixner, Angew. Chem. Int. Ed. 2021, 60, 18867.
[2] P. Malý et al., Nature 2023, 616, 280.

HL 29.91 Tue 18:00 P1

Detection Strategies for Highspeed Impulsive Stimulated Raman Scattering — •Laura Hüllmandel, Julia Lang, and Georg Herink — Universität Bayreuth

Impulsive stimulated Raman scattering is an established method for resolving transient coherent superpositions of optical phonons in matter. Inside a laser cavity, however, this nonlinear interaction between multiple ultrashort temporal solitons can accumulate and determine their trajectories [1]. In this contribution, we study different regimes of the coupling between solitons via optical phonons. Based on extra-cavity spectroscopic experiments on crystalline media, we compare interferometric and spectrally-resolved sampling modes and, in particular, we discuss practical aspects in enhancing Raman signal quality. These new insights contribute to the understanding of phonon-driven soliton coupling and the development of time-domain intra-cavity Raman spectroscopy.

[1] A. Völkel et al., "Intracavity Raman Scattering Couples Soliton Molecules with Terahertz Phonons.", Nature Communications 13.1 (2022).

HL 29.92 Tue 18:00 P1

Two-dimensional spectroscopy setup for the investigation of excitons and polaritons in 2D materials — •Trideep Kawde, Pavel Trofimov, Matteo Russo, Anton Trenczek, David Koch, and Hélène Seiler — Freie Universität Berlin, 14195, Berlin, Germany

Coherent two-dimensional (2D) electronic spectroscopy is a powerful tool for probing interactions between electronically excited states and map their evolution in both energy and time domains. Here we introduce a coherent two-dimensional spectrometer tunable over the 460-950 nm spectral range to investigate the exciton and polariton dynamics in 2D materials. We employ a hollow-core fiber setup for broadband visible continuum generation. Pulse shapers are used to produce phase-locked sequences of pulses. A custom sample area has been designed specifically for 2D materials, typically featuring high degrees of spatial inhomogeneity and small sizes (few tens of micrometers). Linear spectroscopies can be performed at the same position as the 2D spectroscopy experiments, including angle-resolved spectroscopy to investigate polariton dispersion. With our setup we will be able to reveal insights into excitonic and polaritonic properties in 2D materials.

HL 29.93 Tue 18:00 P1

Measurement of ultrashort electron pulse durations using a transient electric field — •Lukas Nöding, Arne Ungeheuer, Ahmed Hassanien, Mashood Tariq Mir, Thomas Baumert, and Arne Senftleben — University of Kassel, Institute of Physics, Kas- sel, Germany

Ultrafast electron diffraction is a well-known method for conducting time-resolved measurements on molecules and condensed matter. In this approach, electron diffraction is performed with an electron pulse at a variable time after optical excitation of the sample. The duration of the electron pulse directly determines the temporal resolution. A streaking setup utilizing free electrons is implemented to measure the duration of the electron pulse. Therefore, a transient electron deflector, was designed. Its main feature is a metal surface parallel to the path of the electron pulse. A femtosecond laser pulse is focused from the side onto this metal surface. As the beam incides, electrons are released from the metal. Due to their momentum, they separate from the surface, create an electric field perpendicular to the surface and then recombine. The build-up and the subsequent fading of this transient electric field is used to streak the electron pulse, because different electrons in the pulse experience different field strengths. By that, the duration of the pulse is mapped into a spatial broadening of the pulse. The broadening is captured by the detector as a streak. We will show results measured with different numbers of electrons per pulse and compare them with simulations. Moreover, the evaluation process and the fitting algorithms for the electron streak will be explained.

HL 29.94 Tue 18:00 P1

Ultrafast dynamics reveal proximity induced changes in Graphite — •Mashood Tariq Mir, Ahmed Hassanien, Arne Ungeheuer, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics, D-34132 Kassel, Germany

Layered transition metal dichalcogenides (TMDs) are at the forefront of materials research due to their diverse electronic and structural properties. Among these materials, 1T-TaS2 exhibits a complex temperature-dependent phase diagram characterized by charge density waves (CDWs) of varying commensurabilities. When integrated into heterostructures, novel interfacial phenomena emerge, enabling the study of proximity effects in atomically thin materials. This work investigates the light-induced dynamics of a van der Waals heterostructure composed of 1T-TaS2 and graphene using ultrafast electron diffraction (UED). Femtosecond laser pulses induce rapid structural changes, revealing a proximity-induced CDW in graphene. This observation demonstrates how interfacial coupling can imprint the characteristic periodic lattice modulation of CDWs onto an otherwise non-CDW material. By controlling lattice heating, we probe the reversible phase transition of 1T-TaS2 from the nearly commensurate to the incommensurate phase and its influence on the interfacial properties of the heterostructure.

HL 29.95 Tue 18:00 P1

Determination of Arrival Time in Ultrafast Electron Diffraction in Specimen Close Proximity with High Accuracy — •Ahmed Hassanien, Mashood Tariq Mir, Arne Ungeheuer, Lukas Nöding, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

The ability to determine time zero in a pump-probe experiment qualitatively indicates its ability to capture dynamics and quantitatively serves as a measure of its temporal resolution. There are only a few methods for determining the time zero in ultrafast electron diffraction (UED) [1,2]. Here, we propose a robust and easy-to-implement method to determine time zero in the immediate vicinity of the sample with sub-picosecond accuracy using Fourier-transformed electron micrography (FT-EM). In the same analogy as the Debye-Weller effect in crystalline solids, the attenuation of the peak amplitude in FT-EM patterns for a metal grid blurred by femtosecond optically-induced transient electrostatic lensing (TEL) allowed us to determine time zero to better than 500 fs. To demonstrate our method, we measured the time zero in the vicinity of a graphite flake, for which we also performed a routine UED measurement by exciting with the same optical pump fluence, well below the damage threshold for either material. Using the accurately determined time zero, we were able to identify the earlier onset of the out-of-plane coherent optical phonon mode in graphite. References: [1] Olshin, Pavel K., et al. APL 120.10 (2022). [2] Dwyer, Jason R., et al. Philos. Trans. of the Royal Society A: Math., Phys. and Eng. Sci. 364.1840 (2006): 741-778.

HL 29.96 Tue 18:00 P1

Investigation of dynamics and character of excitons in WSe_2 multilayers — •Anna Weindl[1], Matthias Brem[1], Jennifer Lehner[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan

We report about our time-resolved Faraday ellipticity (TRFE) experiments on multilayers of the transition metal dichalcogenide WSe_2. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the temporal dynamics in WSe2 multilayers. These previous results have shown that pseudospin oscillations appear in the TRFE signal when we apply an in-plane magnetic field to our multilayer samples. Current results show that the oscillations have two different frequencies, a shorter one earlier in time and a longer one later in time. In differential transmission measurements, the lifetimes show a fast and slow decay on the same time scales. This suggests two different exciton dynamics or species. Now we try to characterize and manipulate these oscillations by playing with different experimental parameters. Varying the angle of the magnetic field, adding an electric field or investigating the layer dependence are examples for our toolbox of parameters to gain further insights in the dynamics of the multilayers.

[1] Raiber et al., Nat Commun 13, 4997 (2022).

HL 30: Focus Session: Young Semiconductor Forum

The young semiconductor forum gives a platform for post-docs at all career stages to present themselves and their scientific ideas. It consists of an oral session with invited talks and immediately afterwards, a poster session, where further participants present a poster about their work and/or scientific vita. With this format, we hope to attract both postdocs and senior researchers and decision makers to join this forum: for postdocs, to give them a platform to present themselves, and for professors, to meet the next generation of scientists.

Organized by Alexander Holleitner and the AGyouLeaP (Susanne Liese, Alexander Schlaich, and Christoph Kastl)

Time: Wednesday 9:30–12:15 Location: H13

Invited Talk HL 30.1 Wed 9:30 H13

Exploring semiconducting epigraphene grown by polymer-assisted sublimation growth — •Teresa Tschirner, Julia Guse, Stefan Wundrack, Frank Hohls, Klaus Pierz, and Hans Werner Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Epitaxial graphene on SiC is a potential candidate in a variety of applications, such as the fabrication of 2D heterostructures and the intercalation of graphene layers with other materials for engineering new electronic material systems. Important for the quality of the graphene is the 0th layer, or buffer layer, which is covalently bonded to the SiC substrate. The buffer layer itself can be functionalized by intercalation. In a recent study it was shown that an electronic bandgap can be opened in the otherwise gapless buffer layer. The semiconducting epigraphene (SEG) on SiC has a bandgap of 0.6 eV and high room temperature mobilities (5000 cm^2/Vs), much larger than silicon and other 2D-semiconductors [1]. In this study we grow high-quality buffer layers not only across single terraces as in the aforementioned study but on millimeter scale, due to an advanced growth technique preventing step bunching and large terrace step heights. We use a polymer-assisted sublimation growth (PASG) method, where pretreatment of the SiC substrate supplies additional carbon and stabilizes the SiC surface by rapid buffer layer-formation preventing step-bunching. We investigate the growth parameters for homogeneous buffer layer formation with our PASG method and systematically study its structural properties and characteristics. [1] J. Zhao et al., Nature 625, 60 (2024).

Invited Talk HL 30.2 Wed 10:00 H13

Huge Enhancement of the Giant Negative Magnetoresistance with Decreasing Electron Density — •Lina Bockhorn[1], Christian Reichl[2], Werner Wegscheider[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases often show a remarkably robust negative magnetoresistance at zero magnetic field. Below 800 mK, this phenomenon divides into two distinct parts [1-4]: a temperature-independent narrow peak around $B = 0$ T, arising from the interplay of smooth disorder and elastic scattering at macroscopic defects [2, 3], and a temperature-dependent giant negative magnetoresistance (GNMR) at higher magnetic fields. The theoretical understanding of the GNMR remains an open question, as it involves several independent parameters in addition to electron-electron interaction possibly leading to hydrodynamic transport effects. To gain insights into the nature of the GNMR, we investigate this effect as a function of electron density at various temperatures and currents. Our results show a significant dependence of GNMR on electron density [4], indicating that variations in scattering potentials [5] are not considered appropriately in theoretical models. [1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011). [2] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014). [3] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016). [4] L. Bockhorn et al., Phys. Rev. B 109, 205416 (2024). [5] Y. Huang et al., Phys. Rev. Materials 6, L061001 (2022).

Invited Talk HL 30.3 Wed 10:30 H13

Ultrafast quantum optics with single-photon emitters in 2D materials — •Steffen Michaelis de Vasconcellos — Physikalisches Intitut, Universität Münster, Germany

Single-photon sources are essential components for building quantum networks, though achieving optimal control remains a significant challenge in advancing quantum technologies. Recently, 2D van der Waals materials, such as transition metal dichalcogenides (TMDs) and hexagonal boron nitride (hBN), have emerged as promising platforms for solid-state quantum light emitters, enabling new possibilities for creating, tuning, and integrating quantum emitters into photonic devices [1].

In my talk, I will review the development of single-photon emitters in 2D materials, focussing particularly on the robust emitters in hBN, which efficiently emit single photons even at room temperature. We demonstrate the efficient collection of single-photons by 3D-printed microlenses [2] and explore ultrafast coherent control of individual hBN quantum emitters [3]. Understanding the underlying dephasing mechanisms is key to designing devices that meet the requirements for future quantum technologies. Our work paves the way towards controlled hybrid quantum systems integrating electronic and phononic excitations.

[1] S. Michaelis de Vasconcellos, et al., Single-Photon Emitters in Layered Van der Waals Materials, phys. status solidi (b) 259, 2100566 (2022) [2] J. A. Preuß, et al., Nano Lett. 23, 407 (2023) [3] J. A. Preuß, et al., Optica 9, 522 (2022)

15 min. break

Invited Talk HL 30.4 Wed 11:15 H13

Realistic simulation of quantum emitter dynamics made easy — •Moritz Cygorek — TU Dortmund, Germany

Few-level quantum emitters such as quantum dots are a main workhorse for cutting edge research in quantum science, e.g., for nonclassical light generation. A practical challenge is the strong interaction with the physical environment such as phonons, which gives rise to a plethora of effects such as decoherence, phonon-assisted transitions, and renormalization. The intricacy of environment effects and computational challenges have in the past rendered the theoretical analysis an expert topic requiring an in-depth understanding of various theoretical methods.

Here, I demonstrate how the concept of process tensor matrix product operators (PT-MPOs) enables quick-and-easy, yet numerically exact simulations of very general open quantum systems. A computational framework is presented that can be used as a black box by the practitioner, which (i) requires no expert knowledge, (ii) leverages path integrals and tensor networks for exceptional speed and accuracy, (iii) is based on C++ for computational and memory efficiency, (iv) yet can be controlled by parameter files and requires no explicit programming, (iv) while also providing Python bindings for easy postprocessing.

Moreover, I demonstrate applications to solid-state cavity-QED relating to concrete experiments: single- and entangled photon generation, multitime correlation functions and dynamically dressed Mollow spectra, as well as phonon effects on cooperative emission and superradiance.

Invited Talk HL 30.5 Wed 11:45 H13

Data-driven Design of Next Generation 2D Materials and Their Heterostructures — •Rico Friedrich — TU Dresden — Helmholtz-Zentrum Dresden-Rossendorf — Duke University, USA

Two-dimensional (2D) materials and their heterostructures provide an extensive platform for realizing advanced electronic and magnetic functionalities at the nanoscale. While individual 2D systems are traditionally obtained from bulk layered compounds bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of semiconducting non-vdW 2D materials derived from non-layered crystals [1] opens up a new direction.

As outlined by our recent data-driven investigations employing autonomous *ab initio* calculations [2, 3], several dozens of new candidates showcase a wide range of appealing electronic, optical, and in particular magnetic properties owing to the (magnetic) cations at the active surfaces of the sheets. Further generalizing the data-driven modelling approach to all inorganic compounds provides fundamental insights into the exfoliation and cleavage of crystals. At the same time, chemical tuning by surface passivation provides a valuable handle to further control the electronic and magnetic properties of these next generation 2D compounds [4]. These features thus make non-vdW 2D materials an attractive platform for fundamental as well as applied nanoscience.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[4] T. Barnowsky *et al.*, Nano Lett. **24**, 3974 (2024).

HL 31: Focus Session: Young Semiconductor Forum Poster

The young semiconductor forum gives a platform for post-docs at all career stages to present themselves and their scientific ideas. It consists of an oral session with invited talks and immediately afterwards, a poster session, where further participants present a poster about their work and/or scientific vita. With this format, we hope to attract both postdocs and senior researchers and decision makers to join this forum: for postdocs, to give them a platform to present themselves, and for professors, to meet the next generation of scientists.

This part is the poster session.

Organized by Alexander Holleitner and the AGyouLeaP (Susanne Liese, Alexander Schlaich, and Christoph Kastl)

Time: Wednesday 12:15–13:00 Location: H13

HL 31.1 Wed 12:15 H13

Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, and Manfred Bayer — Experimentelle Physik 2a, TU Dortmund University, Dortmund, Germany

We demonstrate self-sustained auto-oscillations in a dissipative electron-nuclear spin system (ENSS) in semiconductors, where spontaneous breaking of translational symmetry in time produces robust limit-cycle dynamics across a broad range of parameters, including laser power, temperature, and magnetic field. These periodic oscillations exhibit coherence times extending to hours, reflecting ideal "time atom" ordering within the auto-oscillatory system.

Additionally, we uncover synchronization within excited subsystems without additional modulation, identifying its microscopic origins. Under periodic driving, modulation of parameters such as excitation power and pump polarization yields parametric resonances, signaling a transition to discrete auto-oscillatory behavior. Key phenomena include frequency entrainment, Arnold tongues, bifurcation jets, and a devil's staircase, showcasing the ENSS's versatility in exploring nonlinear dynamics, with broad implications for both fundamental physics and semiconductor applications.

HL 31.2 Wed 12:15 H13

Reducing waste through substrate reuse: a pathway to cost-effective iii-v optoelectronics — •radouane ennadir — 3IT, Sherbrooke University, Sherbrooke, QC, Canada

III-V materials, such as Gallium Arsenide (GaAs), are widely used in optoelectronic devices due to their superior electronic and optical properties. However, the high cost of III-V substrates, primarily made from Ge or other expensive materials, represents a significant barrier to the widespread adoption of these technologies.

Our research focuses on reducing waste in the production of III-V optoelectronics through the reuse of Germanium (Ge) substrates. In this study, we propose a novel approach to mitigate substrate waste by reusing Ge substrates in the fabrication of III-V optoelectronics. By carefully optimizing the recycling process, including substrate cleaning, surface treatment, and the integration of new III-V layers, we aim to significantly reduce material costs without compromising device performance. This approach not only enhances the sustainability of optoelectronic manufacturing but also provides a cost-effective pathway to large-scale production of III-V-based devices. The findings of this study contribute to both environmental sustainability and economic viability in the growing field of optoelectronics, opening up new opportunities for the development of advanced, cost-effective optoelectronic devices.

HL 31.3 Wed 12:15 H13

1D exciton confinement in monolayer $MoSe_2$ near ferroelectric domain walls in periodically poled $LiNBo_3$ — •Pedro Soubelet, Yao Tong, Asier Astaburuaga Hernandez, Andreas V. Stier, and Jonathan J. Finley — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Monolayer transition metal dichalcogenides are an emergent platform for exploring and engineering quantum phenomena in condensed matter. Due to their atomic thickness, the excitonic response is highly influenced by the dielectric environment. In this work, we explore the optical properties and exciton kinetics of monolayer thick $MoSe_2$ straddling domain wall boundaries in ferroelectric periodically poled $LiNbO_3$ (PPLN). Spatially resolved photoluminescence (PL) experiments reveal sorting of neutral and charged excitons across the boundary. Our results reveal evidence for extremely large in-plane electric fields (≃4000 kV/cm) at the domain wall (DW), whose effect is manifested in the routing of free charges and trions towards oppositely poled domains, resulting in a nonintuitive spatial PL intensity pattern. In a second step, we engineer the PPLN substrate and the 2D heterostructure to exploit the non-uniform in-plane electric field exerted by the DW to confine neutral excitons in a 1D dipolar gas. Reducing the dimensionality holds an excellent potential for unlocking strong exciton-exciton interaction regimes, enabling exploration of exotic quantum phases of matter and designing advanced optoelectronic devices.

HL 31.4 Wed 12:15 H13

Probing strong electron-phonon coupling in graphene by resonance Raman spectroscopy with infrared excitation energy — •Simone Sotgiu[1,2], Tommaso Venanzi[1], Lorenzo Graziotto[1], Francesco Macheda[1], Taoufiq Quaj[2], Elena Stellino[1], Bernd Beschoten[2], Christoph Stampfer[2], Francesco Mauri[1], and Leonetta Baldassarre[1] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

Resonance Raman spectroscopy (RRS) has been a key asset to study the interplay between electronic and vibrational properties of graphene. We report on RRS measurements with an excitation photon energy down to 1.17 eV on mono (MLG) and bilayer (BLG) graphene, to study how low-energy carriers interact with lattice vibrations. Thanks to the excitation energy close to the Dirac point, we unveil in the MLG a giant increase of the intensity ratio between the double-resonant 2D and 2D* Raman peaks with respect to graphite [1]. In BLG, the low excitation energy hampers some of the resonant Raman processes giving rise to the 2D peak. Consequently, the sub-features composing the 2D mode are spectrally more separated with respect to visible excitations. We compare experimental measurements on BLG with ab initio theoretical calculations and we trace back such modifications on the joint effects of probing the electronic dispersion close to the band splitting and enhancement of electron-phonon matrix elements [2]. [1] T. Venanzi et al., Phys. Rev. Lett. 2023, 130, 256901 [2] L. Graziotto et al., Nano Lett. 2024, 24, 1867

HL 31.5 Wed 12:15 H13

Effects of atomistic fluctuations on the excitonic fine-structure in alloyed colloidal quantum Dots — •Anne Nadine Tewonoue Djota, Surender Kumar, and Gabriel Bester — Institute of physical chemistry and physics, University of Hamburg

The electron-hole exchange interaction in the presence of spin-orbit coupling leads for an atomistic calculation to a small energy splitting of the excitonic state known in this context as the fine structure splitting (FSS). Although this splitting is typically small, it has large consequences for the optical properties. For instance, the photoluminescence originates from these few states and is governed by the splitting (giving rise to temperature dependence) and polarization of these low energy excitonic states. So far most of the theoretical modeling has assumed that high symmetry structures lead to a simple dark-bright splitting with a large degeneracy of the excitonic states. In this work, we show based on atomistic calculations, that even globally perfectly symmetric structures (i.e., as far as an atomistic construction permits a "spherical" quantum dot) show a qualitatively different FSS as soon as alloying is introduced. The alloying effect is significantly stronger than any global shape anisotropy where the symmetry is broken for instance by geometrical elongation of the quantum dot. On the other hand, alloying a quantum dot through processes such as cation exchange is inherently random. As a result, different random alloy configurations with the same size and composition can exhibit significantly different FSS.

HL 31.6 Wed 12:15 H13

Resistance standards from artifact wire coils to graphene quantum Hall resistance — •Yefei Yin[1], Mattias Kruskopf[1], Stephan Bauer[1], Teresa Tschirner[1], Klaus Pierz[1], Frank Hohls[1], Rolf J. Haug[2], and Hans W. Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Historically, resistance standards were made by physical artifact wire coils before 1990 and quantum resistors based on GaAs heterostructures after 1990. However, conventional GaAs quantum Hall resistance (QHR) standards with the quantized resistance $R_H = h/2e^2$ are operating under high magnetic flux densities B > 10 T, limited currents I < 50 μA, and low temperatures T < 1.5 K, which significantly hinder the dissemination of primary resistance standards. In this work, we developed practical primary QHR standards based on n- and p-type epitaxial graphene. This study first systematically demonstrated that p-type epitaxial graphene can also be used for primary resistance standards, as accurate (10^{-9} accuracy) as GaAs and n-type graphene counterparts for realizing

the SI unit ohm in quantum metrology. [1] The n-type graphene QHR standards achieved the world best performance so far with a 10^{-9} accuracy under relaxed conditions (B = 4.5 T, I = 232.5 μA, T = 4.2 K) simultaneously. [2-3] Our graphene QHR standards have been utilized in the national metrology institutes in European countries. [1] Appl. Phys. Lett., 125, 064001 (2024). [2] Adv. Phys. Res. 1, 2200015 (2022). [3] Phys. Rev. Applied, 2024

HL 31.7 Wed 12:15 H13

Hybridized excitons in 2D van der Waals materials — •Andreas Stier — Walter Schottky Institut und TUM School of Natural Sciences, TU München, Garching, Deutschland

I will review our recent progress on magneto optical spectroscopy of atomically thin materials in magnetic fields up to 91 T with an emphasis on the spin-valley physics of neutral and charged excitons.

In monolayer (ML) semiconductors, magneto-absorption spectroscopy revealed the diamagnetic shifts of the exciton Rydberg states, which allowed the first direct experimental measure of the reduced mass and binding energy. Surprisingly, investigating the photoluminescence, we observe the emergence of a new excitonic peak, which we discuss in the framework of the theoretically predicted linear dispersing exciton branch originating from intervalley exchange interactions.

For heterostructures (HS) of a 2D semiconductor with graphene, we find a new multi-step proximity effect due to band folding in the HS, where we show that the spin-valley physics can be used to quantify interlayer hybridization. In HS from ML MoSe2 and the layered antiferromagnetic (AFM) semiconductor CrSBr, we show the formation of new exciton states depending on the twist angle. These excitons exhibit clear signatures of proximity coupling to the magnetic state of the AFM layer, such as hysteretic response to in- and out of plane B fields. We discuss these results in the framework of Ising-type spin-orbit proximity coupling.

HL 31.8 Wed 12:15 H13

Shaped pulses enable robust coherent control of quantum dots: perspectives for quantum technologies — •Vikas Remesh — Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

Shaped laser pulses have been remarkably effective in investigating and controlling various light-matter interactions in a broad area of research. In quantum technologies, the techniques to shape complex spatiotemporal waveforms have found renewed interest, for instance in coherent control of quantum dots [1]. In this talk, I will navigate through the impact of pulse shaping techniques in nanospectroscopy and how it enabled efficient preparation schemes in quantum dots, based on our recent works [2], including the pioneering off-resonant coherent control of quantum dots, compact plug-and-play method of exciting multiple quantum dots and accessing dark excitons in quantum dots for advanced entanglement generation. Afterwards, I will conclude with my vision on the future scope of nanophotonics-assisted-quantum technology roadmap. [1] Photonic Quantum Technologies: Science and Applications 1, 53 (2023) [2] Nano Letters 22, 6567 (2022), Materials for Quantum Technology 3, 025006 (2023), APL Photonics 8, 101301 (2023), npj Quantum Information 10, 17 (2024), Advanced Quantum Technologies, 2300352 (2024), arXiv:2409.13981, arXiv:2406.07097, arXiv:2404.10708

HL 31.9 Wed 12:15 H13

First-Principles Investigation of NV Centers in Silicon Carbide Polytypes — •Timur Biktagirov, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Optically addressable spin defects in semiconductors offer versatile platforms for quantum applications, including computing, communication, and sensing. Among these, nitrogen-vacancy (NV) centers in silicon carbide (SiC) polytypes have emerged as a promising class of quantum defects, analogous to the NV center in diamond. In contrast to diamond, SiC is a technologically mature material with large-scale production capabilities, advanced doping techniques, and compatibility with CMOS fabrication methods. Additionally, the emission wavelengths of NV centers in SiC lie in the near-infrared range, making them particularly suitable for applications in single-photon emission. In this work, we discuss recent advancements in the ab initio investigation of NV centers in the 4H, 6H, and 3C polytypes of SiC. Simulating the magneto-optical properties of these spin centers, which are crucial for quantum applications, requires a detailed and accurate description of both the host material and the embedded defect. Accordingly, we demonstrate how supercell density functional theory (DFT) and recent implementations based on DFT can be employed to model key properties, including intra-defect optical transition energies, electron-electron and electron-nuclear spin interactions, and electron-phonon coupling. These theoretical insights provide a foundation for optimizing NV centers in SiC for next-generation quantum technologies.

HL 31.10 Wed 12:15 H13

Transport properties of quantum dots for single-electron pumps — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Frank Hohls, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, 31668 Braunschweig, Germany

A single-electron pump (SEP) is a device emitting a well-defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e, this results in a current of $I = nef$. Since the revision of the SI system, the elementary charge e hereby is an exact value, so that SEPs provide a suitable basis for a quantum current standard. The accuracy of this current is directly related to erroneous cycles, where the emitted number of electrons deviates from n. Our SEP devices are based on electrostatically defined quantum dots in GaAs/AlGaAs two-dimensional electron gases. In such devices, the tunnel barriers as well as the energy levels are controllable via gate voltages. Based on multiple quantum dot devices we here investigate relations between transport properties and SEP operation characteristics.

HL 32: Nitrides: Preparation and Characterization I

Time: Wednesday 9:30–11:00 Location: H15

HL 32.1 Wed 9:30 H15

Optical properties of asymmetric cubic AlGaN/GaN quantum wells — •Erik Graper[1], Elias Baron[1], Martin Feneberg[1], Tobias Wecker[2], Donat J. As[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany

Group III-nitrides, particularly AlGaN and GaN, are essential materials for high-performance electronic and optoelectronic devices. While conventional hexagonal AlGaN/GaN high-electron-mobility transistors (HEMTs) operate in normally-on mode, cubic AlGaN/GaN structures enable normally-off operation - a crucial advantage for energy-efficient power electronics. These cubic AlGaN/GaN heterostructures offer additional benefits such as the absence of internal polarization fields in (001) orientation.

In this study, we investigate asymmetric cubic AlGaN/GaN double quantum wells (2.5 nm and 0.6 nm) with varying barrier thicknesses, grown by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation. We employed complementary spectroscopic techniques to analyze quantum well coupling, combining photoluminescence (PL) measurements using continuous-wave lasers (266 nm and 325 nm) with photoluminescence excitation (PLE) spectroscopy using a tunable pulsed laser (325 - 354 nm). The acquired spectra were analyzed to determine wavelength dependent luminescence of the 2.5 nm quantum well.

HL 32.2 Wed 9:45 H15

Nanoscale characterization of cascaded GaN/InGaN LEDs with tunnel junction — •Konstantin Wein, Gordon Schmidt, Frank Bertram, Holger Eisele, Peter Veit, Olga August, Christoph Berger, Armin Dadgar, André Strittmatter, and Jürgen Christen — Otto-von-Guericke-University Magdeburg, Germany

In this work, comprehensive cathodoluminescence (CL) and electron beam induced current (EBIC) characterization directly performed in a scanning transmission electron microscopy (STEM) were performed on an InGaN/GaN double cascaded LED using a GaN:Ge/GaN:Mg tunnel junction (TJ). Cascaded LEDs benefit from monolithic multi-wavelength emission, lower injection current density (lower droop), and smaller chip sizes compared with standard LEDs. In low temperature (T = 17 K) highly spatially resolved CL, each individual layer is identified by its characteristic emission. The GaN:Si layers exhibit NBE emission at 365 nm corresponding to donor-bound exciton recombination, in contrast to the GaN:Mg layers which exhibit donor-acceptor pair recombination emitting at 380 nm. The intensity profile across the InGaN MQWs of both active regions gives access to the transport and capture of the excess carriers and excitons. The direct comparison of the local CL emission with the EBIC signal exhibits not only the local quantum efficiency as well as transfer of carriers (diffusion/drift) but also the current spreading/injection distribution of the vertical device. The impact of functional layers like electron blocking layers or TJs on the transport of carriers is directly visualized on the nano-scale.

HL 32.3 Wed 10:00 H15

Understanding the Effect of Defects in Ta3N5 Thin Films on Charge Carrier Dynamics — •Jan Luca Blänsdorf[1], Lukas M. Wolz[1], Matthias Kuhl[1], Johannes Dittloff[1,2], Nina Miller[1], Gabriel Grötzner[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany

Transition-metal nitrides are a highly interesting material space for solar-energy conversion due to their suitable bandgap for visible light absorption and high theoretical solar-to-hydrogen efficiencies. An intensively studied example is Ta3N5, with a bandgap of 2.2 eV and favorable band alignment for solar water splitting. However, its photoelectrochemical performance is limited by oxygen impurities and nitrogen vacancies. Here, we used transient absorption spectroscopy on the microsecond timescale to reveal the impact of different defects on charge carrier dynamics in Ta3N5. Therefore, we synthesized Ta3N5 thin films with different concentrations of nitrogen vacancies and oxygen impurities. Their structure, defect and photoelectrochemical properties were correlated with charge carrier dynamics to identify current performance limitations.

HL 32.4 Wed 10:15 H15

Accessing and evaluating the full growth window of PAMBE grown AlGaN/GaN nanowires — •Rudolfo Hötzel[1], Marten Wilkens[1], Florian Krause[1], Andreas Rosenauer[1,2], Stephan Figge[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, 28359 Bremen, Germany

Typically group III/V nanowires synthesized by PAMBE are grown under a surplus of nitrogen. Under metal-rich conditions nanowire broadening is reported [1] leading to increased coalescence until self-stabilisation to stoichiometric conditions is reached. To establish stoichiometry single GaN nanowires consisting of multilayers of GaN grown with varying Ga fluxes were analyzed by STEM-EDX. The dependence of growth rates on temperature and fluxes could be consistently fitted with previously reported growth models [1] with the Ga desorption rate as the only free parameter. However a lateral broadening was not observed even for deep Ga-rich conditions. We attribute this to higher growth temperatures leading to an increased Ga desorption from the side facets. Based on these findings AlGaN/GaN nanowires were grown under deep metal-rich conditions. We observed that high Al/Ga fluxes lead to the formation of AlN regions due to the higher formation enthalpy of AlN with Ga accumulating on the c-face because of demixing. A homogenous incorporation of Al under deep metal-rich conditions was only possible for low Al/Ga flux ratios which are limited by the growth temperature. [1] S. Fernández-Garrido et al., Nano Lett. 13, 3274-3280 (2013)

HL 32.5 Wed 10:30 H15

Nanoscale multi-spectroscopic characterisation of InGaN pseudo-substrates grown on nanowire arrays — •Aidan Flynn Campbell, Jingxuan Kang, Huaide Zhang, Oliver Brandt, Lutz Geelhaar, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

The efficiency of nitride light-emitting diodes (LEDs) in the amber and red spectral ranges is severely limited by the high strain in (In,Ga)N quantum wells with increasing In content when grown on GaN. Thus, reducing the lattice mismatch between the active region and adjacent layers is highly desirable. Our approach exploits the lateral elastic strain relaxation facilitated by nanowires fabricated top-down from a single-crystalline layer, epitaxial overgrowth of a subsequent layer achieves a strain free pseudo-substrate. In this study, we characterise the optical, chemical, and crystallographic properties of such overgrown layers, which are key in understanding and optimising our epitaxial overgrowth fabrication route.

We utilise experimental techniques such as continuous-wave and time-resolved cathodoluminescence (TRCL), energy-dispersive X-ray spectroscopy (EDX), and high-resolution electron backscatter diffraction (HR-EBSD). We demonstrate low dislocation densities, low compositional variations and low crystal misorientation across coalescence boundaries. Furthermore, the factors influencing defect formation and the relevance of dislocation propagation are investigated and correlated with the resulting luminescence efficiency of the overgrown layers.

HL 32.6 Wed 10:45 H15

Measuring solute concentrations in ammonothermal solutions via in situ X-ray absorption - estimating detection limits for novel nitrides — •Rajesh Chirala, Ege N. Civas, and Saskia Schimmel — Chair of Electron Devices (LEB), Dept. EEI, FAU Erlangen-Nürnberg, Cauerstr. 6, 91058 Erlangen, Germany

The ammonothermal method [1] is effective for producing high quality single crystals of binary and ternary nitrides [2], which are emerging semiconductor materials [3]. Despite the challenging process conditions (100 to 300 MPa, 400 to 800 °C), in situ measurement techniques such as X-ray imaging [4] allow to study reaction kinetics and solubilities, which are highly relevant to bulk crystal growth. In case of GaN, the quantitative determination of the concentration of Ga containing intermediates was already demonstrated [5].

By simulating the X-ray absorption of novel nitrides in an ammonothermal autoclave, we estimate element-specific detection limits for solute concentrations and derive strategies for detecting lighter elements or lower concentrations. Amongst the others, effectiveness of using a combination of lower X-ray energies and higher X-ray dose will be analyzed.

[1] R. Dwilinski et al., Acta Phys. Pol. A 88, 833, 1995.
[2] J. Häusler, W. Schnick, Chemistry 24, 11864, 2018.
[3] D. Jena et al., Jpn. J. Appl. Phys. 58, SC0801, 2019.
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HL 33: Nitrides: Devices

Time: Wednesday 11:15–13:00 Location: H15

HL 33.1 Wed 11:15 H15

Influence of barrier height variations on the efficiency of AlGaN-based 225nm LEDs — •Markus A. Blonski[1], Jakob Höpfner[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[2], Paula Vierck[1], Tim Wernicke[1], Michael Kneissl[1,2], and Markus Weyers[2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Deep ultraviolet (DUV) light emitting diodes (LEDs) with emission wavelengths shorter than 225 nm exhibit low external quantum efficiencies (EQEs). Since the AlGaN multi-quantum well (MQW) active region remains a significant limiting factor for EQE, the effects of the barrier height in the MQW region on the radiative recombination efficiency (RRE), carrier injection efficiency (CIE) and light extraction efficiency (LEE) are examined. For this, the barrier composition is varied from $Al_{0.82}Ga_{0.18}N$ over $Al_{0.86}Ga_{0.14}N$ to $Al_{0.89}Ga_{0.11}N$. The lowest barrier leads to the highest peak EQE at 0.05 % and the highest barrier to an EQE peak below 0.02 %. The RRE, CIE and LEE are determined using continuous wave and pulsed electroluminescence measurements, determination of optical polarization and Monte Carlo raytracing simulations. The analysis shows that an increase in barrier height leads to an increase in RRE and LEE and a significant decrease in CIE for an overall decrease in EQE. Drift diffusion simulations indicate a notable increase in electron spillover across the $Al_{0.98}Ga_{0.02}N$ electron blocking layer to the p-side, attributable to a reduced band offset between barrier and electron blocking layer, reducing the CIE.

HL 33.2 Wed 11:30 H15

Homoepitaxy on AlN-bulk substrates with different off-cut angles — •Sebastian Krüger[1], Sarina Graupeter[1], Massimo Grigoletto[1,2], Marcel Schilling[1], Sylvia Hagedorn[2], Carsten Hartmann[3], Thomas Straubinger[3], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Laser diodes in the UVC spectral range require high-quality AlN and AlGaN layers with low threading dislocation densities (TDD) and smooth surfaces. AlN substrates with a TDD of $< 10^4$ cm^{-2} are the ideal choice. In this work we investigate the influence of substrate off-cut (0.1° to 0.5°) and growth parameters (e.g. TMAl flow, V/III-ratio) on the morphology of homoepitaxially grown AlN buffer layers. A transition from step flow growth for a 0.2° miscut AlN substrate to step bunching for miscuts of 0.39° and above is observed for a growth temperature of 1070°C, a TMAl flow of 35 μmol/min and a V/III-ratio of 15. For a miscut of 0.27° step flow growth is still present but the terrace width shows significant variation. The RMS roughness increases from 0.11 nm (on 0.2°) to 0.45 nm (on 0.39°). For 0.5° miscut, the substrate terrace width is even smaller, i.e. the diffusion length must be reduced to avoid step bunching e.g. by increasing the V/III-ratio. Between V/III ratios of 15 and 60 we found morphologies such as island growth and step meandering with the lowest RMS roughness of 0.11 nm for a TMAl flow of 35 μmol/min and a V/III-ratio of 15.

HL 33.3 Wed 11:45 H15

Stabilizing Ta_3N_5 Thin Films Photoelectrodes by Defect Engineering — •Lukas M. Wolz[1], Gabriel Grötzner[1,2], Tim Rieth[1,2], Laura I. Wagner[1,2], Matthias Kuhl[1], Johannes Dittloff[1,2], Guanda Zhou[1,2], Saswati Santra[1,2], Verena Streibel[1,2], Frans Munnik[3], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Tantalum nitride (Ta_3N_5) is a highly investigated photoelectrode material due to its favorable optoelectronic properties for photoelectrochemical (PEC) energy conversion. However, intrinsic defects such as nitrogen vacancies and oxygen impurities play a crucial role in defining their optical, electronic, and photoelectrochemical properties. While the role of these defects in PEC activity is well investigated, their impact on material stability remains underexplored. We investigate the relationship between atomic-scale defects and macroscale PEC stability in Ta_3N_5 thin films. To reveal the impact of each defect type on the material properties, we introduced different defect concentrations in Ta_3N_5 by using three different precursors in the synthesis process. Low oxygen concentrations are found to increase long-range order but lead to high concentrations of deep-level defects, leading to increased charge recombination and decreased material stability. Conversely, higher oxygen contents result in reduced structural order but beneficially passivate deep-level defects, leading to improved stability.

HL 33.4 Wed 12:00 H15

Studying the carrier distribution of multicolor far-UVC LEDs by temperature dependent electroluminescence measurements — •Jakob Höpfner[1], Franz Biebler[1], Florian Kühl[1], Marcel Schilling[1], Anton Muhin[1], Massimo Grigoletto[1,2], Martin Guttmann[2], Gregor Hoffmann[3], Friedhard Römer[3], Tim Wernicke[1], Berndt Witzigmann[3], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), 12489 Berlin, Germany — [3]Lehrstuhl für Optoelektronik, Department EEI, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

The low current injection efficiency (CIE) is one of the root causes for the poor external quantum efficiency of AlGaN based far-UVC LEDs. To improve the CIE it is necessary to gain insights into the carrier distribution and transport in the AlGaN multiple quantum well active region. Therefore, heterostructures were grown by metalorganic vapour phase epitaxy (MOVPE) with a varying number of QWs (2 –20) emitting at 233 nm and one single QW with an emission wavelength of 250 nm. This allows us to probe the carrier transport with the help of temperature dependent electroluminescence measurements (100 K - 340 K). The experimental findings were correlated with drift-diffusion simulations and Monte-Carlo ray-tracing simulations. Experiment and simulations show that the holes are weakly confined in the 233 nm emitting QWs and exhibit a long diffusion length over many QWs mainly due to thermal escape from the shallow barriers.

HL 33.5 Wed 12:15 H15

Influence of strain reduced HTA-AlN/sapphire templates with different offcuts on the performance of UVC LEDs — •Sarina Graupeter[1], Finn Kusch[1], Paula Vierck[1], Sylvia Hagedorn[2], Markus Weyers[2], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

High temperature annealing (HTA) of sputter dposited AlN layers on (0001) sapphire substrates allows for fabrication low threading dislocation densitiy templates (TDD of 4 x $10^8\,cm^2$) enabling UVC LEDs with improved external quantum efficiency and lifetime. However, due to the thermal expansion mismatch of the sapphire and the AlN, the AlN layers are under high compressive strain after cooling down from HTA at 1700°C. This can lead to strain relaxation and formation of dislocation half-loops during the subsequent growth of AlN and AlGaN layers, thus decreasing the radiative recombination efficiency (RRE). By growing a Si-doped AlN layer on HTA-AlN the in-plane compressive strain ϵ_{xx} is reduced by around 30% from -0.3 to -0.2. The impact of such an interlayer on the electro-optical properties of UVC-LEDs has been investigated with focus on the RRE. The RRE has been determined using cw and pulsed EL-measurements with the Titkov-Dai method. Using an AlN:Si interlayer shows an increase of the EQE value from 0.8% to 1%. Emission powers as high as 1.9 mW at 50 mA can be realized for UVC LEDs on strain reduced templates.

HL 33.6 Wed 12:30 H15

Characterisation of a Pt on-chip counter electrode on a GaN/AlGaN-ISFET Wheatstone bridge as pH-sensor — •Alexander Hinz[1], Niklas Krantz[1], Stephan Figge[1], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliotheksstraße 1, 28359 Bremen, Germany

The influence of a Pt on-chip counter electrode on field effect transistors as pH-sensors was investigated. The intention was to reduce the size of the complete sensor structure consisting of ISFET, counter and reference electrode. In addition, the function of the Pt on-chip electrode was be compared to setup using an external Pt counter electrode to discuss stability and leakage. Furthermore, a Wheatstone bridge design is used to compensate temperature drifts. A reduction of this drift to 0.02 mV/°C was achieved. The long-time behavior of the temperature drift and also of pH changes was also analysed.

HL 33.7 Wed 12:45 H15

Efficiency analysis of 233 nm far-UVC LEDs with varied DPD AlGaN layer thickness beyond 298 K — •Paula Vierck[1], Jakob Höpfner[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Markus Blonski[1], Tim Wernicke[1,2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand Braun Institut (FBH), Berlin, Germany

Light emitting diodes (LEDs) emitting in the far ultraviolet-C (far-UVC) spectral range offer applications in skin safe disinfection and gas sensing. In this work we analyze far-UVC LEDs with a distributed-polarization doped (DPD) p-AlGaN layer as this offers a promising alternative to Mg-doping. By compositionally grading the Al content of the AlGaN layer, a 3D hole gas can be generated exceeding the free hole concentration of conventionally Mg doped samples. The theoretically calculated charge profile depends on the grading and can be controlled by changing the DPD layer thickness or the alloy composition. In this work, five samples with DPD layer thicknesses between 25 nm and 150 nm were investigated by electroluminescence spectroscopy and numerical simulations. With decreasing DPD layer thickness we find an increase in the peak external quantum efficiency (EQE) with a maximum EQE of 0.37 % for a DPD thickness of 25 nm due to an increased hole concentration. Further analysis at temperatures of up to 353 K revealed a notable decline in the devices EQE down to 0.15 % at 353 K for a 25 nm thick DPD. This work will provide an analysis of the different contributing factors to the EQE drop with insights provided by simulations.

HL 34: Focus Session: Quantum Emission from Chaotic Microcavities (joint session HL/DY)

In this joint focused session of the divisions DY, HL, and TT, we bring together two dynamic areas of research: semiconductor quantum emitters and chaotic cavities. While quantum emitters in cavities represent an established building block for quantum information technologies, chaotic microcavities may promise novel design routes towards optimized cavity performance parameters. Experts from both fields will provide an overview of the current state of research, exploring the potential of chaotic and unconventional microcavities to enhance the emission of quantum states.

Organized by Sonja Barkhofen (University of Paderborn) and Christian Schneider (University of Oldenburg).

Time: Wednesday 9:30–12:15 Location: H17

Invited Talk HL 34.1 Wed 9:30 H17

From complex internal dynamics to emission characteristics control in quantum billiards — •Martina Hentschel — 1 Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

The field of mesoscopic physics has given access to new classes of fascinating model systems ranging from ballistic quantum dots via microcavity lasers to graphene billiards over the past decades. Their rich internal dynamics, subject to quantum chaos and often successfully accessed employing wave-particle correspondence in real and phase space, is directly related to their emission properties. Here, we illustrate this close connection for various examples and system classes. For optical microcavities, we vary the internal dynamics by changing the geometric shape of the resonator and explain how the far-field emission characteristics is determined by the underlying steady probability distribution and a possibility to achieve directional emission required for microlasing devices with

the Limaçon geometry. Placing sources into the cavity will affect the internal dynamics of the cavity by, taking the particle point-of-view, effectively changing the set of initial conditions, as observed for optical cavities as well as for graphene billiards in the form of Dirac fermion optics. A further way to change the dynamics of a system is the existence of anisotropies that can either be intrinsically present such as in bilayer graphene in the form of trigonal warping [1], or can be induced to a given system by, for example, applying a mechanical strain. [1] L. Seemann, A. Knothe, and M. Hentschel, New J. Phys. 26, 103045 (2024).

Invited Talk HL 34.2 Wed 10:00 H17

Positioning of microcavities around single emitters — •Tobias Huber-Loyola — Technische Physik, Physikalisches Institut, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Single emitters in solids are great sources of single and entangled photons for usage in quantum information technologies. Many emitters possess high internal quantum efficiency, majority of the emission into the zero-phonon line and controllable single charge spins that can be used as quantum memories or as resource to generate chains of entangled photons. However, due to their solid-state host, which usually comes with a high refractive index, the outcoupling of photons requires the use of nanophotonic structures such as waveguides or microcavities. In this talk, I will show how we place microcavities around pre-registered quantum dots using hyperspectral imaging and e-beam lithography and I will give an overview of how placement accuracy has different effects on the emitted photons' properties based on the type of cavity.

Invited Talk HL 34.3 Wed 10:30 H17

Exploring Wave Chaos and Non-Hermitian Physics: Future Prospects for Quantum Emission from Chaotic Microcavities — •Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, Germany

Optical microcavities play a fundamental role in many fields of basic and applied research in physics. A chaotic microcavity is a type of cavity where the light ray dynamics is (partially) chaotic [1]. This can occur in a microdisk cavity with a deformed boundary shape. Chaotic microcavities are ideal for studying ray-wave correspondence, or wave chaos, in open systems, allowing direct comparisons with experiments [2]. These cavities can also exhibit non-Hermitian phenomena such as reflectionless scattering modes [3] and exceptional points [4].

The light emission from chaotic microcavities has been studied exclusively within the classical domain. The effects of electromagnetic field quantization, including phenomena like entanglement, single-photon states, and squeezed light, remain unexplored in this context. In this talk, I will review my group's recent efforts to investigate classical emission from chaotic microcavities and quantum emission from semiconductor quantum dots embedded in conventional microcavities. Additionally, I will discuss the prospects for achieving genuine quantum emission from chaotic microcavities.

[1] H. Cao and J. Wiersig, Rev. Mod. Phys. 87, 61 (2015)
[2] X. Jiang et al., Science 358, 344 (2017)
[3] X. Jiang et al., Nat. Phys. 20, 109 (2023)
[4] C.-H. Yi et al., Phys. Rev. Lett. 120, 093902 (2018)

15 min. break

Invited Talk HL 34.4 Wed 11:15 H17

Correlations and statistics in cavity embedded quantum dot sources of quantum light — •Ana Predojevic — Stockholm University, Stockholm, Sweden

Single quantum dots coupled to photonic cavities are established emitters of single photons and entangled photon pairs. The cascaded generation of photon pairs intrinsically contains temporal correlations that negatively affect the ability of such sources to perform two-photon interference, hindering applications. I will show how such correlation interacts with decoherence and temporal postselection, and under what conditions temporal postselection could improve two-photon interference visibility. Our study identifies crucial parameters of the source and shows the way to achieve optimal performance. The single photons emitted by a quantum dot exhibit quantum statistics, which is usually verified in an autocorrelation measurement. Single photons can be subjected to more extensive tests of quantum nature, such as non-Gaussianity. However, there is little evidence that such a measurement can be made on pairs of photons. I will show that pairs of photons exhibit strongly non-classical properties that can be quantified. Our result is applicable to a wide range of quantum light sources and measurement methods.

Invited Talk HL 34.5 Wed 11:45 H17

Nonlinear Phenomena in Exciton-Polaritons from Bound States in the Continuum — •Dario Ballarini — CNR-NANOTEC, Lecce, Italy

Exciton-polaritons in semiconductor microcavities have demonstrated remarkable collective behaviors and nonlinear interactions. In this work, we introduce an alternative platform to study strong light-matter interactions within a waveguide configuration. Among other interesting phenomena and applications, such as dispersion engineering of waveguide exciton-polaritons or exciton tuning through the Stark effect [1,2], we highlight the demonstration of parametric nonlinearities, polariton lasing from bound-in-the-continuum (BIC) states, and the recent realization of polariton BICs operating at room temperature in 2D materials [3-5].

[1] Electrically controlled waveguide polariton laser, Optica 7, 1579 (2020). [2] Reconfigurable quantum fluid molecules of bound states in the continuum, Nature Physics 20, 61 (2024). [3] Polariton Bose-Einstein condensate from a bound state in the continuum, Nature 605, 447 (2022). [4] Emerging supersolidity from a polariton condensate in a photonic crystal waveguide, arXiv:2407.02373 (2024). [5] Strongly enhanced light-matter coupling of monolayer WS2 from a bound state in the continuum, Nature Materials 22, 964 (2023).

HL 35: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

See O 61 for details of this session.

HL 36: Materials and Devices for Quantum Technology II

Time: Wednesday 15:00–18:00 Location: H13

HL 36.1 Wed 15:00 H13

High aspect ratio wurtzite GaAs nanowires as a platform for hexagonal SiGe — •Marvin Marco Jansen[1], Wouter H.J. Peeters[1], Marcel A. Verheijen[1,2], and Erik P.A.M. Bakkers[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherland — [2]Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands

One of the most promising pathway to create a silicon based laser is the recently developed hexagonal silicon germanium (hex-SiGe) shells around wurtzite (WZ) gallium arsenide (GaAs) nanowires (NWs) for which efficient direct band gap emission was shown. However, studies have highlighted the limitations of the core/shell NW system. A main challenge is the recently discovered aspect ratio limitation in WZ GaAs NWs ascribed to a dynamic variation of the growth conditions. Here, we report on the crystal phase control of GaAs NWs down to the monolayer regime opening up new pathways for superlattices as well as high aspect ratios GaAs NWs. To achieve this, Ga pulses are executed by momentarily halting the As supply, leading to an accumulation of Ga atoms within the catalyst particle. This process leads to the increase of the contact angle of the catalyst particle enabling a controlled transition from the WZ phase to the zinc blende (ZB), and then back to the WZ phase. By using the ZB inclusion as a marker during the growth process, we successfully carried out a detailed investigation into the evolution of the NW growth, considering its diameter, length, and the pulse frequency.

HL 36.2 Wed 15:15 H13

Shaped pulses enable robust coherent control of quantum dots: perspectives for quantum technologies — •Vikas Remesh — Institute für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

Shaped laser pulses have been remarkably effective in investigating and controlling various light-matter interactions in a broad area of research. In quantum technologies, the techniques to shape complex spatiotemporal waveforms have found renewed interest, for instance in coherent control of quantum dots [1]. In this talk, I will navigate through the impact of pulse shaping techniques in nanospectroscopy and how it enabled efficient preparation schemes in quantum dots, based on our recent works [2], including the pioneering off-resonant coherent control of quantum dots, compact plug-and-play method of exciting multiple quantum dots and accessing dark excitons in quantum dots for advanced entanglement generation. Afterwards, I will conclude with my vision on the future scope of nanophotonics-assisted-quantum technology roadmap. [1] Photonic

Quantum Technologies: Science and Applications 1, 53 (2023) [2] Nano Letters 22, 6567 (2022), Materials for Quantum Technology 3, 025006 (2023), APL Photonics 8, 101301 (2023), npj Quantum Information 10, 17 (2024), Advanced Quantum Technologies, 2300352 (2024), arXiv:2409.13981, arXiv:2406.07097, arXiv:2404.10708

HL 36.3 Wed 15:30 H13

Single-Electron Shuttling for Scalable Silicon Quantum Computers: Modeling, Simulation and Optimal Control — •Lasse Ermoneit[1], Burkhard Schmidt[1], Thomas Koprucki[1], Jürgen Fuhrmann[1], Tobias Breiten[2], Arnau Sala[3], Nils Ciroth[3], Ran Xue[3], Lars R. Schreiber[3,4], and Markus Kantner[1] — [1]Weierstrass Institute, Berlin, Germany — [2]Technical University Berlin, Germany — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Germany — [4]ARQUE Systems GmbH, Aachen, Germany

While spin qubits in gate-defined Si/SiGe quantum dots provide excellent prospects for scalability, the lithographic processing, signal routing and wiring of large qubit arrays at a small footprint pose a significant challenge. A potential solution is to divide the qubit register into compact, dense qubit arrays linked by an interconnecting quantum bus shuttle, that allows for coherent transfer of quantum information by physically moving electrons along a channel. Limitations in qubit shuttling fidelity arise from the interaction of the electron with material defects within the channel that can cause non-adiabatic transitions to excited orbital states. Since those have an altered effective g-factor, this leads to a spin precession with an indeterministic phase. In this contribution, we theoretically explore the capabilities for bypassing defect centers using optimally engineered control signals that allow for a quasi-adiabatic passage of the electron through the channel without reducing the shuttling velocity. Our approach is based on quantum optimal control theory and Schrödinger wave packet propagation.

HL 36.4 Wed 15:45 H13

Spectral Hole linewidths and donor-acceptor dynamics in ultra-pure 28-Si:P — •Nico Eggeling[1], Finja Tadge[1], N.V. Abrosimov[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

Donor-bound excitons in ultra-pure silicon show significant inhomogeneous broadening, which can be studied in detail using spectral hole burning[1]. Surprisingly, for decreasing pump intensities, the linewidth of these holes does not approach the natural transition linewidth, resulting from the dominating Auger effect at low temperatures[2]. Instead, time-dependent experiments show that the width and decay of the spectral holes change significantly with temperature and magnetic field, which an intricate model including donor-acceptor pair recombination can explain.

[1] J. J. Berry, et al. Appl. Phy. Lett. **88**, 061114, (2006).
[2] Yang, et al. Appl. Phy. Lett. **95**, 122113, (2009).

HL 36.5 Wed 16:00 H13

The Kitaev transmon qubit: design, readout and operation — •Tobias Kuhn and Monica Benito — Augsburg University, Augsburg, Germany

Fermionic-parity qubits are very stable but cannot be operated in isolation. Coupling two parity qubits allows us to construct parity-spin qubit states within one global parity [1]. Its degeneracy and non-locality should improve T_2 and T_1 times [2]. A parity qubit can be realized in a double quantum dot connected via a common superconducting lead, where elastic cotunneling t as well as crossed Andreev reflection Δ preserve parity. This minimal Kitaev chain possesses degenerate distinct-parity states at the sweetspot $\Delta = t$[1]. Weakly coupling two minimal Kitaev chains inside a transmon loop introduces an additional Josephson potential which is a consequence of the emerging parity-spin qubit [3]. This hybrid device combines the advantages of both quantum dots and transmons to promise a high-fidelity qubit device we call Kitmon (Kitaev transmon). We theoretically analyze even and odd global parity subspaces of the Kitaev junction and show that flux spectroscopy in a circuit QED implementation [4] determines global parity. Additionally, we derive an effective Hamiltonian depending on the transmon excitation state, which is useful for single qubit operations and qubit readout. [1] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012) [2] G.-L. Guo, H.-B. Leng, and X. Liu, New J. Phys. **26**, 063005 (2024) [3] D. M. Pino, R. S. Souto, and R. Aguado, Phys. Rev. B **109**, 075101 (2024) [4] L. Peri, M. Benito, C. J. B. Ford, and M. F. Gonzalez-Zalba, npj Quantum Inf **10**, 1 (2024)

HL 36.6 Wed 16:15 H13

Towards the goal of reliably storing single-photons from a quantum dot — •Ioannis Caltzidis[1], Patricia A. Kallert[1], Chase Wallace[2], Sean Keenan[3], Nicolas Claro-Rodríguez[1], Santiago Bermúdez-Feijóo[1], Sonja Barkhofen[1], Margherita Mazzera[3], Eden Figueroa[2], and Klaus D. Jöns[1] — [1]Institute for Photonic Quantum Systems (PhoQS), Center for Optoelectronics and Photonics Paderborn (CeOPP) and Department of Physics, Paderborn University, Germany — [2]Quantum Memories Group, Heriot-Watt University, Edinburgh, Scotland, United Kingdom — [3]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA and Brookhaven National Laboratory, Upton, NY, USA

In quantum networks, precise single-photon arrival times are crucial for effective entanglement swapping protocols. Therefore, quantum memories are curcial to store photons until read out simultaneously and synchronously routed to further processing, e.g. Bell measurements. To operate a varm vapor memory in our laboratories we present initial results demonstrating our ability to generate short optical pulses in the desired frequency domain optimized for the atomic transitions of rubidium. We further probe the interaction of short pulses with the atomic medium in the presence or absence of different supsidiary light-fields. This series of experiments aims to probe the parameter space of our system with the goal of storing single photons fom quantum dots in a rubidium based EIT Memory.

15 min. break

HL 36.7 Wed 16:45 H13

Stability of Majorana modes in disordered topological insulator nanowires — •Leonard Kaufhold — Institute for theoretical physics, Cologne, Germany

The possibility of Majorana bound states (MBS) in nanowire hybrid devices has sparked great interest over the past decade due to their potential application in quantum computing. In this talk, we evaluate theoretically the possibility to realize MBS in topological-insulator (TI) nanowires proximity-coupled to an s-wave superconductor with regards to one main obstacle: disorder, be it from charged impurities within the bulk of the TI or short ranged surface defects. Based on extensive numerical investigation of screening effects as well as the resulting surface states, we demonstrate, that Majorana modes can be achieved under realistic conditions.

HL 36.8 Wed 17:00 H13

Signature of topological transitions in Na-Sb-Bi alloys via Compton scattering — •Aki Pulkkinen[1], Veenavee Kothalawala[2], Kosuke Suzuki[3], Bernardo Barbiellini[2,4,5], Hiroshi Sakurai[3], Ján Minár[1], and Arun Bansil[4,5] — [1]New Technologies-Research Centre, Pilsen, Czech Republic — [2]School of Engineering Science, LUT University, Finland — [3]Graduate School of Science and Technology, Gunma University, Japan — [4]Department of Physics, Northeastern University, USA — [5]Quantum Materials and Sensing Institute, Northeastern University, USA

We investigate the topological transition in Na-Sb-Bi alloys using x-ray Compton scattering experiments, combined with first-principles modeling of the electronic structure. A robust signature of the semiconductor-to-Dirac semimetal transition is identified in the spherically averaged Compton profile. We demonstrate the evolution of the electronic structure across the topological transition as a function of Bi concentration using the coherent potential approximation (CPA) within the fully relativistic, full potential Korringa-Kohn-Rostoker (KKR) method implemented in the SPRKKR package. Spherically averaged Compton profiles are estimated by averaging over directional profiles over a set of special directions within the KKR method. We demonstrate how the number of electrons involved in the topological transition can be estimated, providing a new descriptor to quantify the strength of the spin-orbit coupling driving the transition. Our study also highlights the sensitivity of the Compton scattering technique in capturing the spillover of Bi 6p relativistic states onto Na sites.

HL 36.9 Wed 17:15 H13

Circular photonic crystal grating design for charge-tunable quantum light sources in the telecom C-band — •Chenxi Ma[1], Jingzhong Yang[1], Pengji Li[1], Eddy Rugeramigabo[1], Michael Zopf[1], and Fei Ding[1,2] — [1]Leibniz University Hannover, Institute of Solid State Physics, Hannover, Germany — [2]Leibniz University Hannover, Laboratory of Nano and Quantum Engineering, Hannover, Germany

Efficient generation of entangled photon pairs at telecom wavelengths is a key ingredient for long-range quantum networks. While embedding semiconductor quantum dots into hybrid circular Bragg gratings has proven effective, it conflicts with p-i-n diode heterostructures which offer superior coherence. We propose and analyze hybrid circular photonic crystal gratings, incorporating air holes to facilitate charge carrier transport without compromising optical properties. Through numerical simulations, a broad cavity mode with a Purcell factor of 23 enhancing both exciton and biexciton transitions, and exceptional collection efficiency of 92.4

HL 36.10 Wed 17:30 H13

Control of NV centre generation in pulsed plasma chemical vapor deposition (CVD) grown diamonds — •Ravi Teja Aditya[1], Felix Hoffmann[1], Patrik Stranak[1], Volker Cimalla[1], and Rüdiger Quay[1,2] — [1]Fraunhofer Institute for Applied Solid State Physics, Tullastraße 72, D-79108 Freiburg, Germany — [2]Department for Sustainable Systems Engineering INATECH, University of Freiburg, 79108 Freiburg, Germany

Nitrogen vacancy (NV) centres in diamond have emerged to be an integral part in many quantum computing and quantum sensing applications. High and precise NV density is required especially for quantum sensing applications. There is a need for control of nitrogen incorporation and NV yield without compromis-

ing crystal quality and growth rate. Although higher power levels ensure higher nitrogen incorporation, it is often limited by temperature. Investigating pulsed plasma chemical vapor deposition (CVD) for this purpose proved to be beneficial to control the NV generation. A pulsed plasma generator was used to reach higher power levels while maintaining an appropriate temperature by adjusting the duty cycle accordingly. Time resolved optical emission spectroscopy (OES) was used to observe the plasma composition during microwave pulses. A pulse length dependent activation of CN radicals was observed which led to a variation in NV densities in grown films. We present the results of variation of NV densities in diamond films caused by variation in pulse length, MW power and duty cycle.

HL 36.11 Wed 17:45 H13

Charge-tunable quantum dot single photon sources for quantum repeater experiments — •Peter Gschwandtner, Quirin Buchinger, Constantin Krause, Sebastian Krüger, Silke Kuhn, Tobias Huber-Loyola, and Sven Höfling — Julius-Maximilian-Universität Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik, Germany

Semiconductor quantum dots (QD) are promising candidates for entangled photon sources (SPS) for quantum network purposes [1]. Single charge spins in QDs could serve as the quantum memory in the quantum repeater [2] or as a local entangler to create a photonic state for a memory-free quantum repeater [3].

In this talk, we present our experimental results for electrically contacted charge-tuneable p-i-n InAs QDs embedded in a circular Bragg grating (CBG). The cavity design enables us to control the charged exciton states of the quantum dots. The CBG exhibits high Purcell enhancement in a broad wavelength range. A novel labyrinth design of the CBG allows for electrical contacting without impeding other performance characteristics [4].

[1] D. Vajner et al., Adv. Quantum Technol. (2022), 10.1002/qute.202100116 [2] H.-J. Briegel, W. Dür, J. I. Cirac and P. Zoller, Phys. Rev. Lett. 81, 5932*5935 (1998), 10.1103/PhysRevLett.81.5932 [3] K. Azuma, K. Tamaki and H.-K. Lo, Nature communications 6, 6787 (2015)., 10.1038/ncomms7787 [4] Q. Buchinger et al., Appl. Physics Letters (2023), 10.1063/5.0136715

HL 37: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)

The session is the first part of the focus session on the physics of the van der Waals magnetic semiconductor CrSBr, with a main session on Friday morning. The focus session is jointly organized by HL and MA.

Time: Wednesday 15:00–15:30 Location: H15

HL 37.1 Wed 15:00 H15

Doping-control of excitons and magnetism in few-layer CrSBr — •Farsane Tabataba-Vakili[1,2,3], Anna Rupp[2], Huy Nguyen[2], Anvar Baimuratov[2], and Alexander Högele[2,3] — [1]Institute of Condensed Matter Physics, Technische Universität Braunschweig, Braunschweig, Germany — [2]Fakultät für Physik, Munich Quantum Center, and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, München, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

In two-dimensional (2D) magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-layer CrI3. Within the class of 2D magnets, air-stable CrSBr stands out as an antiferromagnetic semiconductor with a high Néel temperature, excitons coupled to the magnetic order, and exciton-magnon coupling. In this talk, I will present our work on doping-control of excitons and magnetism in few-layer CrSBr [1]. We demonstrate that both exciton and magnetic transitions are sensitive to field-effect charging, exhibiting bound exciton-charge complexes and doping-induced metamagnetic transitions. We further visualize magnetic domain formation induced by magnetic field or charge-doping at the metamagnetic transition all-optically by raster-scan reflectance imaging. Our work identifies few-layer CrSBr as a rich platform for exploring collaborative effects of charge, optical excitations, and magnetism.

[1] F. Tabataba-Vakili et al., Nat. Commun. 15, 4735 (2024).

HL 37.2 Wed 15:15 H15

Proximity-Induced Exchange Interaction and Prolonged Valley Lifetime in $MoSe_2$/CrSBr Van-Der-Waals Heterostructure with Orthogonal Spin Textures — •Andreas Beer[1], Klaus Zollner[1], Caique Serati de Brito[1,2], Paulo E. Feria Junior[1], Philipp Parzefall[1], Talieh S. Ghiasi[3], Josep Ingla Aynés[3], Samuel Mañas-Valero[4], Carla Boix-Constant[4], Kenji Watanabe[5], Takashi Taniguchi[5], Jaroslav Fabian[1], Herre S. J. van der Zant[3], Yara Galvão Gobato[2], and Christian Schüller[1] — [1]UR, Regensburg, Germany — [2]UFSCar, São Carlos, Brazil — [3]TU, Delft, Netherlands — [4]ICMol, València, Spain — [5]NIMSC, Tsukuba, Japan

We report a comprehensive optical study of a ML-$MoSe_2$ on the layered A-type antiferromagnetic semiconductor CrSBr. The band alignment of the material combination is under debate. Here, we adopt the type-III band alignment picture. By performing co-circular polarized PL and reflection contrast (RC) experiments, we observe that the atomic proximity of the materials leads to an unexpected breaking of time-reversal symmetry, despite the originally perpendicular spin texture in both materials, which are further supported by first-principles calculations. Moreover, time-resolved PL and time-resolved RC measurements identify a very long-lived dynamic charge-transfer process in the heterostructure, consistent with a type-III band alignment. Our findings suggest band bending, and efficient Förster resonance energy transfer within the heterostructure. Finally time resolved Kerr ellipticity measurements reveal a two magnitudes prolonged valley lifetime.

HL 38: Nanomechanical systems (joint session HL/TT)

The session covers the physics of nanomechanical systems.

Time: Wednesday 15:00–15:45 Location: H17

HL 38.1 Wed 15:00 H17

Optimizing an Integrated Photonic Racetrack Resonator for Optomechanical Synchronization — •Agnes Zinth[1] and Menno Poot[1,2,3] — [1]Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Institute for Advanced Study, Technical University of Munich, Garching, Germany

In the field of optomechanics, synchronization will be an essential tool in fields like sensing and quantum technologies. Towards this goal, we develop a photonic integrated optomechanical device consisting of a silicon nitride racetrack cavity with partly suspended waveguide that can vibrate freely. A second beam is added to improve the optomechanical coupling. The observed mechanical modes do not match in frequency, so we use a predisplaced beam instead [1]. The remaining frequency distance can be tuned by the laser power. As the light propagates in the predisplaced beam and only past the PhC beam, it shifts further than the photonic crystal one due to thermal effects. To synchronize them with optomechanical backaction, we also need to enhance the optical cavity. Therefore, we modify the transition from supported to suspended parts. Two different approaches lead to the desired improved optical quality. Currently, we are investigating their impact on the mechanics. We believe that, in the next generation of devices, we can synchronize the racetrack and photonic crystal beam.

[1] Geometric tuning of stress in predisplaced silicon nitride resonators. Nano Letters, 22(10), 4013-4019.

HL 38.2 Wed 15:15 H17

Quantum Mechanics in Two-Dimensional Dynamic Spaces — •Benjamin Schwager and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

In the study of systems with reduced dimensions one encounters quantum particles under spatial constraints. Their dynamics have to be modeled based on a configuration space that is a Riemannian manifold, in general, and the resulting quantum wave equations contain correction terms in dependence of its geometric properties. We consider particles which are confined to a flexible thin material shell by studying the Schrödinger equation on moving domains. The

model assumes a static observer and couples the deformation dynamics of the material to the quantum dynamics it hosts via additional potential fields. Effects caused by the interplay of geometry and the temporal evolution of the underlying configuration space will be discussed.

HL 38.3 Wed 15:30 H17

Towards cavity optomechanics using 2D materials — •Petricia Sara Peter[1,2], Lukas Schleicher[1,2], Anne Rodriguez[1,2], Leonard Geilen[2,3], Alexander Musta[2,3], Benedict Brouwer[2,3], Alexander Holleitner[2,3], and Eva Weig[1,2] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Walter Schottky Institute, TU Munich, Germany

Two-dimensional (2D) materials, such as hexagonal boron nitride (hBN), are promising candidates for advancing cavity optomechanics due to their low mass, high mechanical strength, and unique optical properties. This work focuses on the fabrication of freely suspended hBN membranes on silicon oxide (SiO_2) and silicon nitride (Si_3N_3) substrates, utilizing a water-assisted wet transfer technique. Compared to the dry transfer method, this approach minimizes inhomogeneous stress and preserves optimal mode shapes, improving mechanical quality factors. A Michelson interferometer is used to measure the mechanical properties of the resulting drumhead resonators, including vibrational resonances, mode shapes, and quality factors. These results provide important insights into the performance and quality of the resonator, laying the groundwork for incorporating 2D materials into cavity optomechanical studies.

HL 39: Poster III

The third poster session covers most recent results on the optical and thermal properties of semiconductors, as well as on nitrides and organic semiconductors, and semiconductor lasers.

Time: Wednesday 15:00–18:00 Location: P3

HL 39.1 Wed 15:00 P3

Termperature dependent electroluminescence spectroscopy of far-UVC-LEDs with varying AlGaN quantum well thickness — •Max Dittmer[1], Jakob Höpfner[1], Markus Blonski[1], Tim Kolbe[2], Sylvia Hagedorn[2], Hyun Kyong Cho[2], Jens Rass[2], Sven Einfeldt[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1] — [1]TU Berlin, Insitute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Insitut (FBH), Berlin Germany

AlGaN far-UVC-LEDs with emission wavelengths below 240 nm require AlGaN layers with such high aluminium molefractions that p-doping with magnesium is inefficient due to its high ionization energy. An alternative method of p-doping is distributed polarization doping (DPD), which induces charge carriers by polarization charges. We will present the results of temperature dependent electroluminescence spectrocopy on 233 nm AlGaN LEDs with DPD gradient, grown by metal organic vapor phase epitaxy (MOVPE). We investigated the impact of the quantum well (QW) width from 1.3 nm to 7.6 nm. Most importantly we found the 2.6 nm LED to be the most efficient at room temperature. The LEDs exhibit an S-shape in the emission energy in dependence of the temperature and the highest internal quantum efficiency of 55%, was measured at 200 K.

HL 39.2 Wed 15:00 P3

MATRIX: GaN diode arrays for proton monitoring and imaging — •Nico Brosda[1], Stéphane Higueret[2], Thê-Duc Lê[2], Andreas Wieck[1], Maxime Hugues[3], Matilde Siviero[3], and Jean-Yves Duboz[3] — [1]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Université de Strasbourg, CNRS, IPHC UMR 7178, F-67000 Strasbourg, France — [3]Université Côte d'Azur, CNRS, CRHEA, 06560, Valbonne, France

The MATRIX project is pioneering advancements in proton therapy for cancer treatment by developing novel, highly durable detectors that enhance real-time control of irradiation doses. Proton detection is achieved by measuring the current induced in the active regions of PIN GaN diodes. Our GaN-based devices are fabricated as linear diode arrays of 128 elements and two-dimensional imaging arrays up to 11×11 elements, covering an area of 1 cm^2 with up to 500 μm spatial resolution. Thanks to the microelectronics processes, a much higher resolution can be obtained if needed. Results concerning the sample structure and fabrication process are presented. The design of bonding contacts proved to have a significant impact on the measured signal and, thus, the imaging quality. A bonding fanout on the GaN samples introduced notable signal distortions at the edges of the proton irradiation field. The underlying electron external emission mechanism responsible for this distortion was modeled, and a correction method was developed. An adapted sample design improved the device quality and removed the signal distortion. These findings pave the way for optimizing future GaN-based proton detector arrays.

HL 39.3 Wed 15:00 P3

Investigating the Electrical Properties of Distributed Polarization Doped $Al_xGa_{1-x}N$ Heterostructures via Capacitance-Voltage Measurements — •Thibaut Ehlermann[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin — [2]Ferdinand-Braun-Institut (FBH)

Distributed Polarization Doping (DPD) enables the generation of charge carriers in wide-bandgap semiconductors like AlGaN by utilizing the material's inherent polarization properties without the introduction of impurities. Linearly graded AlGaN DPD layers were grown by metal-organic vapor phase epitaxy (MOVPE). The starting Al mole fraction was always 100%. The thickness and end mole fraction were varied. The charge carrier concentration N_A was determined from CV-measurements. For a 100 nm thick AlGaN DPD layer (x=100% –> 60%), the charge carrier concentration is $N_A = 1.4 \cdot 10^{18} \frac{1}{cm^3}$, closely matching the theoretical value of $N_A = 1.72 \cdot 10^{18} \frac{1}{cm^3}$, based on the calculated intrinsic polarization. Thicker DPD layers lead to a lower doping concentration and AlGaN DPDs (x=100% –> 80%) result in lower doping concentrations in agreement with the calculated values. The consistency of the results suggest that DPD is a reliable and promising way for p-type doping in AlGaN.

HL 39.4 Wed 15:00 P3

Temperature Dependence of the Quantum Efficiency of UV LEDs emitting from 226 nm to 300 nm — •Max Eysell[1], Jakob Höpfner[1], Marcel Schilling[1], Norman Susilo[1], Anton Muhin[1], Massimo Grigoletto[1,2], Tim Kolbe[2], Arne Knauer[2], Sylvia Hagedorn[2], Markus Weyers[2], Jens Rass[2], Hyun Kyong Cho[2], Tim Wernicke[1], Sven Einfeldt[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

UV-LEDs are of huge interest for e.g. air, surface, and water disinfection. However, the widespread application of UV-LEDs is constrained by their external quantum efficiency (EQE) which is decreasing further as the emission wavelength shortens. To gain insight into the carrier transport and recombination mechanisms, a detailed analysis of the EQE of UV-LEDs and the three contributors: the carrier injection, the radiative recombination and the light extraction was performed.

The emission power of LEDs with emission wavelengths of 226 nm, 233 nm, 265 nm and 305 nm are investigated by temperature dependent electroluminescence measurements in the range of $25 - 80^{\circ}C$. A reduction in emission power and EQE has been observed going from UVB to the far-UVC spectral range. A thermal droop in the emission power was observed for all samples which is caused by the decline of all three contributions. The magnitude of this thermal droop becomes higher with decreasing wavelength which we attribute to an increased electron leakage suggested by Schrödinger-Poisson drift-diffusion simulations.

HL 39.5 Wed 15:00 P3

Theoretical Study on the (In, Ga)N/GaN heterojunction — •Maximilian Lauer[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Semiconductor materials have a wide range of applications and their electronic properties can be easily tuned by alloying and changing their composition x. Understanding the properties of semiconductor alloys, such as indium gallium nitride $In_xGa_{1-x}N$, is therefore an important area of research. Two such properties are the band gap of the semiconductor and its band alignment with substrate and conduction materials.

While the band gap of the random alloy (In, Ga)N is a well-established quantity, the band alignment is less well understood.

Our research aims to better understand the band alignment and interface states at a GaN/(Ga,In)N heterojunction and its impact on the electronic properties of the system.To achieve this, we performed DFT calculations using the Korringa-Kohn-Rostoker (KKR) formalism with the coherent potential approximation (CPA). From these calculations we computed the layer-resolved density of states (DOS) for varying $In_xGa_{1-x}N$ compositions. This approach can be further used to simulate the effects of doping on the electronic properties or to study the transport properties of such a system.

HL 39.6 Wed 15:00 P3

Moiré exciton polaritons in twisted photonic lattices at room temperature — •Tobias Schneider[1], Chunzi Xing[2], Yu Wang[3], Xiaokun Zhai[2], Xinzheng Zhang[3], Haitao Dai[2], Xiao Wang[4], Anlian Pan[4], Zhenyu Xiong[5], Hao Wu[5], Yuan Ren[5], Stefan Schumacher[1,6], Xuekai Ma[1], and Tingge Gao[2] — [1]Physics dept. and CeOPP, Paderborn University, Germany — [2]Department of Physics, School of Science, Tianjin University, Tianjin 300072, China — [3]The MOE Key Laboratory of Weak-Light Nonlinear Photonics and International Sino-Slovenian Join Research Center on Liquid Crystal Photonics, TEDA Institute of Applied Physics and School of Physics, Nankai University, Tianjin 300457, China — [4]College of Materials Science and Engineering, Hunan University, Changsha 410082, China — [5]Lab of quantum detection and awareness, Space Engineering University Beijing 101416, China — [6]PhoQS, Paderborn University, Germany

Due to their support of many exotic physical phenomena such as Mott insulators or the fractal quantum Hall effect, moiré lattices have attracted great interest. In this work, rhombic optical moiré lattices are realized in microcavity exciton polaritons[1]. These lattices consist of two stacked 1D periodically patterned stripes which are twisted to a specific angle. This structure allows the resulting bands to be tuned via modulating the lattice parameters such as the periodicity, the potential depth of the stripes, and the rotation angle. In addition, moiré polaritons in twisted 2D honeycomb lattices are also observed. [1] C. Xing et al., arXiv:2408.02431 (2024).

HL 39.7 Wed 15:00 P3

Ultradoped GeSn plasmonic antennas for IR photodetection — •Guillermo Godoy[1,2], Ali Azimi[3], Fritz Berkmann[3], Oliver Steuer[1], Slawomir Prucnal[1], Shengqiang Zhou[1], Ing-Song Yu[4], Inga A. Fischer[3], and Yonder Berencén[1] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden Germany — [2]Dresden University of Technology, Dresden Germany — [3]BTU Cottbus-Senftenberg, Cottbus Germany — [4]National Dong Hwa University, Hualien Taiwan

Ligth mater interaction due to localized surface plasmon resonances (LSPRs) can generate hight electical field enhacement, enabling biosensing and hot-electron photodetection devices. While metallic nanoparticles like Au and Al are commonly used, their optical losses increase at longer wavelengths, limiting applications in the mid-infrared (MIR) range, such as air pollution detection. Highly doped group-IV semiconductors, particularly GeSn alloys, offer a cost-effective alternative with lower losses and CMOS compatibility. The cut-off wavelength for plasmonic resonances depends on the carrier effective mass, and GeSn alloys with its lower electron effective mass enables plasmonic resonances from shorter wavelengths.This work explores strategies to achieve highly doped GeSn alloys for plasmon-enhanced photodetection, utilizing MBE or CVD-grown GeSn layers on Si substrates. These layers will be doped in-situ or ex-situ via ion implantation, followed by non-equilibrium annealing to enhance crystal quality and dopant activation, showcasing their potential for advancing MIR photodetection.

HL 39.8 Wed 15:00 P3

Optical and phonon properties of In-rich InGaN alloys and InN/InGaN multiple quantum well structures — •Svitlana Polesya[1], Masako Ogura[1], Sergiy Mankovsky[1], Gregor Koblmüller[2], and Hubert Ebert[1] — [1]University of Munich, 81377 Munich, Germany — [2]Technical University of Munich, 85748 Garching, Germany

In two-dimensional systems like multiple quantum well structures, thermalization of hot carriers can be strongly suppressed. InN/InGaN multilayered (ML) materials are seen as promising candidates to show this property. In order to optimize these materials, ab initio calculations have been performed on the electronic and phonon band structure, as well as on the optical properties of In-rich $In_xGa_{(1-x)}N$ alloys and the short period ML systems $[InN]_m/[In_xGa_{(1-x)}N]_n$. All calculations have been done with the VASP package. The HSE exchange-correlation potential has been used with further GW0 corrections. Electron-hole interactions were taken into account by solving the Bethe-Salpeter equation. The calculations on alloys were done via the superlattice technique considering for each In concentration x all non-equivalent atomic arrangements. This is crucial as the atomic distribution has a significant impact on the phonon band structure of the alloys. For the layered $[InN]_m/[In_xGa_{(1-x)}N]_n$ system the optical properties were calculated for various concentrations x. The important role of the interface between the quantum well ($[InN]_m$) and the quantum barrier ($[In_xGa_{(1-x)}N]_n$) on the optical properties as well as phonon band gap is shown.

HL 39.9 Wed 15:00 P3

Ultra-sensitive absorption measurements of perovskites nanocrystals, protein crystals and photo-switchable lipids — •Ayesha Khan[1], Simone Strohmair[1], Ines Amersdorffer[1,2], David Hunger[3], and Thomas Hümmer[1,2] — [1]Qlibri GmbH, Munich, Germany — [2]Ludwig Maximilian University of Munich, Munich, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Optical studies of nano-scale systems through spectroscopy and imaging can reveal intrinsic optical properties of materials including resolving the exitonic fine structure of systems. However, due to diminutive absorption of nano-scale systems, it is challenging to perform absorption spectroscopy. For a nano-scale system placed inside an optical resonator, the light passes through the sample thousands of times, enhancing the absorption and thus, allowing measurements.

Here we present the use of a fiber-based, open-access micro-cavity to image and obtain hyperspectral maps of absorption for different nano-scale, solid state materials including perovskites nanocrystals, protein crystals and photo-switchable lipids.

The successful measurements of different nano-scale systems promise that fiber-based microcavities can become standard tools for absorption measurements of these systems.

HL 39.10 Wed 15:00 P3

Intensity-dependence of the excitonic third-harmonic generation in bilayer MoS2 — •Ruixin Zuo[1], Matthias Reichelt[1], Cong Ngo[1], Xiaohong Song[2], and Torsten Meier[1] — [1]Department of Physics, Paderborn University, D-33098 Paderborn, Germany — [2]School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570288, China

The large exciton binding energies make layered transition metal dichalcogenides an ideal platform for exploring exciton physics in two-dimensional systems. We numerically and theoretically investigate three-photon transitions to the excitonic states in a bilayer MoS2 and demonstrate that beyond the linear order intraband transitions dominate over interband transitions. Beyond the perturbative limit, transitions to and from the continuum that represent fifth- and higher-order nonlinearities contribute to the excitonic response at the third harmonic where they destructively interfere with the third-order excitations. Applying an in-plane static electric field characteristically modifies the k-resolved fourth-order and higher-order nonlinearities and accordingly the interference at the excitonic resonance. We demonstrate that the yield of the third harmonic generation may rise with increasing static field strength. This finding can be interpreted to arise from a shift from destructive to constructive interference between the lowest- and higher-order excitations. Exciton ionization prevails at even higher static field strengths and results in a decrease of the third harmonic generation.

HL 39.11 Wed 15:00 P3

Implementation and Validation of a Herzberg-Teller Approach for Phonon-Assisted Photoluminescence — •Tobias Dittmann, Torben Steenbock, and Gabriel Bester — Insitut für physikalische Chemie, Universität Hamburg

Phonon-assisted PL from electronically excited states leads to the occurrence of phonon side-bands, which can shape the PL spectrum. A Franck-Condon framework based on Huang-Rhys factors efficiently describes phonon side-bands in nanostructures containing up to a few hundred atoms.[1] However, the FC approximation is usually not suited for the emission from a dark state. Therefore, we extend the method towards a Herzberg-Teller (HT) level which allows a more accurate description of the emission from a dark state. Additionally, our method includes the description of spin-orbit effects, offering an advantage over other implementations of the HT framework, particularly for structures containing heavy elements.

In a first stage of the project, we investigate various graphene quantum dots and observe that the inclusion of HT terms introduces both quantitative and qualitative differences compared to the FC spectrum. These findings underscore the critical importance of incorporating HT terms for accurate modelling. In future work, we intend to apply this method to bigger structures containing heavy elements, in order to benefit from the advantages of our implementation.

[1] Wu, Han, Dittmann, Wang, Zhang and Bester, Nanoscale, 2024, DOI: 10.1039/D4NR02458C

HL 39.12 Wed 15:00 P3

Electronic structure and energy landscape of $B_{Si}Si_i$-related defects — Aaron Flötotto[1], Wichard Beenken[1], Kevin Lauer[1,2], Stefan Krischok[1], and •Erich Runge[1] — [1]Technische Universität Ilmenau, Institute for Physics, Ilmenau, Germany — [2]CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Boron is an important dopant for silicon. Together with an adjacent interstitial Si atom, it forms the so-called $B_{Si}Si_i$ defect, which has been proposed as a source of light-induced degradation (LID) in solar cells made from boron-doped Czochralski-grown silicon. Furthermore, the $B_{Si}Si_i$ defect is an intermediate configuration in many models for boron diffusion in silicon.

In a recent comprehensive density-functional-theory-based study [1], we have calculated the energy landscape around the $B_{Si}Si_i$ defect and related defects involving one B atom and one interstitial Si atom for different chemical potentials of electrons corresponding to neutral, positively, and negatively charged supercells. Among the found meta-stable defect configurations, we identify possible recombination centers based on the defect-dependent electronic density of states and the minimal energy paths between them. The resulting potential energy landscape is checked against empirical models for boron diffusion and LID.

[1] A. Flötotto et al., Phys. Rev. Mater. (accepted)

HL 39.13 Wed 15:00 P3

Origin of strong interband transitions in antimony — •Julia Vehndel, Nils Holle, Sebastian Walfort, and Martin Salinga — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, phase change materials (PCMs) have attracted considerable interest as photonic memory elements due to a high contrast in optical properties between crystalline and amorphous states. In order to identify ideal PCMs for specific applications, the intricate connection between electronic structure, bonding and permittivity needs to be understood.

Here, we employ ab-initio simulations based on density functional theory to calculate the optical properties of the single-elemental PCM antimony in the visible and near-infrared. We analyze the permittivity in k-space for both crystalline and amorphous states. Most strikingly, the strong interband transitions at lower energies can be related to the electron and hole pockets in the first Brillouin zone of the crystalline state.

HL 39.14 Wed 15:00 P3

Optical properties of α-$(Cr_xGa_{1-x})_2O_3$ — •Dmitry Sayenko, Clemens Petersen, Jakob Seifert, Christiane Dethloff, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

Due to its high bandgap energy in the order of 4.6 – 5.0 eV and its high predicted electrical breakdown field of about 8 MV cm^{-1}, Ga_2O_3 is a promising material for transparent electronic devices and high power applications [1]. Of special interest is the corundum-structured α-phase as it has the largest band gap energy of the Ga2O3 polymorphs. Further, its band gap energy can be tuned by alloying with Cr without changing its crystal structure. Here we present the dielectric function of α-$(Cr_xGa_{1-x})_2O_3$ as a function of the cation composition. The sample was grown by combinatorial pulsed laser deposition. As expected, the onset of absorption increases with increasing Ga concentration from around 3.2 eV for $x \approx 0.74$ to 4.2 eV for $x \approx 0.13$. Whereas we observe for all concentrations a negative birefringence in the visible range, i.e. $n_{eo} < n_o$, the polarization of the energetically lowest transition changes with Cr concentration. For large Cr concentration the absorption sets in at first for light polarized perpendicular to the c-axis whereas for large Ga concentration the first absorption is observed for light parallel to the c-axis. This change of the polarizability leads to a decrease of the birefringence with decreasing Cr concentration, but $n_{eo} < n_o$ holds for all x.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

HL 39.15 Wed 15:00 P3

Calibration methods in Raman spectroscopy — •Susanne Moritz, Ron Hildebrandt, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

For low symmetry materials, polarization resolved measurements are required for a precise investigation, especially of the Raman tensor [1, 2]. Here we present strategies for calibrating and determining the polarization state of the incident and scattered light. In addition to the polarizing optics, e.g. polarizers, we also consider the impact of all involved optical elements such as mirrors and beam splitters. We show, that these non-idealities can have an impact on the determined Raman tensor elements. Taken into account the non-idealities of the polarizing optics the uncertainty of the deduced tensor elements can be reduced by 20%.

[1] C. Kranert *et al.*, Phys. Rev. Lett. **116**, 127401 (2016).
[2] C. Kranert *et al.*, Sci. Rep. **6**, 35964 (2016).

HL 39.16 Wed 15:00 P3

Spectral Signatures and Kinetics of Y6 Aggregates and Disordered Phase via Absorption Spectroscopy — •Daniel Kroh[1,2], Xinyue Xu[2], Trevor Smith[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, EPII, Universität Bayreuth, Bayreuth, Germany — [2]School of Chemistry, University of Melbourne, Melbourne, Australia

Recent advancements in single-junction organic solar cells (OSCs) utilizing nonfullerene acceptors (NFAs) have significantly increased power conversion efficiencies (PCEs) to over 19%. This remarkable progress is largely attributed to the introduction of the "Y-series" NFAs, with Y6 being the most notable example. Motivated by these achievements, numerous research groups are investigating the relationship between film morphologies and their exceptional optoelectronic properties, especially when blended with the donor material PM6.

In our study, we employed temperature-dependent steady-state UV-Vis absorption and photoluminescence spectroscopy combined with Franck-Condon analysis to identify the spectral signatures of two types of aggregates and the disordered phase of Y6 in solution. We observed that all three phases are also present in neat Y6 films and blend films with PM6. Through transient absorption measurements, we further explored the excitation kinetics and transient absorption spectral signatures of these phases, providing deeper insights into their behavior.

HL 39.17 Wed 15:00 P3

Empowering Thermoelectric Performance of ZnSb via Bonding Interaction Regulation — •Meng Jiang[1,2], Fangyi Hu[1], Qihao Zhang[2], Lianjun Wang[2], Wan Jiang[2], Matthias Wuttig[1], and Yuan Yu[1] — [1]Physical Institute 1, RWTH Aachen University, Aachen, 52074, Germany. — [2]Donghua University, Shanghai, 201620, China.

ZnSb compounds have garnered significant attention due to its green nature, low cost and high Seebeck coefficient. However, its thermoelectric performance has been limited by a relatively low power factor and high lattice thermal conductivity. Recent studies have demonstrated that regulating bonding interactions offers an effective strategy to optimize the thermoelectric properties. Specifically, metavalent bonding shows unprecedented success in predicting and optimizing a series of high-performance thermoelectric materials. This reignites research interest in ZnSb. We explored a one-step synthesis strategy for ZnSb and specifically investigated optimizing mechanisms of Cd and Mg. By regulating bonding interactions to optimize electrical conductivity, the room-temperature power factor was enhanced from 2.5 to 4 μW cm-1 K-2. This improvement, coupled with a reduction in lattice thermal conductivity, resulted in a zT of 0.6 at 600 K. Our work highlights the potential of bonding interaction regulation as an effective approach for enhancing the thermoelectric performance of ZnSb. More, future research would focus on unraveling the intricate mechanisms linking bonding and microstructure to achieve even higher performance.

HL 39.18 Wed 15:00 P3

Challenges and Opportunities for Thermoelectric Coolers — •Fangyi Hu, Meng Jiang, Matthias Wuttig, and Yuan Yu — I. Physikalisches Institut (IA), RWTH Aachen University, 52074 Aachen, Germany

Thermoelectric (TE) materials allow a direct interconversion between heat and electricity, providing an eco-friendly and sustainable energy solution. Particularly, thermoelectric coolers based on the Peltier effect achieve high-precision temperature control without any refrigerant. Bi2Te3-based materials have beenused in commercial TE cooling due to their high near-room-temperature figure-or-merit (ZT). Yet, the low earth abundance of Te restricts the large-scale application of this compound. Discovering Te-free materials with comparable cooling performance is an urgent task. This requires a small bandgap and low thermal conductivity for the material at low temperatures. The recently developed concept of metavalent bonding provides a new avenue for discovering potential candidates. Besides materials, the device design and effective heat dissipation on the hot side are of critical importance. This Poster will summarize the challenges and opportunities for TE cooling materials and devices. We hope that it can shed light on the development of new TE coolers.

HL 39.19 Wed 15:00 P3

Quantum-chemical calculations of structure, electronic properties, and spectra of a model for PBDB-T:ITIC heterojunctions — Montassar Chaabani[1], Samir Romdhane[2], and •Wichard J. D. Beenken[2] — [1]Advanced Materials and Quantum Phenomena Laboratory, Physics Department, Faculty of Sciences of Tunis, University of Tunis El Manar, Tuins, Tunesia — [2]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

We modeled PBDB-T:ITIC heterojunctions by applying DFT on dimers built of various conformers of a PBDB-T segment and the ITIC molecule. These variations represented the non-uniformity of the interface between the donor and the acceptor in the organic solar cell. Based on this model, we calculated electronic and optical properties most relevant for charge separation at the interface using DFT and TD-DFT, respectively. For almost half of our modeled dimers, we found that the band offsets between them and the pristine donor and acceptor materials resulted in charge carrier trapping leading to inefficient charge separation as well as non-geminate recombination. When we calculated the exciton binding energy by TD-DFT using either the B3LYP or the HSE06 functional, we obtained very different qualitative and quantitative results. We, therefore, compared our results with experimental data from ultraviolet photoelectron spectroscopy, CV, ER-EIS, PL, absorption spectroscopy, EQE and EL. Finally we discuss the impact of our findings on characteristic photovoltaic parameters, particularly the open circuit voltage and the short-circuit current.

HL 39.20 Wed 15:00 P3

Investigation of the optical coupling of lasing ZnO nanowires — •Ann-Kathrin Kollak, Lukas Raam Jäger, Francesco Vitale, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Semiconductor nanowires offer potential for miniaturizing optical circuits. Good candidates for this application are ZnO nanowires, because their bottom-up growth via the Vapor-Liquid-Solid (VLS) mechanism allows for high quality crystal structures. When optically pumped, ZnO nanowires simultaneously act as an active medium and a laser cavity, emitting UV light mainly waveguided to their end facets. To study the interaction of these nanometer-scale lasers via evanescent field coupling, two nanowires were positioned in contact next to each other on a SiO_2 substrate using a nanomanipulator. In a micro-PL (photoluminescence) setup, the nanowire pair was optically excited using the

third harmonic of an Nd:YAG laser (355 nm). The pair's emission was collected with the same setup, allowing the investigation of the spatially resolved PL and lasing spectra, as well as their linear polarization parallel to the substrate. The data obtained indicate that ZnO nanowire cavities can couple with one another. Depending on the geometry of the nanowire pair and the pumping conditions, optical modes that extend into both cavities can appear in addition to modes confined to only one nanowire. In other cases, the coupled modes dominate the lasing behavior.

HL 39.21 Wed 15:00 P3

Impact of stress current on reverse-bias electroluminescence images of 850 nm oxide-confined VCSELs — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Sebastian Haberkern[1], Helmut Meinert[1], Alexander Moll[1], Ilya E. Titkov[2], Oleg Yu. Makarov[2], and Nikolay N. Ledentsov[2] — [1]Esslingen University of Applied Sciences, Flandernstrasse 101, 73732 Esslingen, Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Germany

Vertical-cavity surface-emitting lasers (VCSEL) employing different doping of the cavity region are studied utilizing reverse current-voltage (*IV*) characteristics as well as reverse bias electroluminescence (ReBEL). Reverse *IV* characteristics exhibits avalanche breakdown enabling an estimation of the electric field in the cavity region. ReBEL emission is observed at locations where avalanche breakthrough current has its maximum. The oxide-confined VCSELs are characterised before and after high current operation. Virgin devices have a homogeneous device center in ReBEL images. Upon a short high current burn-in VCSELs evolved a homogeneous ring at the oxide-aperture perimeter. This ring structure decays into 2 point-like areas after long-term current stress. These observations in ReBEL images can be understood in terms of recently published VCSEL simulation results which gave evidence of local current crowding at the oxide-aperture during high current laser operation.

HL 39.22 Wed 15:00 P3

Tuning nanowire lasers via hybridization with organic molecules — •Philipp Swatosch, Edwin Eobaldt, Marco Grünewald, Olga Ustimenko, Kalina Peneva, and Carsten Ronning — Friedrich Schiller Universität Jena, Deutschland

Among the numerous nanomaterials, semiconductor nanowires have drawn significant scientific interest as promising candidates for nanoscale coherent light sources and all-optical circuits. This attention is due to their exceptional waveguiding properties and inherent ability to lase under high excitation. However, precise control over their lasing characteristics, such as emission wavelength and lasing threshold, is essential for various applications. In this regard, hybridizing nanowires with customized molecules presents a potential approach, providing new control mechanisms through efficient charge and energy transfer processes at the heterointerface. To demonstrate this concept, we hybridized ZnO nanowires with perylene-based organic dyes. These chromophores are particularly advantageous as their optical gap can be easily tuned over a wide spectral range through chemical functionalization. This study employs comparative micro-photoluminescence measurements to investigate the impact of these molecules on the lasing properties of the nanowires.

HL 39.23 Wed 15:00 P3

Development of a VCSEL-chip in the red spectral range with integrated photodiode for chlorophyll fluorescence analysis — •Raphael Buffler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum-Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart

Chlorophyll fluorescence analysis provides information on photosynthetic activity of plants and thus also on their health. Changes in the environmental conditions can be monitored on large scale and, water and nutrients can be added as needed. In order to induce the fluorescence of chlorophyll in the range from 660 nm to 750nm , optical excitation at 650 nm can be used. In this work, a semiconductor chip will be developed that contains both, the light source for excitation and the photodiode for fluorescence detection. The chip is based on the AlGaAs & AlGaInP material systems, which can realise the band gaps for the required wavelengths. The light source is designed as a vertical-cavity surface-emitting laser (VCSEL), which allows for the vertical emission of the excitation light and the vertical irradiation of the photodiode. A stacked arrangement is used, where the VCSEL is grown by metal-organic vapor-phase epitaxy (MOVPE) on top of the photodiode structure on a GaAs wafer. First electro-optical characteristics of the VCSEL and the photodiode such as P-U-I curves, emission wavelength and photodiode responsivity are presented.

HL 39.24 Wed 15:00 P3

Monolithic 850 nm VCSEL array for Quantum Key Distribution via the Decoy State Protocol — •Katharina Dahler, Michael Zimmer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The need for secure data communication has increased in recent years. In contrast to classical key distribution, the use of quantum key distribution (QKD) offers fundamental advantages, such as complete secrecy. However, QKD poses numerous challenges regarding the use of single photons. With this in mind, the decoy-state protocol offers the possibility of realizing QKD with classical light sources such as attenuated semiconductor lasers. Here, we present the electro-optical characterization of a monolithic 850 nm vertical-cavity surface-emitting laser (VCSEL) array, for QKD via the BB84 and decoy state protocol. The complete VCSEL array consists of eight individual VCSELs arranged in a coplanar contact design, with four VCSELs serving as signal states and four as decoy states. A highly homogeneous growth is needed due to the requirement of indistinguishable light pulses regarding the emission wavelength. In order to realize the four necessary polarization states and to counteract the electro-optical effect, each VCSEL features a monolithically integrated surface grating in the top layer of its light emission window. Electro-optical device characteristics regarding light polarization via surface gratings and spectral homogeneity of the VCSEL array are presented.

HL 39.25 Wed 15:00 P3

A machine learning potential for tellurium — •Andrea Corradini, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Elemental tellurium has drawn attention in recent years, due to its possible technological application as switching device in phase change memories [1]. Recent computational studies are addressing the behaviour of elemental Te under operating conditions with a focus on the crystallization dynamics [2]. In addition, experiments have found anomalous thermodynamic maxima in undercooled liquid Te around 615 K, i.e. 130 K below the melting point [3]. Thermodynamic maxima behave in a very similar way as those in undercooled liquid water. Hence the question whether elemental Te shows a liquid-liquid phase transition, analogously to what is claimed for water. In this work, we develop a robust machine learning potential to study elemental Te and try to answer this question.

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[1] Shen et al., Science 374, 1390*1394 (2021)
[2] Zhou et al., arXiv:2409.03860 [cond-mat.mtrl-sci]
[3] Sun et al., PNAS 119 (28), e2202044119 (2022)

HL 40: 2D Semiconductors and van der Waals Heterostructures IV

The session covers the magnetic and topological properties of 2D semiconductors and van der Waals heterostructures.

Time: Wednesday 15:30–19:00 Location: H15

HL 40.1 Wed 15:30 H15

Dielectric tensor of the layered magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Sebastian Schaper[1], Marie-Christin Heissenbüttel[1], Aleksandra Lopion[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

Two-dimensional materials exhibit unique properties due to their atomically thin structure and weak van der Waals (vdW) coupling between layers resulting in layer dependent properties. As in the case of the layered magnetic semiconductor CrSBr, individual layers are ferromagnetically ordered below the Neel temperature (TN= 132K), while adjacent layers are coupled antiferromagnetically. Due to the highly anisotropic electronic bands in CrSBr, electronic and excitonic states at the fundamental band-gap behave quasi-one-dimensional [1]. To develop a better understanding of the extraordinary light-matter interaction in CrSBr, we access the materials dielectric tensor in the paramagnetic phase by spectroscopic imaging ellipsometry that is hard to access by alternative approaches such as reflectance measurements due to the strong anisotropy. In

agreement with theory, we extract highly anisotropic dielectric functions along the crystallographic main axes with strong excitonic resonances particularly in the plane. [1] J. Klein et al. ACS Nano, 17, 6, 5316-5328 (2023).

HL 40.2 Wed 15:45 H15

Raman Polarization Switching in CrSBr — •Priyanka Mondal[1], Daria I. Markina[1], Lennard Hopf[1], Lukas Krelle[1], Sai Shradha[1], Julian Klein[2], Mikhail M. Glazov[3], Iann Gerber[4], Kevin Hagmann[1], Regine v. Klitzing[1], Kseniia Mosina[5], Zdenek Sofer[5], and Bernhard Urbaszek[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Massachusetts Institute of Technology, Cambridge, United States — [3]St. Petersburg, Russia — [4]Université de Toulouse,Toulouse, France — [5]University of Chemistry and Technology, Prague,Czech Republic

Semiconducting CrSBr is a layered A-type antiferromagnet, with individual layers antiferromagnetically coupled along the stacking direction. Due to its unique orthorhombic crystal structure, CrSBr exhibits highly anisotropic mechanical and optoelectronic properties acting itself as a quasi-1D material. CrSBr demonstrates complex coupling phenomena involving phonons, excitons, magnons, and polaritons. Here we show through polarization-resolved resonant Raman scattering the intricate interaction between the vibrational and electronic properties of CrSBr. For samples spanning from few-layer to bulk thickness, we observe that the polarization of the A_g^2 Raman mode can be rotated by 90 degrees, shifting from alignment with the crystallographic *a* (intermediate magnetic) axis to the *b* (easy magnetic) axis, depending on the excitation energy. In contrast, the A_g^1 and A_g^3 modes consistently remain polarized along the *b* axis, regardless of the laser energy used. We access real and imaginary parts of the Raman tensor in our analysis, uncovering resonant electron-phonon coupling.

HL 40.3 Wed 16:00 H15

Resonant Inelastic Light Scattering on CrSBr — •Jan-Hendrik Larusch[1], Pierre-Maurice Piel[1], Nicolai-Leonid Bathen[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van der Waals material CrSBr is an optically active semiconductor and an air-stable 2D magnet with ferromagnetic (FM) ordering within each layer and antiferromagnetic (AFM) coupling between adjacent layers, alongside triaxial magnetic anisotropy. Additionally, CrSBr has a highly anisotropic electronic band structure, rendering it a quasi-one-dimensional electronic system, resulting in linearly polarized excitons that are strongly bound [1]. Distinct differences in excitonic emission signatures arise depending on the transition in magnetic ordering from AFM to FM states [2]. To study the coupling between excitons and collective excitations, we employ magnetic field-dependent resonant inelastic light scattering (RILS) experiments at temperatures well below the Néel temperature (~4K). While first-order phonon modes in Raman spectra remain mostly unaffected by magnetic ordering, RILS reveals resonantly enhanced as well as additional, magnetic field-dependent modes. The later are interpreted as spin-density excitations aka magnon modes. The combined PL and RILS study reveal strong interactions between electronic, excitonic, lattice and spin degrees of freedom. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023) [2] M.C. Heißenbüttel et al. (2024). arXiv:2403.20174.

HL 40.4 Wed 16:15 H15

Disentangling three anisotropic resistivities of the topological insulator α-Bi_4Br_4 — •Jonathan K. Hofmann[1,2], Serhii Kovalchuk[1,3], Yuqi Zhang[4,5,6], Vasily Cherepanov[1], Timofey Balashov[1], Zhiwei Wang[4,5,6], Yugui Yao[4,5,6], Irek Morawski[3], F. Stefan Tautz[1,2], Felix Lüpke[1,7], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Lehrstuhl für Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Institute of Experimental Physics, University of Wrocław, Poland — [4]Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement, Ministry of Education, School of Physics, Beijing Institute of Technology, China — [5]Beijing Key Lab of Nanophotonics and Ultrafine Optoelectronic Systems, Beijing Institute of Technology, China — [6]International Center for Quantum Materials, Beijing Institute of Technology, China — [7]II. Physikalisches Institut, Universität zu Köln, Germany

The higher-order topological insulator α-Bi_4Br_4 is a promising, highly anisotropic quasi one-dimensional van der Waals material. Using a four-tip scanning tunneling microscope, we combine four-point resistance measurements in the square geometry on a bulk sample of α-Bi_4Br_4 with four-point resistance measurements on thin flakes in a linear configuration to disentangle the anisotropic resistivity tensor at room temperature (RT) and at 77 K: At RT, the resistivity along the chain direction is 6.4 times smaller than the resistivity perpendicular to the chains. At 77 K, this anisotropy reduces to 5.0. The vertical anisotropies are ~ 1300 and ~ 6500, at RT and 77 K, respectively.

15 min. break

HL 40.5 Wed 16:45 H15

Spin Hall effect in van-der-Waals ferromagnet — •Tomoharu Ohta[1,2], Nan Jiang[3,4,5], Yasuhiro Niimi[3,4,5], Kohei Yamagami[6], Yoshinori Okadada[6], Yoshichika Otani[7,8], and Kouta Kondou[4,8] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Depertment of Physics, Osaka University, Osaka, Japan — [4]Institute for Open and Transdisciplinary Research Initiatives (OTRI), Osaka, Japan — [5]Center for Spintronics Research Network (CSRN), Osaka, Japan — [6]Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan — [7]Institute for Solid State Physics, The University of Tokyo Chiba, Japan — [8]RIKEN Center for Emergent Matter Science (CEMS), Saitama, Japan

We investigated the spin Hall effect (SHE) in a vdW ferromagnet Fe5GeTe2 (FGT) with a TC of 310 K utilizing the spin torque ferromagnetic resonance method. In synchronization with the emergence of the ferromagnetic phase resulting in the anomalous Hall effect (AHE), a noticeable enhancement in the SHE was observed below TC. On the other hand, the SHE shows a different temperature dependence from the AHE below 120 K: the effective spin Hall conductivity clearly enhanced below TC unlike the anomalous Hall conductivity, might be reflecting variation of band-structure accompanied by the complicated magnetic ordering of the FGT. The results provide a deep understanding of the SHE in magnetic materials to open a new route for novel functionalities in vdW materials-based spintronic devices.

HL 40.6 Wed 17:00 H15

Pseudo-magnetotransport simulations in strained graphene — •Alina Mrenca-Kolasinska[1] and Ming-Hao Liu[2] — [1]AGH University, Krakow, Poland — [2]National Cheng Kung University, Tainan, Taiwan

Graphene, a 2D material consisting of carbon atoms, despite its simple structure and composition can host intriguing phenomena. Application of inhomogeneous strain can lead to pseudomagnetic field (PMF), predicted to have opposite sign in the K and K 0 valley. Special strain profiles have been designed to generate uniform pseudomagnetic field in graphene [1, 2].

In this work we consider transport in pseudo magnetic field in these strain configurations. By deforming the sheet we can control the PMF, and design geometries which allow us to demonstrate interesting transport phenomena. These include electron focusing and snake states observed without external magnetic field present. For efficient modeling of quantum transport within these scenarios in large-scale systems close to realistic size devices, we extend the scalable tight-binding model [3] to accurately capture the effect of displacement field in the Hamiltonian. Our investigations open new possibilities for control over the valley degree of freedom.

[1] F. Guinea, et al., Phys. Rev. B 81, 035408 (2010).
[2] F. Guinea, M. I. Katsnelson, and A. K. Geim, Nat. Phys. 6, 30 (2010).
[3] M.-H. Liu, et al., Phys. Rev. Lett. 114, 036601 (2015).

HL 40.7 Wed 17:15 H15

Strong magnetic proximity effect in van der Waals heterostructures driven by direct hybridization — •Claudia Cardoso[1], Antonio T. Costa[2], Allan H. McDonald[3], and Joaquin Fernandez-Rossier[2] — [1]S3 Centre, Istituto Nanoscienze, CNR, Via Campi 213/a, 41125 Modena, Italy — [2]International Iberian Nanotechnology Laboratory, 4715-330 Braga, Portugal — [3]Physics Department, University of Texas at Austin, Austin, Texas 78712, USA

Proximity effects may induce an electronic property of a material, to an adjacent material in which that property is not present. Here we propose a class of magnetic proximity effects based on the spin-dependent hybridisation. We consider the hybridisation between the electronic states at the Fermi energy in a nonmagnetic conductor and the narrow spin-split bands of a ferromagnetic insulator.

Unlike conventional exchange proximity, this proximity effect has a strong impact on the nonmagnetic layer and can be further modulated by application of an electric field.

Using density functional theory calculations, we illustrate this effect in graphene placed next to a monolayer of CrI_3, a ferromagnetic insulator. The calculations show a strong hybridisation of the graphene bands with the narrow conduction band of CrI_3 in one spin channel only. Furthermore, the results confirm that the hybridisation strength can be modulated by an out-of-plane electric field, paving the way for applications.

HL 40.8 Wed 17:30 H15

Magnetotransport in heterostructures of MBE-grown BS/BSTS and graphene — •Marina Marocko[1], Matthias Kronseder[1], Tobias Rockinger[1], Takashi Taniguchi[2], Kenji Watanabe[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

A number of novel phenomena have been observed or predicted in heterostructures of topological insulators and graphene. Similar to transition metal dichalcogenides, topological insulators are expected to dramatically increase the intrinsically very low spin-orbit coupling (SOC) in graphene due to the proxim-

ity effect. This opens the way for a range of potential applications, including a spin transistor based on the spin-orbit valve effect.

In our recent experiments, we used a thin MBE-grown film of BS/BSTS topological insulator to induce SOC in graphene. This material has the advantage of adjustable stoichiometry and thus increased possibilities of band structure engineering. The SrTiO3 substrate used for the MBE growth of BS/BSTS also serves as a gate dielectric.

Magnetotransport measurements at 1.7K show a very distinct and narrow weak antilocalization peak around zero magnetic field, which is a sign of induced SOC in graphene. The fitting procedure yields approximate values of the Rashba and valley-Zeeman spin-orbit coupling. We discuss how the extracted SOC values compare with theoretical predictions.

HL 40.9 Wed 17:45 H15

Exploring the valley splitting and valley dynamics of WSe_2 proximity-exchange coupled to CrI_3 — •Natalie Kuhn[1], Marc Schütte[1], Jo Henri Bertram[1], Frank Volmer[1], K. Watanabe[2], T. Taniguchi[3], Christoph Stampfer[1,4], Lutz Waldecker[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Research Centre for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [4]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Proximity exchange coupling between 2D magnets and monolayers of transition metal dichalcogenides (TMDs) can lift valley degeneracy of the TMD. This is promising for the field valleytronics, as valley splitting is expected to increase valley lifetimes.

In this study, we investigate the proximity exchange coupling in van der Waals heterostructures made of monolayer WSe_2 and few-layer CrI_3, a 2D antiferromagnet. The proximity-induced valley splitting of WSe_2 is spatially probed by reflection contrast measurements of WSe_2 excitons. We observe distinctly different regions in WSe_2 identified by their reversed valley splitting. Their origin is explored by their magnetic field dependent reversals, i.e. hysteresis curves that are induced by reversing the magnetization of the interface layer of CrI_3. Using time-resolved Kerr rotation measurements we find a strong enhancement of WSe_2 valley lifetimes of the spin split valence bands.

HL 40.10 Wed 18:00 H15

Excitonic traps in freely suspended 2D membranes — •Alexander Musta[1,3], Leonard Geilen[1,3], Lukas Schleicher[2,3], Benedict Brouwer[1,3], Petricia Sara Peter[2,3], Anne Rodriguez[2,3], Eva Weig[2,3], and Alexander Holleitner[1,3] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Chair of Nano and Quantum Sensors, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

We present studies on the strain profile of large-area suspended transition-metal-dichalcogenides monolayers by photoluminescence measurements. Variations in the strain profile lead to band bending, which results in a redshift of the excitonic spectrum. Additionally, we observe an increase in intensity at the center of the suspended structures. We correlate the excitonic luminescence profiles with mechanical characterizations of the membranes, including AFM measurements and spatial mode mapping.

HL 40.11 Wed 18:15 H15

Rabi Splitting in Quantum Wells and TMDCs: Influence of Many-Particle Coulomb Correlations — •Henry Mittenzwey[1], Felix Schäfer[2], Markus Stein[2], Oliver Voigt[1], Lara Greten[1], Daniel Anders[2], Isabel Müller[2], Florian Dobener[2], Marzia Cuccu[3], Christian Fuchs[4], Kenji Watanabe[5], Takashi Taniguchi[5], Alexey Chernikov[3], Kerstin Volz[4], Sangam Chatterjee[2], and Andreas Knorr[1] — [1]ITP, Technische Universität Berlin, D-10623 — [2]LaMa, Justus-Liebig-University Giessen, D-35392 — [3]IAPP and ct.qmat, Technische Universität Dresden, D-01062 — [4]WZMW, Philipps-University Marburg, D-35032 — [5]NIMS, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan

In this joint theory-experiment collaboration, we study the Rabi splitting of excitons under simultaneous strong light-matter and Coulomb interaction on ultrafast timescales.

It turns out, that in a setting, where Coulomb and optical interaction are comparable (MQW), the Rabi splitting almost linearly follows the optical field amplitude similar to an ideal two-level system. On the other hand, in a setting with dominating Coulomb interaction ($MoSe_2$), the Rabi splitting depends sublinearly on the optical field strength and it significantly deviates from an ideal two-level system. Within the developed theoretical approach based on Heisenberg equations of motion and a correlation expansion of many-body interactions, we identify the origin of this sublinear trend due to six-particle exciton-to-biexciton transitions.

HL 40.12 Wed 18:30 H15

Inhomogeneous Broadening of Dark Rydberg Excitons in TMDC Monolayers Probed by Ultrafast Frequency-Resolved Autocorrelation Spectroscopy — •Katem Mitkong, Tom Jehle, Daniel C. Lünemann, Lukas Lackner, Juanmei Duan, Christian Schneider, and Christoph Lienau — Institute of Physics, Carl von Ossietzky University, Oldenburg, Germany

Monolayers of Transition Metal Dichalcogenides (TMDCs), as two-dimensional materials, exhibit unique optical properties influenced by their dielectric environment. The reduced dimensionality enhances the exciton binding energy, enabling the formation of Rydberg exciton series even at room temperature. In this study, broadband nonlinear Interferometric Frequency-Resolved Autocorrelation (IFRAC) spectroscopy with few-cycle time resolution is used to probe the optically dark 2p exciton state in WS2 monolayers. The result readily distinguishes coherent second harmonic generation (SHG) from incoherent two-photon photoluminescence emission (TPPLE) without requiring polarization control. We observe the 2p dark exciton state at 2.20 eV, with TPPLE linewidths that depend on excitation power. Comparison with Lindblad Master equation solutions shows significant inhomogeneous broadening of the 2p resonance, about three times greater than that of 1s excitons. This broadening, attributed to the extended spatial wavefunction of 2p excitons relative to 1s excitons, underscores their increased sensitivity to inhomogeneities such as local strain and dielectric fluctuations. This finding suggests potential applications in nanoscale sensing technologies.

HL 40.13 Wed 18:45 H15

Expanding the lithography toolbox - 2D devices and beyond — •Vasilis Theofylaktopoulos — Heidelberg Instruments Nano AG, Bändliweg 30, 8048 Zurich, Switzerland

Lithography is used in 2D devices to contact them with precisely placed electrodes, shape the building blocks or to control other properties such as doping or strain. Thermal scanning probe lithography is an up and coming method that can assist in all of the above.[1] In this talk the working principle of tSPL will be introduced and examples of its application will be given in the field of 2D electronics, photonics and metasurfaces.[2,3,4]

The NanoFrazor is a tSPL tool offering complimentary features to established lithography techniques such as photolithography, ebeam and focused ion beam. It uses a heated cantilever to write features with sizes bellow 15nm. At the same time grayscale patterning is possible with a resolution of 2nm. A reader is integrated at the tip allowing for parallel imaging to the patterning enabling markerless overlay. This simplifies the placement of features on 2D materials which are easily imaged under the resist. A laser can be used with the same resist stacks to create larger features >500nm such as contact pads. Finally, the process patterning the resist through sublimating it can yield devices with better electronics properties compared to ebeam.[5]

[1] S. T. Howell, A. Grushina, F. Holzner, and J. Brugger, Thermal scanning probe lithography - a review, Microsyst. Nanoeng., vol. 6, no. 1, p. 21, Apr. 2020, doi: 10.1038/s41378-019-0124-8.

[2] X. Liu et al., Thermomechanical Nanostraining of Two-Dimensional Materials, Nano Lett., vol. 20, no. 11, pp. 8250-8257, Nov. 2020, doi: 10.1021/acs.nanolett.0c03358.

[3] M. C. Giordano, G. Zambito, M. Gardella, and F. Buatier De Mongeot, Deterministic Thermal Sculpting of Large Scale 2D Semiconductor Nanocircuits, Adv. Mater. Interfaces, vol. 10, no. 5, p. 2201408, Feb. 2023, doi: 10.1002/admi.202201408.

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HL 41: Spin Phenomena in Semiconductors

Time: Wednesday 15:45–16:30 Location: H17

HL 41.1 Wed 15:45 H17

The charge cycle of the silicon vacancy in diamond — •Joshua Claes, Bart Partoens, and Dirk Lamoen — University of Antwerp, Antwerp, Belgium

Color centers in wide bandgap semiconductors are point defects with strongly localized electrons, resembling atom-like systems that can be optically controlled. These defects hold great promise for advancing quantum technologies, including quantum sensing and quantum computing. Among them, the silicon vacancy (SiV) center in diamond stands out as a particularly promising candidate due to its narrow optical emission and long spin coherence time, lasting up to 1 second at cryogenic temperatures in its neutral state.

A key challenge for the practical use of such defects is the precise measurement of their spin state. Photoelectric detection of magnetic resonance (PDMR) is a promising technique that measures the spin state by inducing charge state transitions and capturing the released electron or hole. In this work, we employ density functional theory with the HSE06 hybrid functional to calculate the onset energies and optical cross-sections for charge state transitions of the SiV center in diamond, ranging from -2 to 0.

Using this data, we model the PDMR experiment to predict charge transitions as a function of the laser frequency applied, providing insights into the defect's behavior under experimental conditions.

HL 41.2 Wed 16:00 H17

Carrier spin coherence in inas/inalgaas quantum dots emitting in the telecom range — •Vitalie Nedelea — Technische Universität Dortmund, Dortmund, Germany

This study focuses on the carrier spin coherence in quantum dots(QDs), which are promising candidates for entanglement with an emitted photon as well as entanglement of two remote spins induced by measuring of two indistinguishable photons. The Samples, grown by molecular beam epitaxy, consist of 5.5nm InAs monolayers separated by InAlGaAs barriers. A Si δ-doped layer, at a distance of 15 nm from the QD layer, provides resident electrons. Differential transmission reveals a double exponential decay behaviour, with a short exciton(X) decay time of 0.5ns and the long indirect molecular X decay time of 2ns. The dependence of the Larmor frequencies on the transversal magnetic field (BV) gives us information about the carrier g-factor, |ge|=1.88 for the electron and |gh|=0.6 for the hole. The hole spin dephasing saturates at a higher value of T2*=1.4ns than the electron T2*=0.6ns, which could be explained by the weaker hyperfine coupling of the hole. The decay of the FR signal as a function of fm gives TS=0.3μs and extrapolating the power dependence to zero gives the spin relaxation time T1=0.5μs. The wide spread of g-factors and long spin relaxation times are promising candidates for the spin mode locking (SML) effect. In the ensemble of QDs, the sum of the multiple oscillating signals with Larmor frequencies corresponding to ωR contributes to the SML. Measured dependence of the SML on the BV reveal that the signal is related to the hole spins.

HL 41.3 Wed 16:15 H17

Optically induced spin electromotive force in ferromagnetic-semiconductor quantum well structure — •Olga Ken[1,2], Igor Rozhansky[2], Ina Kalitukha[1,2], Grigory Dimitriev[2], Mikhail Dorokhin[3], Boris Zvonkov[3], Dmitri Arteev[2], Nikita Averkiev[2], and Vladimir Korenev[2] — [1]TU Dortmund, Dortmund, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Lobachevsky State University of Nizhny Novgorod, Russia

We study hybrid structures which consist of ferromagnetic (FM) layer and a semiconductor quantum well (QW) and present here a systematic approach combining the optical and electrical detection of the spin-dependent electron transfer with nanoscale spatial resolution. Spin-dependent transfer is manifested in three spectacular effects: PL circular polarization under unpolarized excitation, dependence of the PL intensity from the QW on the circular polarization degree of the excitation, and spin-dependent photo-voltage across the junction. We show that in GaMnAs/GaAs/InGaAs heterostructure all the three parameters demonstrates similar non-linear magnetic field dependences with hysteresis loop saturating in ~100 mT [1]. This indicates the interaction of charge carriers in the QW with the FM, i.e. the FM proximity effect [2].

[1] I.V. Rozhansky et al. Nano Letters 23, 3994 (2023).
[2] V. L. Korenev et al. Nature Commun. 3, 959 (2012).

HL 42: Quantum Dots and Wires: Optics I

Time: Wednesday 16:45–18:30 Location: H17

Invited Talk HL 42.1 Wed 16:45 H17

Quantum key distribution with single photons from quantum dots — Joscha Hanel[1], •Jingzhong Yang[1], Jipeng Wang[1], Vincent Rehlinger[1], Zenghui Jiang[1], Frederik Benthin[1], Tom Fandrich[1], Jialiang Wang[1], Fabian Klingmann[2], Raphael Joos[3], Stephanie Bauer[3], Sascha Kolatschek[3], Ali Hreibi[4], Eddy. Patrick Rugeramigabo[1], Michael Jetter[3], Simone. Luca Portalupi[3], Michael Zopf[1,5], Peter Michler[3], Stefan Kueck[4], and Fei Ding[1,5] — [1]Leibniz Universität Hannover, Hannover, Germany — [2]Fraunhofer-Institut für Photonische Mikrosysteme, Dresden, Germany — [3]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [5]Laboratorium für Nano-und Quantenengineering, Hannover, Germany

Quantum key distribution (QKD) ensures secure communication against eavesdroppers. On-demand quantum light sources, such as semiconductor quantum dots (QDs), enhance QKD security and loss tolerance due to their deterministic single-photon emission with high brightness and low multiphoton rates. Here, we demonstrate high-speed modulation of telecom C-band single photons emitted from a QD embedded in a circular Bragg grating. Using a phase-modulator in a Sagnac-loop interferometer, a 16-bit pseudo-random sequence is encoded into polarisation states in real time at a 76 MHz clock rate, achieving an ultra-low quantum bit error rate of ~1%.

HL 42.2 Wed 17:15 H17

Development and deterministic fabrication of electrically controlled quantum dot molecule bullseye resonators — •Setthanat Wijitpatima[1], Normen Auler[2], Binamra Shrestha[2], Sven Rodt[1], Arne Ludwig[3], Dirk Reuter[2], and Stephan Reitzenstein[1] — [1]Institute of Solid-State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Department of Physics, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

Quantum information can be encoded in the polarization states of photons as flying qubits and decoded in the spin states of solid-state systems as stationary qubits, providing robust platforms for quantum information processing. Quantum dot molecules (QDMs) are particularly promising for this purpose, as their singlet-triplet qubits are immune to spin dephasing, enabling temporally stable spin-photon interfaces. Toward real-world applications, QDM devices with high photon extraction efficiency (PEE) are required, motivating the integration of QDMs into nanophotonic structures, such as circular Bragg gratings (CBGs) which yield broadband enhancement of PEE and moderate Purcell enhancement. However, applying the CBG concept to QDMs has been challenging since precise electrical control is crucially needed to operate QDMs properly. In this work, we demonstrate the fabrication of QDM-CBG devices, providing a crucial step toward scalable and efficient quantum technologies.

HL 42.3 Wed 17:30 H17

Magnetic field dependence of the Auger recombination rate in a single quantum dot — •Nico Schwarz[1], Fabio Rimek[1], Hendrik Mannel[1], Marcel Zöllner[1], Britta Maib[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

In solid state physics, the quantum dot (QD) as a single photon emitter is an ideal system to study the Auger effect in a confined nanostructure. The Auger effect is an electron-electron scattering effect in which the energy of the electron-hole recombination is transferred to a third carrier, leading to a non- radiative recombination of, e.g., the trion [1]. This Auger recombination should be suppressed in high-photon-yield, low-dephasing single-photon emitters. We used two-color, time resolved resonance fluorescence spectroscopy with a high spectral resolution on a single quantum dot to differentiate between the differ- ent recombination paths: Auger, spin-flip and spin-flip Raman recombination [2]. We observe an unexpected behaviour of the Auger recombination rate, which shows a decrease from B = 0 to 2 T, followed by an increase to 4 T , before decreasing again by a factor of approx. three up to 8 T. These new findings may be the starting point for further theoretical and experimental studies to unterstand or even supress this scattering effect, in which the environment seems to play an important role. [1] P. Lochner et al., Nano Lett. **20**, 1631-1636 (2020). [2] H. Mannel et al., JAP **134**, 154304 (2023).

HL 42.4 Wed 17:45 H17

Studying the optical properties of AgInS2-based quanutm dots — •Yizhuo Xi, Julian Mann, Jochen Feldmann, and Sushant Ghimire — Chair for photonics and optoelectronics, Nano-institute Munich and department of physics, Ludwig-Maximilians-University, Königstr.10, 80539 Munich, Germany

I-III-VI quantum dots have attracted considerable interest for their non-toxic nature, tunable bandgap, and excellent stability. However, these quantum dots contain intrinsic sub-gap defects, which can act as donor-acceptor pairs. In this work, we synthesize AgInS2 quantum dots showing a dual emission spectrum. A narrow but weak free-exciton emission is observed near the band edge, while a broad and intense emission, associated with donor-acceptor-type defects, appears in the lower energy region. After coating the core particles with a gallium sulfide shell, the free-exciton luminescence is strongly improved, and the recombination at donor-acceptor pairs is suppressed. This demonstrates the successful elimination of defects in AgInS2/GaSx core/shell quantum dots, which is further evidenced in the absorption spectrum by the removal of a defect-related Urbach tail. In essence, we find that the donor-acceptor pair defects in these AgInS2 quantum dots are mainly located on the surface, and the excitonic character emerges upon their elimination through the growth of a gallium sulfide shell.

HL 42.5 Wed 18:00 H17

Deoxidization induced InAs(P) single photon emitter formation on InP substrate — •Yiteng Zhang[1], Xin Cao[1], Doaa Abdelbarey[1], Zenghui Jiang[1], Markus Etzkorn[2], Chenxi Ma[1], Tom Fandrich[1], Arijit Chakraborty[1], Tom Rakow[1], Eddy Rugeramigabo[1], Michael Zopf[1,3], and Fei Ding[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167, Hannover, Germany — [2]Technische Universität Braunschweig,LENA, Institut für Angewandte Physik, Universitätsplatz 2, 38106 Braunschweig — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167, Hannover, Germany

Efficient quantum light sources at telecom O-band and C-band are essential for long-haul quantum communication to minimize photon dispersion and loss. While semiconductor quantum dots (QDs) grown by Stranski-Krastanov and droplet epitaxy methods show promise, their reproducibility is hindered by complex growth parameters. Here, we present a straightforward method to fabricate self-assembled InAs(P) QDs emitting single photons at telecom O-band using molecular beam epitaxy. By deoxidizing and annealing InP(001) substrates in an arsenic atmosphere, QDs form naturally without additional metal deposition. Statistical analysis reveals size distribution and density comparable to QDs from conventional methods. Cryogenic photoluminescence confirms single-photon emission. This approach offers a reproducible and efficient pathway to telecom-wavelength single-photon sources, advancing quantum information technologies.

HL 42.6 Wed 18:15 H17

Excitonic structure of G center computed by unfolded tight-binding model — •Jakub Valdhans[1] and Petr Klenovský[1,2] — [1]Masaryk University, Brno, Czech Republic — [2]Czech Metrology Institute, Brno, Czech Republic

We have studied the carbon G center in bulk silicon and germanium using the empirical tight-binding (ETB) model for calculating unfolded band structures with configuration interaction (CI) correction for an exciton. The G center in B configuration (emissive) being a candidate for a telecom single photon source has two substitutional carbons and one interstitial atom embedded in the bulk for 6 possible configurations. Using advantage of low computation effort of ETB, it is possible to calculate and analyze behavior of electronic transitions with respect to a variation of bond distance between substitutional carbons and interstitial atom, and with using band offset as external tuning parameter.

HL 43: Twisted Materials / Systems (joint session TT/HL)

Time: Wednesday 17:00–18:30 Location: H31

See TT 39 for details of this session.

HL 44: Focus Session: Quantum Technologies in Deployed Systems I

Recent advancements in quantum cryptography, quantum computing, and quantum sensing are driving researchers to develop a universal quantum network*known as the quantum internet, which will enable secure connections among quantum computers, as well as to networks of quantum sensors, through quantum cryptography. Building a functional quantum internet is one of the most ambitious goals in quantum technology for the coming decades.

The focus sessoin aims to provide a comprehensive overview of the corresponding platforms and advances in quantum technologies, and is organized by Simone L. Portalupi (U. Stuttgart), Michal Vyvlecka (U. Stuttgart) and Michael Zopf (U. Hannover).

Time: Wednesday 18:00–18:45 Location: H13

HL 44.1 Wed 18:00 H13

Advancing Quantum Communication with Deterministic Quantum Light Sources from Laboratory- to Field-Experiments — •Mareike Lach, Koray Kaymazlar, Pratim Saha, Martin von Helversen, and Tobias Heindel — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

The advances in the field of non-classical light generation using solid-state quantum light sources fostered the exploration of applications in quantum communication and networking. This interdisciplinary field thereby increasingly evolves from laboratory-scale to field-experiments [1]. In this contribution we address the design, set-up and characterization of stand-alone compact modules for field-deployable quantum communication systems. In this context key components of the transmitter- and receiver-stations for quantum key distribution protocols are discussed, including mobile quntum light sources, fast qubit-state encoders, and qubit-state analyzers. Advancing the field-deployment of quantum technologies will foster both the progress in explorativ research projects as well as the transfer to their commercialization.

[1] D.A. Vajner et al., Advanced Quantum Technologies, doi:10.1002/qute.202100116 (2022)

HL 44.2 Wed 18:15 H13

Automated in situ optimization and disorder mitigation in a quantum device — •Jacob Benestad[1], Torbjørn Rasmussen[2,3], Bertram Brovang[2], Oswin Krause[4], Saeed Fallahi[5,6], Geoffrey C. Gardner[6], Michael J. Manfra[5,6,7,8], Charles M. Marcus[2], Jeroen Danon[1], Ferdinand Kuemmeth[2], Anasua Chatterjee[2,3], and Evert van Nieuwenburg[9] — [1]Department of Physics, Norwegian University of Science and Technology — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — [3]QuTech and Kavli Institute of Nanoscience, Delft University of Technology — [4]Department of Computer Science, University of Copenhagen — [5]Department of Physics and Astronomy, Purdue University — [6]Birck Nanotechnology Center, Purdue University — [7]Elmore Family School of Electrical and Computer Engineering, Purdue University — [8]School of Materials Engineering, Purdue University — [9]Lorentz Institute and Leiden Institute of Advanced Computer Science

We investigate automated in situ optimisation of a quantum point contact (QPC) device with 9 adjustable electrostatic gates atop the split-gate constriction, using the Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) with a metric for how "step-like" the conductance is when the channel is constricted. The optimization algorithm is first tested on tight-binding simulations to show how it could adapt to a disorder potential, followed by implementing it in an experiment to show a marked improvement in the quantization of device conductance.

HL 44.3 Wed 18:30 H13

Fast and high-fidelity composite gates in superconducting qubits: Beating the Fourier leakage limit — •Hristo Tonchev[1], Boyan Torosov[2], and Nikolay Vitanov[1] — [1]Center for Quantum Technologies, Department of Physics, Sofia University, James Bourchier 5 blvd., 1164 Sofia, Bulgaria — [2]Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko chaussée, 1784 Sofia, Bulgaria

We present a method for quantum control in superconducting transmon qubits, which overcomes the Fourier limit for the gate duration imposed by leakage to upper states. The technique utilizes composite pulses, which allow for the correction of various types of errors that naturally arise in a system. We use our approach to produce complete and partial population transfers between the qubit states, as well as two basic single-qubit quantum gates. Our simulations show a substantial reduction of the typical errors and gate durations. Three different independent verifications are made to justify these claims.

HL 45: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:00 Location: H13

HL 45.1 Thu 9:30 H13

Optical Simulations of Nanophotonic Back Contacts for Light Management in Ultrathin CIGSe Solar Cells — •Daniel Jiménez Tejero[1], Merve Demir[1], Bodo Fuhrmann[2], Roland Scheer[1], Ralf Wehrspohn[1], and Alexander Sprafke[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle (Saale) — [2]MLU, Interdisziplinäres Zentrum für Materialwissenschaften, Nanotechnikum Weinberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

The development of ultrathin-film Cu(In,Ga)Se_2 (CIGSe) solar cells aims to reduce material usage and expand applications such as bifacial or tandem solar cells. However, CIGSe absorber layers with thicknesses below 1 μm exhibit diminished light absorption, particularly for wavelengths near the bandgap, leading to decreased power conversion efficiency. This can be counteracted by utilising functional back contacts that effectively increase the optical path length within the absorber layer through scattering, reflection, and nanophotonic mechanisms.

This work employs nano-optical simulations to investigate the potential of SiO_2 nanostructures on a flat gold back contact for enhancing the performance of CIGSe solar cells. By solving the Maxwell equations using the finite element method, the quantum efficiency and photocurrent under ideal charge carrier collection conditions are computed, enabling a comparison of various nanostructure geometries viable for fabrication. We find photocurrents higher than those of conventional CIGSe solar cells with an absorber thickness of 4 μm, indicating the potential of our light management approach.

HL 45.2 Thu 9:45 H13

Stabilizing Perovskite Solar Cells by Organic Salts Under One Full Sun and Maximum Power Point Tracking — •Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Bashudev Bhandari[2,3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany

The use of organic halide salts to passivate metal halide perovskite (MHP) surfaces have been studied extensively. Passivating the surface defects of the MHP is of critical importance for realizing high-efficiency and stability of perovskite solar cells (PSCs). Here we discuss the success of a multifunctional organic salt used as passivation material for grain boundary defects and as molecular sealing layer in terms of stabilization. To assess the stability of PSCs, maximum power point tracking is seemingly the most realistic condition for the ageing test. Here, PSCs made from the four cation RbCsMAFA based perovskite absorber layer were aged under full light with maximum power point tracking and in addition they were tested periodically by IV-characterization, in order to yield all photovoltaic parameters for improved understanding of the ageing process.

HL 45.3 Thu 10:00 H13

Hyperuniform discordered structures for Light Management in Ultrathin CIGSe Solar Cells — •Katharina Trockel[1], Merve Demir[1], Frank Syrowatka[2], Ralf Wehrspohn[1], Roland Scheer[1], and Alexander Sprafke[1,2] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Interdisciplinary Center of Materials Science, 06120 Halle, Germany

Ultrathinfilm Cu(In,Ga)Se2 (CIGSe) solar cells are highly attractive due to their reduced material consumption and low manufacturing costs. While conventional CIGSe solar cells can achieve efficiencies of up to 21 %, increasing the efficiency of ultrathin solar cells remains a key research objective to enhance their competitiveness. A promising approach involves extending the optical path length in the absorber layer by integrating textured structures at the back or front contact of the solar cell. Most studies focus on periodic textures.

In this work, we investigate hyperuniform disordered (HuD) structures for light management in ultrathin CIGSe solar cells. The HuD structures are fabricated using polymethyl methacrylate (PMMA) particles deposited onto the back contact of the solar cells. These particles are covered with an indium tin oxide (ITO) layer and subsequently removed via a calcination process. The resulting ITO layer functions as a textured back contact, improving both light scattering and electrical performance.

First experimental results on the implementation of CIGSe solar cells with integrated HuD structures will be presented.

HL 45.4 Thu 10:15 H13

A Theoretical study of charge transport properties in perovskite analogues for high performance solar cells. — •Prerna Prerna[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Perovskite materials have emerged as promising candidates in solar cell technology, offering exceptional efficiency and affordability. Their remarkable performance, surpassing that of conventional inorganic materials, has placed them at the forefront of next-generation solar cell research, attracting significant attention from both academic and industry.

To harness their potential, we are investigating their charge transport properties using first-principles calculations (DFT) within the band transport regime. Our focus includes the calculation of carrier mobility, scattering rates and relaxation time through a detailed analysis of effective mass, deformation potential, and elastic properties. Our studies also incorporate the effects of structural deformations, aiming to align theoretical predictions with experimental results, providing deeper insights into the transport mechanisms in perovskites.

Furthermore, we are exploring the anisotropic nature of perovskites to understand directional dependencies in their electronic and mechanical properties. This anisotropy analysis is crucial for optimizing their performance and tailoring their application in advanced solar technologies. Together, these studies offer a comprehensive approach to enhancing the functionality of perovskites for cutting-edge solar energy solutions.

HL 45.5 Thu 10:30 H13

THz-Driven Phonon Fingerprints of Hidden Symmetry Breaking in 2D Layered Hybrid Perovskites — •Joanna M. Urban[1], Michael S. Spencer[1], Maximilian Frenzel[1], Gaëlle Trippé- Allard[2], Marie Cherasse[1,3], Charlotte Berrezueta Palacios[4], Olga Minakova[1], Luca Perfetti[3], Stephanie Reich[4], Martin Wolf[1], Emmanuelle Deleporte[2], and Sebastian F. Maehrlein[1,5,6] — [1]FHI Berlin — [2]LuMIn, Université Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS — [3]LSI, CEA/DRF/IRAMIS, CNRS, École Polytechnique, Institut Polytechnique de Paris — [4]FU Berlin — [5]HZDR — [6]TU Dresden

Metal halide perovskites (MHPs) are emerging as promising candidates for spintronic applications. In MHPs which lack inversion symmetry, strong spin-orbit coupling induces the Rashba-Dresselhaus effect, allowing spin current control. Here we use intense THz fields to coherently drive lattice dynamics in Ruddlesden-Popper 2D layered perovskites. We identify simultaneous IR and Raman activity of specific inorganic cage modes, suggesting the presence of inversion symmetry breaking despite the globally centrosymmetric crystal structure. By exploring the driving pathways of coherent phonons bearing the signatures of broken inversion symmetry, we lay the groundwork for simultaneous ultrafast control of optoelectronic and spintronic properties in 2D MHPs.

HL 45.6 Thu 10:45 H13

Analysis of real-space transport channels in halide perovskites — •Frederik Vonhoff[1], Maximilian J. Schilcher[1], David R. Reichman[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA

The charge carrier transport is a crucial factor for the performance of halide perovskites as solar energy conversion material. However, standard semiconductor transport theories fail to model the transport properties of halide perovskites because of their unusual transport behavior triggered by the anharmonic nuclear dynamics and its dynamic disorder [1]. For an accurate prediction of electron and hole mobilities of $MAPbI_3$ and $MAPbBr_3$, we capture the anharmonicity with molecular dynamics trajectories as a backbone for a time-dependent real-space hopping model [2,3] parametrized with hybrid density functional theory. With our transport model, we trace back the transport behavior of $MAPbI_3$ and $MAPbBr_3$ to their band structures via the projected density of states and the dynamics in the orbital occupation configurations. The real-space nature of our

model allows us to determine the microscopic transport mechanisms which are driven by three transport channels.

[1] M. J. Schilcher et al, ACS Energy Lett. 6, 2162 (2021)
[2] M. Z. Mayers et al, Nano Lett. 18, 8041 (2018)
[3] M. J. Schilcher et al, Phys. Rev. Mater. 7, L081601 (2023)

15 min. break

HL 45.7 Thu 11:15 H13

Unravelling how solvated PbI_2 Crystallites precede the Crystallization of Lead Halide Perovskites by UV/VIS In-Situ measurements — •Maximilian Spies[1], Simon Biberger[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth, Germany — [2]Dynamics and Structure Formation, University of Bayreuth, Bayreuth, Germany

The fabrication of reproducible, high-quality lead iodide perovskite films via solution-based methods requires a comprehensive understanding of crystallization dynamics. The formation of perovskite films is primarily dictated by the composition of the precursor solution and its processing conditions. In this study, we present an in-situ absorption study, i.e. during spin-coating, of the critical pre-nucleation stage to unravel the formation mechanisms of lead iodide perovskite films. We tracked the evolution of iodoplumbate complexes within the precursor solution and identified a distinctive absorption feature at 3.15 eV, emerging prior to film formation. We attribute this feature to the development of a crystalline PbI_2-DMF solvated (PDS) phase. In particular, we propose that PDS crystallites serve as precursors to the crystalline perovskite phase, acting as nucleation sites within the precursor solution. Notably, the amount of this PDS phase correlates closely with the concentration of the solution layer during spin coating, suggesting that increasing concentration promotes PDS formation. These findings provide valuable insights into the early stages of perovskite crystallization.

HL 45.8 Thu 11:30 H13

Effect of a 2D/3D Heterostructure on Contact Formation of the Double Perovskite $Cs_2AgBiBr_6$ with Hole Transport Layers Revealed by In-Situ KPFM Growth Studies — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of a 2D perovskite interlayer caused by surface modification with organic amines between the absorber and contact layers is widely known to significantly improve the performance of perovskite solar cells. This has already been approved as well for the lead-free double perovskite absorber $Cs_2AgBiBr_6$. To better understand the interaction of the contact layer with the 2D/3D heterostructure, in this work, film growth of Copper Phthalocyanine (CuPc), used as a model hole conductor, onto $Cs_2AgBiBr_6$ modified by different 2D phases was investigated and compared to bare $Cs_2AgBiBr_6$. Employing solar cell geometry, the morphology and work function were inspected intermittently to the evaporation of CuPc by Kelvin Probe Force Microscopy at different average film thickness. The energy alignment was revealed to be more confined on the 2D/3D heterostructures and the growth of CuPc was improved: a more homogenous growth led to formation of closed films even at early stages of deposition. These changes in growth and energy alignment are accompanied by preferential formation of different crystal phases in the CuPc.

HL 45.9 Thu 11:45 H13

The influence of oxygen and water on $MAPbI_3$ absorber materials measured with in-situ TRPL and PES — •P. Stötzner[1], M. Müller[1], T. Schulz[1], P. Pistor[2], R. Scheer[1], and S. Förster[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Universidad Pablo de Olavide Sevilla, Spain

Methylammonium lead halide perovskites ($MAPbI_3$) are promising thin-film solar cell absorber materials, but their response to environmental conditions like moisture and oxygen is not well understood. Here, we present a combined photoelectron spectroscopy (PES) and in-situ time-resolved photoluminescence (TRPL) study conducted in one ultrahigh vacuum system, which allows for studying changes in the chemical composition, the electronic structure and charge carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.

For $MAPbI_3$, we observe a significant reduction of the charge carrier lifetime compared to ex-situ TRPL measurements. To bridge between the different measurement environments, we conducted additional TRPL measurements in a closed cell having the as-grown sample in nitrogen atmosphere, which is pumped to high vacuum. These results show a decreased lifetime in vacuum but an increased lifetime linked to air contact. Consequently, we exposed $MAPbI_3$ samples to water vapor to mimic air contact, resulting in increased lifetime but also in a decomposition of $MAPbI_3$. Pure oxygen exposure did not affect the lifetime. Surprisingly, the simultaneous exposure to both gases did not show the detrimental effect of water.

HL 45.10 Thu 12:00 H13

On the Nature of Light Induced Defects in MAPI Thin Films: Long Pulses in TrPL — •Maxim Simmonds and Eva Unger — Kekuléstraße 5, 12489 Berlin, Germany

Metal-halide perovskite (MHP) semiconductors are highly relevant candidates for the fabrication of next generation solar cells but suffer from instability under continuous irradiation. This has been shown with a non-constant steady state PL during illumination. In order to better understand the evolution of recombination mechanisms at play, we usetime resolved photoluminescence (trPL) and differential lifetime plots.

Therefore, in this presentation, we will focus on methylammonium-lead-iodide (MAPI) thin films and the (ir)reversible introduction of traps triggered by quasi-continuous illumination. For this, we develop a method that uses long pulses of light in combination with trPL counting schemes, calling it long pulsed trPL (LP-trPL). From the method, we observe the inclusion of long lived and non-deep trapping sites due to continuous illumination. The data also suggests a highly asymmetric mechanism of trap formation, where trap annihilation is much slower than observed formation. We conclude that previously described mechanisms of iodine outgassing is compatible with the observed shallow nature of traps introduced as well as the asymmetric process of formation/annihilation.

HL 45.11 Thu 12:15 H13

Phase evolution of sequential evaporated (FA/Cs)SnI_3 halide perovskite thin films via in situ X-ray diffraction — •Pu-Chou Lin[1], Josha Damm[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Photovoltaics Group, Martin-Luther-University, 06120 Halle, Germany — [2]Departamento de Sistemas Físicas, Universidad Pablo de Olavide, 41013 Sevilla, Spain

Tin-based halide perovskites, particularly $FASnI_3$ and $CsSnI_3$, offer promising potential for photovoltaic applications. This study employs in situ X-ray diffraction to investigate these materials' real-time growth mechanisms and thermal stability during sequential vapor deposition and annealing. Our results demonstrate that the deposition sequence significantly impacts the resulting perovskite film quality. For $FASnI_3$, the SnI_2-FAI stack yields superior, cavity-free films compared to the FAI-SnI_2 stack. This suggests that FAI is the primary diffusing species, with $FASnI_3$ forming at interfaces and completing its formation around 160°C. In contrast, the $CsSnI_3$ system exhibits more complex behavior. The SnI_2-CsI sequence leads to the formation of the intermediate phase Cs_2SnI_6, while the CsI-SnI_2 sequence directly forms $CsSnI_3$ with minimal defect formation. This suggests that SnI_2 is the dominant diffusing species in the Cs-based system. $FASnI_3$ and $CsSnI_3$ undergo thermal degradation at 200°C and 240°C, respectively, through co-desorption of their constituent elements. These findings provide valuable insights into tin-based perovskites' growth mechanisms and thermal stability, which can guide future efforts to improve their performance and long-term stability.

HL 45.12 Thu 12:30 H13

Determining the key parameters of 3C-SiC photoelectrodes for water splitting application — •Marius Wasem[1,2], Sebastian Benz[1,3], Philip Klement[1,2], Joachim Sann[1,3], Jürgen Janek[1,3], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

We investigated the photoelectrochemical properties of n- and p-doped 3C-SiC thin films on n- or p-doped Si substrates, respectively, in a phosphate buffer solution. Key parameters such as the flat band potential and open-circuit potential were determined using various electrochemical methods. The combination of ultraviolet photoelectron spectroscopy and low energy inverse photoelectron spectroscopy measurements yields the estimation of the positions of the Fermi level, as well as the positions of the valence and conduction bands of the differently doped 3C-SiC thin films. Impedance spectroscopy characterized the interfacial processes in more detail. The flat band potential was derived from the space-charge layer capacitance using Mott-Schottky analysis. The determination of these key parameters enabled the construction of an energy level diagram, which explains the electrochemical behavior of n- and p-type 3C-SiC thin films under both dark conditions and illumination.

HL 45.13 Thu 12:45 H13

Circular Dichroism Engineering via Bismuth Doping and Cation Substitution in 2D Lead-Halide Perovskites — •Jan-Heinrich Littmann[1], Keito Mizukami[1,2], Henrik Spielvogel[1], Philip Klement[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Hybrid lead halide perovskites have garnered significant attention for their remarkable semiconductor properties. Their building blocks allows for tuneable features such as the crystal structure and the electronic bandgap. Introducing chiral cations into these materials endows them with chiroptical proper-

ties, such as circularly polarized luminescence (CPL) and spin-polarized charge transport, promising applications in optoelectronics and spintronics. However, the mechanism of chirality transfer remains poorly understood due to complex structure-property relationships. This study delves into the impact of heterovalent Bi^{3+} doping on the genuine circular dichroism (CD) of 2D lead iodide perovskites incorporating methylbenzylamine (MBA) and (pyridyl)ethylamine (PyEA) cations. Bi^{3+} doping, while preserving the band gap, significantly influences the genuine CD, suggesting a doping-dependent chirality transfer mechanism. Our findings provide valuable insights into the structure-property relationships in chiral perovskites and pave the way for the rational design of advanced chiroptical materials.

HL 46: Optical Properties

Time: Thursday 9:30–13:00 Location: H15

Invited Talk HL 46.1 Thu 9:30 H15

Exploring Auto-Oscillations in Semiconductor Electron-Nuclear Spin System — •Alex Greilich, Nataliia E. Kopteva, Vladimir L. Korenev, and Manfred Bayer — Experimentelle Physik 2a, TU Dortmund University, Dortmund, Germany

We demonstrate self-sustained auto-oscillations in a dissipative electron-nuclear spin system (ENSS) in semiconductors, where spontaneous breaking of translational symmetry in time produces robust limit-cycle dynamics across a broad range of parameters, including laser power, temperature, and magnetic field. These periodic oscillations exhibit coherence times extending to hours, reflecting ideal "time atom" ordering within the auto-oscillatory system.

Additionally, we uncover synchronization within excited subsystems without additional modulation, identifying its microscopic origins. Under periodic driving, modulation of parameters such as excitation power and pump polarization yields parametric resonances, signaling a transition to discrete auto-oscillatory behavior. Key phenomena include frequency entrainment, Arnold tongues, bifurcation jets, and a devil's staircase, showcasing the ENSS's versatility in exploring nonlinear dynamics, with broad implications for both fundamental physics and semiconductor applications.

HL 46.2 Thu 10:00 H15

Material selective Nonlinear Optics on Transition-metal Dichalcogenide - ZnO Nanowire Hybrid Structures — •Maximilian Tomoscheit, Benedikt Mathes, Edwin Eobalt, Alexander Zaunick, Carsten Ronning, and Giancarlo Soavi — Institute of Solid State Physics, Friedrich Schiller University Jena

The nonlinear optical (NLO) properties of any material are described by the complex tensor $\chi^{(n)}$, where, for each element of the tensor, the imaginary part mainly appears close to optical resonances. A direct measurement of the complex NLO suscebility is challenging because any NLO measurement is proportional to $|\chi^{(n)}|^2$. A second harmonic generation (SHG) interference measurement from two different materials with $\chi_\nu^{(2)}$ ($\nu = 1, 2$), is also proportional to $\left|\chi_1^{(2)}\right|\left|\chi_2^{(2)}\right|\cos\theta$, where θ is the phasemismatch. For a hybrid system with non overlapping resonances, if the SH photon energy is off-resonant for one material and resonant for the other, the interference term directly probes the complex NLO suscebility of the resonant material. In this work, we study SH interference in a transition-metal dichalcogenide (TMD) ZnO-nanowire (NW) hybrid structure, and we characterize the complex NLO suscebility of the TMD close to the A-exciton resonance. To be able to measure such interference, the ZnO NW needs to be placed along the armchair direction of the TMD, in our case WSe_2. Preliminary measurements and the results of SH polarization and wavelength dependent measurements will be be presented in this talk.

HL 46.3 Thu 10:15 H15

Nonempirical hybrid functional based on metaGGA — •Stefan Riemelmoser[1], Xun Xu[1,2], and Alfredo Pasquarello[1] — [1]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland — [2]Beijing Computational Science Research Center, Beijing, China

Semi-local density functionals such as PBE typically underestimate experimental band gaps by 50%. Hybrid functionals address this "band gap problem" by admixing a fraction of exact exchange to semi-local exchange. The optimal mixing parameter depends on the specific material and can be identified as the inverse dielectric constant. Recently, we have show that dielectric constants obtained using the r^{2}SCAN metaGGA functional are significantly more accurate than dielectric constants obtained using PBE. This can be understood through the improved treatment of electronic self-interaction within the metaGGA framework.

In this talk, we will show that a dielectric-dependent hybrid functional based on r^{2}SCAN can outperform the standard PBE based hybrid in terms of band gaps. Particularly impressive improvements are obtained for narrow gap semiconductors such as Ge and InAs, where PBE wrongly predicts a metallic phase, but r^{2}SCAN can open a gap. The hybrid functional based on r^{2}SCAN also yields accurate effective masses and ionization potentials. Finally, we showcase that our new hybrid functional is an excellent choice for semiconductor applications such as defect calculations.

HL 46.4 Thu 10:30 H15

Room-temperature polariton condensate in a two-dimensional hybrid perovskite — •M. Struve[1], C. Bennenhei[1], H. P. Adl[1], K. W. Song[2], H. Shan[1], N. Mathukhno[1], J. Drawner[1], F. Eilenberg[3], N. P. Jasti[4], D. Cahen[4], O. Kyriienko[2], C. Schneider[1], and M. Esmann[1] — [1]Institut for Physics, Carl von Ossietzky Universität Oldenburg — [2]University Exeter, United Kingdom — [3]Frauenhofer IOF, Jena — [4]Weizmann Instutute of Science, Israel

Chemically synthesized 2D halide perovskites form naturally grown quantum well stacks. Their large binding energy, tunable emission spectra and high oscillator strength makes them promising platforms for room temperature polaritonics but bosonic condensation and polariton lasing at ambient conditions are yet to be shown. In this work we demonstrate cavity exciton-polariton condensation of 2D Ruddelson-Popper iodine perovskites $(BA)_2(MA)_2Pb_3I_{10}$ crystal at room temperature [1]. A polariton condensation threshold of $P_{th}\approx$6.8 fJ with a strong non-linear response is observed. The emergence of spontaneous spatial coherence across the condensate with interferometric measurements is confirmed with a first-order autocorrelation reaching $g^{(1)}\approx$0.6. With our results we lay the foundation for a new class of 2D halide perovskite based room-temperature polariton lasers that offer great potential for hetero-integration with other van-der-Waals materials and combination with photonic crystals. [1] M.Struve et al., arXiv 2024, https://doi.org/10.48550/arXiv.2408.13677

HL 46.5 Thu 10:45 H15

Determination of optical losses at 265 nm in multimode AlGaN waveguides — •Verena Montag[1], Martin Guttmann[2], Bruno Marx[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs) like, e.g., biochemical sensing, solar-blind communication, and UV Raman spectroscopy require materials with a large bandgap energy to enable low optical losses. Currently, no ideal material has been identified that enables low loss waveguides and simultaneously the implementation of active and passive components in the UV spectral range. AlGaN is a promising material which is already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN, especially the absorption losses in AlGaN waveguides have not yet been studied in detail in the UVC spectral range. In this work, 200 μm wide AlGaN waveguides, UV-LEDs, and detectors were monolithically fabricated on AlN/sapphire wafers and the waveguide losses are determined. We were able to measure photocurrents > 1 nA using an integrated AlGaN-based photodiode. Also, an exponential decrease of the photocurrent with increasing waveguide length could be observed. However, Monte Carlo ray tracing simulations show that apart from absorption losses in the AlGaN waveguides also scattering losses from surface roughness have to be considered in order to fully explain the results.

15 min. break

Prize Talk HL 46.6 Thu 11:15 H15

Development and Application of Computational Simulations to Optimize Organic Photovoltaic Modules — •Annika Janssen — Technische Hochschule Nürnberg — Laureate of the Georg-Simon-Ohm-Prize 2025

Organic photovoltaics (OPV) is one of the emerging solar technologies and has the possibility of more cost-effective and sustainable production compared to conventional silicon cells. The printing technique considered in this thesis is doctor blade printing. In research, this is mainly used to produce OPV, as it is fast and the coating physics is similar to slot-die coating, the technique that is most commonly used for large-scale R2R printing. To produce large modules, a homogeneous coating is important, since the thickness of the layers has an influence on the efficiency of the device. In this work, the influence of the film thickness on the efficiency is investigated experimentally on cell level and the influence of layer thickness variations is studied by means of electrical finite element method (FEM) simulations for large-area modules. Formulas describing the behavior of the injected ink during printing are established. A special focus was put on the analysis of the non-accelerated and the accelerated printing. Using simulations, this work shows that a homogeneous coating achieved by ac-

celerating the doctor blade can improve the efficiency of organic solar modules by 16.22 %.

HL 46.7 Thu 11:45 H15

Ultraflat excitonic dispersion in single layer g-C3N4 — •Francesca Martini, Pietro Nicolò Brangi, Pier Luigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Single-layer graphitic carbon nitride (g-C3N4) is widely regarded as one of the most promising two-dimensional photocatalysts for hydrogen generation via water splitting. Despite its extensive study, limited information is available on its excitonic dispersion and velocity, critical parameters for achieving high charge mobility and efficient photogeneration. In this work, we employ many-body perturbation theory and the Bethe-Salpeter equation to provide a comprehensive description of the optical absorption and finite-momentum energy loss function for both s-triazine and tri-s-triazine structures. Our findings reveal the exciton dispersion and velocity, emphasizing the significant role of localized nitrogen lone pairs in producing remarkably flat excitonic bands with velocities that are two orders of magnitudes smaller than the typical one in two-dimensional materials and of the same order or smaller than the optical phonon frequencies in single layer g-C3N4. As the time-scale for inter-site exciton hopping is longer or similar to a phonon period, our results point to a highly non-conventional exciton propagation.

HL 46.8 Thu 12:00 H15

Investigation of PLD-grown β-CuI — •Aaron Giess, Lukas Trefflich, Gabrielle Benndorf, Marius Grundmann, and Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Copper iodide (CuI) is a transparent semiconductor that is currently of great interest due to its inherent p-type behavior and its high exciton binding energy of 62 meV. Typically, CuI crystallizes in the zincblende structure (γ-CuI) at room temperature. However, CuI can also crystallize in other phases, which are thermodynamically not stable at ambient pressure and temperature. One of these phases is the rhombohedral phase, which is often also called β-phase. Under certain growth conditions, this β-phase appears simultaneously with the γ-phase.

We grew closed thin films of CuI on c-sapphire, using pulsed laser deposition. The influence of the growth-parameters on the occurrence of β-CuI seems to be a multidimensional problem. The most important parameter is the film thickness, with thinner films favouring a higher fraction of the β-phase. The appearance of the β-phase causes additional features in the 2θ-ω scan in XRD, the dielectric function and the optical transmittance. Furthermore, photoluminescence spectra reveal a change of the emission spectra with time, which indicates that a photobleaching processes takes place.

HL 46.9 Thu 12:15 H15

Luminescent Microthermometers Based on ALD-encapsulated Ga_2O_3:Cr DBR Microcavities — •Ruben Neelissen[1], Daniel Carrasco[1,2], Anton Schäning[1], Marco Schowalter[1], Andreas Rosenauer[1], Emilio Nogales[2], Bianchi Mendez[2], Martin Eickhoff[1], and Manuel Alonso-Orts[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany. — [2]Departamento de Fisica de Materiales, Plaza Ciencias 1, Universidad Complutense de Madrid, 28040 Madrid, Spain.

The ability to measure temperature non-invasively, accurately and reliably is an ever reoccurring challenge in various fields such as micro- and nanosystems. Luminescent thermometry sensors can operate in environments where electronic counterparts are ineffective, thanks to their capability for remote sensing while being minimally intrusive.

Gallium oxide (β-Ga_2O_3) is a semiconductor with an ultra-wide bandgap of 4.8 eV and high resilience. Chromium-Ions (Cr^{3+}) in β-Ga_2O_3 result in two well-defined peaks, superimposed to a red-NIR emission, which can be utilized for temperature sensing.

In this work [1] it is demonstrated how confined light of β-Ga_2O_3:Cr microcavities (MCs) can be enhanced by encapsulating them in ALD-grown distributed Bragg reflectors (DBRs). With increasing temperature, the resonant wavelength redshifts due to changes in both the refractive index and the optical length of the MCs. A temperature accuracy of < 0.5 °C for temperatures above -80 °C is demonstrated.

[1] M. Alonso-Orts et al. In: *Advanced Materials Technologies* (2024), p. 2400881.

HL 46.10 Thu 12:30 H15

Theoretical and Experimental Study of Lead Tungstate (PWO-II) Crystal Properties for Electromagnetic Calorimetry — •Ather Ahmad[1], Pavel Orsich[1], Valera Dormenev[1], Hans-Georg Zaunick[1], Kai-Thomas Brinkmann[1], Simone Sanna[2], Martin Becker[3], and Limei Chen[3] — [1]II. Physikalisches Institut, Gießen, Germany — [2]Institut für Theoretische Physik, Gießen, Germany — [3]I. Physikalisches Institut, Gießen, Germany

Lead tungstate ($PbWO_4$ or PWO) is widely recognized as a high-performance scintillator for electromagnetic calorimeters due to its fast response, high density, and radiation hardness. PWO scintillator material is used in several experiments, such as CMS at the LHC (CERN), and the next-generation PWO-II crystals, which are doped to enhance their properties, have been optimized for the PANDA experiment at FAIR in Darmstadt.

To gain a deeper understanding of the material's performance, we have combined theoretical and experimental approaches to study the electronic and optical properties of PWO-II. Raman spectra and light transmission measurements were conducted on PWO-II samples and compared with results from density functional theory (DFT) calculations. In our models, we consider the crystal phases stable at room temperature, revealing characteristic differences in both Raman spectra and light transmission between these phases.

These combined efforts aim to refine the characterization of PWO-II and support the development of advanced calorimeter materials.

HL 46.11 Thu 12:45 H15

Rabi splitting mediated dual electromagnetically induced transparency in metamaterial — •Amit Haldar[1], Kshitij V Goyal[1], Ruturaj Puranik[2], Vivek Dwij[2], Shriganesh Prabhu[2], and Shovon Pal[1] — [1]NISER, HBNI, Jatni, India. — [2]TIFR, HBNI, Mumbai, India.

Electromagnetically Induced Transparency (EIT) and strong coupling are pivotal phenomena in light-matter interactions with profound implications for quantum and material sciences. EIT, resulting from destructive interference in three-level quantum systems, creates a transparency window within an absorption spectrum [1] and is classically emulated in metamaterials via bright-dark-mode interference. This enables applications such as slow-light devices, sensors, and cloaking technologies. Strong coupling, achieved when the interaction strength between a quantum emitter and an electromagnetic field surpasses system losses, leads to hybridized states (Rabi splitting), facilitating coherent energy exchange and insights into coupling mechanisms [2]. This study combines these phenomena using terahertz metamaterials to achieve tunable transitions between single and dual EIT states through strong coupling. This integration enhances the tunability of metamaterial-based devices and deepens our understanding of EIT and strong coupling, bridging classical and quantum perspectives for future applications.

[1] S. Y. Chiam *et al.*, *Phys. Rev. B* **80**, 153103 (2009).

[2] H. S. Kim *et al.*, *Nano Lett.* **20**, 6690 (2020).

HL 47: Focus Session: Quantum Technologies in Deployed Systems II

Recent advancements in quantum cryptography, quantum computing, and quantum sensing are driving researchers to develop a universal quantum network*known as the quantum internet, which will enable secure connections among quantum computers, as well as to networks of quantum sensors, through quantum cryptography. Building a functional quantum internet is one of the most ambitious goals in quantum technology for the coming decades.

The focus sessoin aims to provide a comprehensive overview of the corresponding platforms and advances in quantum technologies, and is organized by Simone L. Portalupi (U. Stuttgart), Michal Vyvlecka (U. Stuttgart) and Michael Zopf (U. Hannover).

Time: Thursday 9:30–12:30 Location: H17

Invited Talk HL 47.1 Thu 9:30 H17

Quantum-Dot Quantum Light Sources in Deployed Systems — •Peter Michler — Institute for Semiconductor Optics and Functional interfaces, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Stuttgart, Germany

Quantum photonic networks require sources of single, indistinguishable and entangled photon pairs with high brightness [1]. Semiconductor quantum dots (QDs) hold great promise to meet these requirements. In many foreseen implementations of quantum photonic networks, full- photonic quantum teleportation is a cornerstone, and the photons must be able to propagate over long

distances in silica fibers with limited absorption and wave packet dispersion. Photons in the so-called telecom bands will experience minimum absorption (C-band) and dispersion (O-band). Moreover, from a practicable point of view, portable rack single- and entangled photon sources are advantageous in deployed systems.

In this talk, we report on the performance of quantum-dot quantum light sources in deployed fibers [2], and demonstrate quantum teleportation with telecom photons from remote quantum emitters [3]. Moreover, QKD with entangled photons is demonstrated in deployed fibers and the performance of a QD based portable rack single- and entangled photon source, which can be operated down to 4 K, is presented.

References: [1] R. Joos et al., Nano Letters 24, 8626 (2024) [2] T. Strobel et al., Optica Quantum 2, 274 (2024) [3] T. Strobel et al., arXiv:2411.12904 (2024)

Invited Talk HL 47.2 Thu 10:00 H17

Field test of semiconductor quantum light sources — •Fei Ding — Leibniz University Hannover, Germany

Semiconductor quantum dots (QDs) are among the most promising quantum light sources, with the potential to revolutionize quantum communication research. For instance, utilizing on-demand single photons and entangled photons in quantum key distribution (QKD) protocols can significantly enhance security and increase the maximum tolerable loss. However, several critical challenges must be addressed to bridge the gap between laboratory experiments and long-distance field tests using QDs. In this talk, I will first review our work over the past years on QD-based single-photon and entangled-photon sources. Following that, I will present our recent field tests of single photon transmissions over a 79 km link between Hannover and Braunschweig, with 25.49 dB loss, equivalent to 130 km in direct-connected optical fiber.

Invited Talk HL 47.3 Thu 10:30 H17

Quantum dot based quantum communication in urban networks — •Rinaldo Trotta — Sapienza University of Rome, Italy

The last two decades have witnessed an impressive progress in the development of single and entangled photon sources based on quantum dots. It has now arrived the moment to explore their full potential in urban quantum-communication scenarios.

In this talk, I will first discuss how single and entangled photons generated by quantum dots can be used to implement advanced quantum communication protocols in a controlled laboratory environment. Then, I will show our efforts towards the construction of a hybrid quantum network, harnessing both fibre and free-space links, within the University campus in the centre of Rome. Finally, I will present field demonstrations of point-to-point entanglement-based quantum key distribution and three-node quantum teleportation with dissimilar quantum dots. A discussion on future challenges and perspectives will conclude the talk.

15 min. break

Invited Talk HL 47.4 Thu 11:15 H17

Quantum communication protocols over a 14-km urban fiber link — •Jürgen Eschner — Universität des Saarlandes, Experimentalphysik, 66123 Saarbrücken, Germany

Quantum communication over urban telecom fibers poses challenges such as environmentally induced polarization fluctuations and lossy splices. We report on the characterization and operation of a 14-km long fiber link across Saarbrücken for quantum communication. The dark fiber has underground and overground sections and ~ 9 dB attenuation. We stabilize its polarization with > 99% process fidelity up to 60 s. For implementing quantum communication protocols we employ a $^{40}Ca^{+}$ single-ion quantum memory, an ion-resonant entangled photon-pair source, and quantum frequency conversion.

We distribute photonic entanglement without significant fidelity degradation. Using heralded absorption of one photon of the entangled pair, we also demonstrate atom-to-photon quantum state teleportation over the fiber link with ~ 84% average fidelity [1].

In a laboratory experiment we also realize a quantum repeater cell based on two $^{40}Ca^{+}$ ions that are asynchronously entangled with their emitted photons. By entanglement swapping via a Mølmer-Sørensen quantum gate on the ions, which are located in the same trap, we generate photon-photon entanglement with ~ 76% average fidelity [2].

[1] S. Kucera et al., npj Quantum Information **10**, 88 (2024)
[2] M. Bergerhoff et al., Phys. Rev. A **110**, 032603 (2024)

HL 47.5 Thu 11:45 H17

Quantum cryptography at deployed communication networks with quantum dots at telecommunication wavelengths — •Anna Friederike Köhler[1], Tim Strobel[1], Michal Vyvlecka[1], Raphael Joos[1], Ilenia Neureuther[1], Timo Schnieber[1], Tobias Bauer[2], Marlon Schäfer[2], Nand Lal Sharma[3], Weijie Nie[3], Ghata Bhayani[3], Caspar Hopfmann[3], Simone Luca Portalupi[1], Christoph Becher[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Campus E2.6, 66123 Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Quantum cryptography leverages quantum effects to achieve unprecedented security. Quantum dot-based nonclassical light sources hold a promise for efficient cryptographic applications, offering on-demand generation of entangled photon pairs with high brightness and negligible multi-photon contribution. These features enable high-speed quantum communication while minimizing security risks. In this work, we demonstrate the BBM92 quantum key distribution protocoll using a GaAs quantum dot source to produce high-fidelity entangled photon pairs. Frequency conversion to telecommunication wavelengths is implemented to enhance transmission efficiency in a deployed intracity silica-based fiber network.

HL 47.6 Thu 12:00 H17

Experimental Quantum Strong Coin Flipping using a Deterministic Single-Photon Source — Daniel Vajner[1], •Koray Kaymazlar[1], Fenja Drauschke[2], Lucas Rickert[1], Martin von Helversen[1], Shulun Li[3], Zhichuan Niu[3], Anna Pappa[2,4], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technische Univeristät Berlin, Germany — [2]Electrical Engineering and Computer Science Department, Technische Univeristät Berlin, Germany — [3]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [4]Fraunhofer Institute for Open Communication Systems - FOKUS, Technical University Berlin, Germany

Strong coin flipping (SCF) is a fundamental cryptographic protocol allowing two distrustful parties to agree on randomly generated bit. In this work, we report the first implementation of a quantum strong coin flipping protocol that yields a quantum advantage compared to both its classical counterpart and an implementation using weak coherent pulses.

The quantum advantage is enabled by employing a state-of-the-art deterministic single-photon source based on a quantum dot embedded in a high-Purcell microcavity. Using a fiber-based electro-optic modulator (EOM) in single-pass configuration in combination with a self-built arbitrary waveform generator we realize fast dynamic, random polarization-state encoding at 80 MHz clock-rate.

Our QSCF implementation enables a coin flipping rate of 1.5 kHz and an average quantum bit error ratio (QBER) below 3%, sufficient to realize a quantum advantage.

HL 47.7 Thu 12:15 H17

Establishing a Quantum Local Area Network in Berlin City using Deterministic Quantum Light Sources — •Martin von Helversen[1], Lucas Rickert[1], Anne Rohwäder[1], Kinga Zolnacz[2], Koray Kaymazlar[1], Daniel Vajner[1], Anna Musial[3], Grzegorz Sek[3], Hanqing Liu[4], Zhichuan Niu[4], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technical University Berlin, Berlin, Germany — [2]Department of Optics and Photonics, Wroclaw University of Science and Technology, Wroclaw, Poland — [3]Department of Experimental Physics, Wroclaw University of Science and Technology, Wroclaw, Poland — [4]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China

Applications of quantum information enabled by solid-state quantum light sources currently witness the transition from laboratory proof-of-concept to field-experiments. In this contribution we present our recent progress in establishing a quantum local area network at the Campus Charlottenburg of TU Berlin. We show results of an actively stabilized free-space optical link with an effective length of 400 m and an end-to-end transmission of >70%. In addition, we operate a fiber-link between two buildings consisting of 6x 650 m of dark optical fiber. Moreover, we discuss the deployment of mobile deterministic single-photon sources based on compact cryocoolers and fiber-pigtailed quantum dot microcavities [FC-CBG] and evaluate the suitability for implementations of different types of cryptographic primitives. [1] Rickert, Lucas, et al., arXiv:2409.08982 (2024) [2] Rickert, Lucas, et al., arXiv:2408.02543 (2024).

HL 48: Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)

Superconducting monolayer transition metal dichalcogenides (TMDs) like $NbSe_2$, TaS_2, and gated WSe_2 or MoS_2, have attracted lot of interest in recent years. On the one hand Ising spin-orbit coupling pins the electron's spin out of plane, and hence is responsible for critical in-plane magnetic fields by far exceeding the Pauli limit. On the other hand, while the underlying pairing mechanism is still under debate, recent experiments provide strong evidence for its unconventional, multiband, nature. The Focus Session will feature experimental and theoretical advances on the superconductivity in monolayer TMDs, with focus on universal features, a possible Luttinger-Kohn mechanism, a nodal or even chiral nature of the gap functions, and their phase diagram.
Organizers: Milena Grifoni (Universität Regensburg), Julian Siegl (Universität Regensburg)

Time: Thursday 9:30–12:45 Location: H36

See TT 44 for details of this session.

HL 49: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

See O 83 for details of this session.

HL 50: 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Thursday 15:00–17:45 Location: H6

See O 88 for details of this session.

HL 51: Transport Properties (joint session HL/TT)

Time: Thursday 15:00–17:15 Location: H13

HL 51.1 Thu 15:00 H13

Quasi-Ballistic Transport in Phase-Pure GaAs/InAs Core/Shell Nanowires — •Farah Basarić[1,2], Vladan Brajović[1,2], Gerrit Behner[1,2], Kristof Moors[1], William Schaarman[1], Raghavendra Juluri[3], Ana M. Sanchez[3], Hans Lüth[1,2], Detlev Grützmacher[1,2], Alexander Pawlis[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Core/shell GaAs/InAs nanowires represent tubular conductors due to their insulating core and confined conducting states in the InAs shell. We investigate nanowires with a crystalline phase purity of the InAs shell, where reduced scattering in electronic transport is expected. Low-temperature gate-dependent transport measurements give us insight into different contributions to the oscillatory behavior in the magnetoconductance, as well as the possibility to probe non-local transport phenomena due to large phase coherence length. With temperature-dependent measurements, we resolved the quasi-ballistic transport regime, and estimate the phase coherence length. Both measurements indicate superior transport properties of phase-pure GaAs/InAs nanowires in contrast to previous reports on non-phase pure nanowires. Our findings are an important optimization step for further development of nanowire-based hybrid devices.

HL 51.2 Thu 15:15 H13

Influence of defects and shape of thin InAs nanowires on their thermal conductivity, assessed via machine-learning potentials — •Sandro Wieser[1], Yu-Jie Cen[1], Georg K. H. Madsen[1], and Jesús Carrete[2] — [1]Institute of Materials Chemistry, TU Wien, Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Nanowires (NWs) grown from the zincblende (ZB) phase of InAs in the (111) direction commonly contain twin boundary defects consisting of narrow wurtzite (WZ) (001) phase regions between ZB sections. To investigate the impact of these and other defects on heat transport, we employ Green-Kubo equilibrium molecular dynamics simulations utilizing cepstral analysis to efficiently process the noise, and an accurate MACE model trained via active learning strategies to achieve transferability for a wide range of surface conditions.

We show that these twin boundaries reduce the thermal conductivity with respect to that of defect-free WZ-phase (001) NWs by a factor of more than two and that surface conditions lead to lower thermal conductivity values for defect-free ultrathin InAs ZB NWs. Analysis of the shape of twinning NWs reveals that structures mimicking experimentally measured surface configurations can enhance heat transport compared to strictly hexagonal NWs. Additional insights are gained from an analysis of line-group symmetries and vibrational properties for various NW shapes. Furthermore, experimentally motivated symmetric and symmetry-breaking surface defects are studied to reveal more and less influential defect sites.

HL 51.3 Thu 15:30 H13

Ab-initio heat transport in defect-laden quasi-1D systems from a symmetry-adapted perspective — •Yujie Cen[1], Sandro Wieser[1], Georg Kent Hellerup Madsen[1], and Jesús Carrete Montaña[2] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Due to their aspect ratio and wide range of thermal conductivities, nanotubes hold significant promise as heat-management nanocomponents. However, one major limitation preventing their widespread use is the typically high thermal resistance that arises from defects or contact with other materials. An intriguing question is the role that structural symmetry plays in thermal transport through those defect-laden sections. However, the ab-initio study of lattice thermal transport is hindered by factors such as the large number of atoms involved and the artifacts introduced by formalism designed for 3D systems.

We employ an Allegro-based machine learning potential to calculate the force constants and phonons of single and multi-layer MoS_2-WS_2 nanotube with near-DFT accuracy and efficient scaling. Subsequently, we combine representation theory with the mode-resolved Green's function method to calculate detailed phonon transmission profiles across defects, and connect the transmission probability of each mode to structural symmetry. while more drastic symmetry breakdowns might be expected to increase scattering and thermal resistance, our results show they actually reduce it by the suppression of selection rules and opening more phonon transmission channels.

HL 51.4 Thu 15:45 H13

Analysis of the electrical transport properties of MBE grown cubic Galliumnitride (c-GaN) sample structures — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor system for 'more-than-Moore' applications such as high-power electronics or optoelectronic devices. The analysis of its electri-

cal transport properties is challenging since the molecular beam epitaxy (MBE) growth of high-quality c-GaN thin films requires a complex substrate architecture in order to accommodate the lattice mismatch between c-GaN and the 3C-SiC template. However, a reliable characterization of the electrical transport properties of c-GaN is crucial for the design of advanced functional devices. Here we analyze the electrical transport properties of the whole sample structure (MBE grown c-GaN/c-AlN thin films onto a 3C-SiC/Si template) with different c-GaN thicknessses using electrochemical impedance spectroscopy (EIS) as well as angle- and temperature-dependent magnetoresistance (MR) measurements. MR measurements reveal the existence of a highly conductive channel while EIS measurements allow the determination of the position of the channel between the c-AlN thin film and the 3C-SiC layer.

15 min. break

HL 51.5 Thu 16:15 H13

Fabrication and Characterisation of Short-channel Junctionless Nanowire Transistors — •Alessandro Puddu — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The downscaling limitations of conventional planar transistors require the investigation of alternative device configurations. Because of their excellent electrostatic control and intrinsic scalability, junctionless nanowire transistors (JNTs) present a feasible solution and are highly desirable for next-generation electronics. The key factor that characterizes the JNTs is the absence of pn-junctions. This provides several benefits, such as an easier fabrication process since the devices do not require abrupt doping profiles within the nanowire channel, which is now uniformly doped.

This work focuses on the fabrication and characterisation of short-channel Si JNTs. A top-down approach based on e-beam lithography (EBL) and inductively coupled plasma reactive ion etching (ICP-RIE) was used to fabricate the Si nanowires. The device characterisation showed improved performances due to the channel length shrinking.

HL 51.6 Thu 16:30 H13

***Ab initio* investigation of drag effect in germanium** — •Dwaipayan Paul and Nakib Protik — Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany

In a system of interacting electrons and phonons, the transport of one induces transport in the other. This phenomenon is known as the electron-phonon drag effect [1]. Now, an important milestone in the history of drag physics is the first recorded measurement of this phenomenon in germanium [2]. Here we present the results of our *ab initio* computations of the thermoelectric transport coefficients of germanium for various temperatures and charge carrier concentrations using the `elphbolt` code [3]. We investigate how the various scattering channels in the system enable this material to exhibit strong drag phenomena.

[1] Gurevich, Yu G., and O. L. Mashkevich. "The electron-phonon drag and transport phenomena in semiconductors." Physics Reports 181.6 (1989): 327-394.

[2] Frederikse, H. P. R. "Thermoelectric power of germanium below room temperature." Physical Review 92.2 (1953): 248.

[3] Protik, Nakib H., et al. "The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations." npj Computational Materials 8.1 (2022): 28.

HL 51.7 Thu 16:45 H13

Anomalous Knudsen effect signaling long-lived modes in 2D electron gases — •Grigorii Starkov and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

Careful analysis of electron collisions in two spatial dimensions leads to the conclusion, that the odd harmonics of the electron distribution function decay much slower in comparison to the even ones at finite temperatures. Focusing on a channel geometry with boundary scattering, we show, that such behaviour of the odd decay rates leads to a characteristic behaviour of the resistance that we dub anomalous Knudsen effect: increasing temperature leads to decreasing resistance, that quickly slows down and turns into growth. The further increase of temperature exhibits the usual Gurzhi peak in the resistance related to the crossover from ballistic to hydrodynamic transport. The simultaneous observation of the Gurzhi peak preceded by an anomalous Knudsen dip can serve as a concrete signature of the long-lived modes in the 2D electron transport at low temperatures.

HL 51.8 Thu 17:00 H13

Quantum confinement and stoichiometry fluctuations in nm-thin SiGe layers — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

We simulate biaxially strained SiGe layers of varying thickness in the range of a few nanometers, as found in the base layer of heterojunction bipolar transistors (HBTs). At this length scale, local fluctuations in atomic concentrations can strongly influence the electronic properties of the device, especially the distribution of dopants like e.g. boron. Even at high doping concentrations, only a single atom is present at a 1 nm^2 cross section of the layer on average.

Employing a new parameterization of silicon and germanium in the framework of extended Hückel theory (EHT), we calculate the local band gap for different permutations of the atomic structure. Various distributions of boron atoms are simulated. We study the impact of locally increased and decreased concentrations on the band gap. By varying layer thickness, we evaluate the effects of quantum confinement and how it impacts transport properties of the thin layer in contrast to bulk material.

HL 52: Oxide Semiconductors II

Time: Thursday 15:00–17:15 Location: H14

HL 52.1 Thu 15:00 H14

Connection between electronic structure and crystal symme- try in bismuth vanadate — •Philip Schwinghammer, Franziska Hegner, Frederico Delgado, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The electronic and structural properties of bismuth vanadate (BVO) were characterized using density functional theory (DFT). Previous work in the literature indicated that semi-local exchange was incapable of correctly reproducing the ground-state structure of BVO, but disagreed on which functional would improve the description. We found that the Heyd-Scuseria-Ernzerhof hybrid functional could accurately predict the monoclinic ground state structure, provided spin-orbit coupling was included. Semi-local density functionals mischaracterize the hybridization of the lone pair Bi6s states and O2p states near the valence band edge, which is corrected by hybrid functionals. Due to the large mass of bismuth, spin-orbit coupling is required for an accurate description of the electronic structure. When both corrections are taken into account, we find that the valence and conduction band edges in BVO are extremely flat, leading to large effective masses along one direction in reciprocal space. The effective carrier masses are affected by the ionic structure, indicating a possible reason for the different photo-catalytic efficiencies of tetragonal and monoclinic scheelite BVO.

HL 52.2 Thu 15:15 H14

Blue shift of the absorption onset and bandgap bowing in rutile $Ge_xSn_{1-x}O_2$ — •Elias Kluth[1], Yo Nagashima[2], Shohei Osawa[3], Yasushi Hirose[3], Jürgen Bläsing[1], André Strittmatter[1], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, 113-0033, Japan — [3]Department of Chemistry, Tokyo Metropolitan University, 1-1 Minamiosawa Hachioji, Tokyo 192-0397, Japan

Rutile-GeO_2 has recently attracted increasing research interest as an ultra wide bandgap oxide similar to Ga_2O_3 with the unique advantage that theoretical calculations predict the possibility of ambipolar doping. In contrast rutile-SnO_2 is a well-established transparent conductive oxide (TCO) widely used in solar cells and displays. Alloying SnO_2 with Ge offers a promising pathway to developing deep ultraviolet (DUV) TCOs. However, investigations into the optical properties of the $Ge_xSn_{1-x}O_2$ system remain limited.

In this study, we employed spectroscopic ellipsometry in the visible and ultraviolet region to determine the ordinary dielectric functions of $Ge_xSn_{1-x}O_2$ thin films grown by pulsed laser deposition (PLD) on rutile-TiO_2 substrates. Our analysis reveals a systematic blue shift of the onset of absorption with increasing Ge content. By evaluating the dielectric functions, we extracted the characteristic transition energies at the absorption onset and determined the bowing parameter of the dipole-allowed direct bandgap to be $b = 0.70$ eV.

HL 52.3 Thu 15:30 H14

$NaNbO_3$, $KNbO_3$, and their solid solutions: A *first-principles* and special quasirandom structures investigation — •Daniel Fritsch — Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany — University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

Ferroelectric materials crystallising in the perovskite structure, like $NaNbO_3$ and $KNbO_3$, have come into focus as lead-free and environmentally friendly alternatives to the widely used piezoelectric ceramic $Pb[Zr_xTi_{1-x}]O_3$ (PZT) [1].

They both exhibit a large range of structural phase transitions and accompanying changes in their ferroelectric behaviour. While the material properties of both end members are relatively well known, this is much less the case for their solid solutions.

Here, we present results for $Na_{1-x}K_xNbO_3$ solid solutions based on *first-principles* calculations for the structural and electronic properties, and so-called special quasirandom structures to investigate the solid solutions [2]. The obtained results will be compared to available experimental findings and other theoretical investigations.

[1] D. Fritsch, Adv. Mater. Sci. Eng. **2018**, 6416057 (2018).
[2] D. Fritsch, Appl. Sci. **12**, 2576 (2022), J. Phys. Condens. Matter **36**, 375702 (2024).

HL 52.4 Thu 15:45 H14

Spintronic properties of the two-dimensional electron gas in KTaO3-based heterostructures. — •Sonali Kakkar[1] and Chandan Bera[2] — [1]Department of Physics, Noida Institute of Engineering and Technology, 19, Institutional Area, Knowledge Park II, Greater Noida, Uttar Pradesh 201306, India — [2]Institute of Nano Science and Technology, Sector-81, Knowledge City, Sahibzada Ajit Singh Nagar, Punjab, 140306, India

A two-dimensional electron gas (2DEG) in oxide interfaces offers a single platform for a wide range of functionalities. Compared to STO-based 3d-2DEG, 2DEG in the polar perovskite oxide KTaO3 (KTO) with 5d-t2g orbitals shows a greater atomic spin-orbit coupling. Moreover, the electronic and spintronic properties of oxide heterostructures are greatly influenced by the inherent crystal structure symmetry. In this work, we have investigated the electronic and spintronic properties in KTO-based heterostructures using density functional theory calculations with the Hubbard parameter (DFT+U). The dependence of the Rashba spin-splitting and the corresponding spin texture in the reciprocal space for 2DEG at the KTO surface and LVO/KTO interface on the crystal orientation highlights the importance of crystal symmetry for the 5d-2DEG in KTO [1]. Furthermore, highly confined, spin-polarized 2DEG at the interfacial TaO2 layer in the 5dxy orbitals of Ta at the interface between the ferromagnetic insulator EuO and the non-magnetic KTO shows Rashba spin texture [2]. [1] S. Kakkar, et al., Physica E Low Dimens. Syst. Nanostruct. 144, 115394 (2022). [2] S. Kakkar, et al., Adv. Phys. Res. 2, 2200026 (2023).

15 min. break

HL 52.5 Thu 16:15 H14

Unraveling the mechanism of resistive switching in titanate-based perovskites — Wahib Aggoune[1,2], •Parrydeep Kaur Sachdeva[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany — [2]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Memristors capable of switching between high and low resistance states while retaining memory, hold promise for non-volatile memory. A recent fascinating experimental work observed high resistive switching (RS) in *off*-stoichiometric paraelectric titanate-based perovskites $ATiO_3$ (A=Sr, Ca) [1]. It suggests that RS is driven by defects, though their exact role remains unclear. Here, we investigate the defects behavior using density functional theory. Under the experimental growth conditions, the complex defect (Ti-interstitial with *A*-vacancies) is thermodynamically stable, pinning the Fermi level close the conduction band. Remarkably, the *off*-center shift of the interstitial atom induces a local polarization and gives rise to localized mid-gap states. Switching between the equivalent *off*-center sites faces energy barriers of 0.1–0.8 eV, depending on the pathway. This switches both polarization direction and the defect charge distribution. Therefore, upon applying a voltage, the overall polarization driven by the local shifts of the defects can be switched. As this also redistributes the defect charge states, it switches the resistance state. Our findings provide insights into the origin of RS toward memristor development.

[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 52.6 Thu 16:30 H14

Ultraviolet Emission from $^6P_{7/2}$ Stark Manifold in Gd-Implanted β-Ga_2O_3 Thin Films — •Martin S. Williams[1,2], Mahmoud Elhajhasan[1], Marco Schowalter[1], Lewis Penman[3], Alexander Karg[1], Fabien C.-P. Massabuau[3], Andreas Rosenauer[1], Gordon Callsen[1], Carsten Ronning[4], Martin Eickhoff[1,2], and Manuel Alonso-Orts[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany — [3]Department of Physics, SUPA, University of Strathclyde, Glasgow, United Kingdom — [4]Institute of Solid State Physics, Friedrich-Schiller-University Jena, Helmholtzweg 3, 07743 Jena, Germany

Monoclinic gallium oxide (β-Ga_2O_3) is a promising ultra-wide band gap semiconductor for the next generation of optoelectronic devices. Despite its attractive material properties, its luminescence spectrum is dominated by defect emission in the visible spectral range and a dominating UV emission in β-Ga_2O_3 has rarely been observed. An enhancement of the UV emission in β-Ga_2O_3 by optically active ion doping in β-Ga_2O_3 is only achieved with gadolinium (Gd^{3+}).

In this work, β-Ga_2O_3 thin films grown by molecular beam epitaxy and atomic layer deposition are implanted with Gd and thermally activated. Four separate luminescence peaks, from the Stark-split $^6P_{7/2} \rightarrow {}^8S_{7/2}$ transition in Gd^{3+}, are individually resolved with linewidth ≤ 2 meV. The influence of growth technique, implantation parameters and annealing temperature is investigated.

HL 52.7 Thu 16:45 H14

Investigation of the bond length dependence and lattice relaxation in zincblende Cu(Br,I) alloys — •Sandra Montag[1], Stefan Merker[2], Michael Bar[1], Richard J. Schenk[1], Eva Zollner[1], Konrad Ritter[1], Timo Pfeiffelmann[1], Sergiu Levcenko[1], Edmund Welter[3], Holger von Wenckstern[1], Marius Grundmann[1], Harald Krautscheid[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

CuI is a promising p-type wide-bandgap semiconductor with various applications in the field of transparent electronics. Among the numerous doping and alloying candidates, the Cu(Br,I) alloy system offers the opportunity to tailor the free hole concentration in functional layers, enabling optimized performance of active devices, such as pn-diodes and transistors. Using X-ray absorption spectroscopy, the fine structure of $CuBr_{1-x}I_x$ powder and thin film samples, with anion composition x varying from 0 to 1, was measured. The analysis of the extended fine structure reveals a nonlinear change of the Cu-Br and Cu-I bond lengths with composition x. This behaviour is different from that reported for III-V and II-VI zincblende alloys, but comparable to the rocksalt $RbBr_{1-x}I_x$ alloy. The observed bond length bowing may therefore be a characteristic feature of group I-VII alloys. To uncover the degree of lattice relaxation with increasing distance from the absorbing atom, the higher neigbour scattering signal is evaluated.

HL 52.8 Thu 17:00 H14

Revealing the incorporation site and local structure of Ni and Se in doped CuI thin films — •Mustafa G. Yazlak[1], Christiane Dethloff[1], Philipp Storm[1], Michael Lorenz[1], Sandra Montag[1], Hans H. Falk[1], Edmund Welter[2], Sofie Vogt[1], Marius Grundmann[1], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

This study investigates polycrystalline CuI thin films with varying nickel (Ni) and selenium (Se) concentrations, grown on glass substrates using Pulsed Laser Deposition (PLD) and co-sputtering. CuI:Ni thin films, with 1*30 at% Ni and thicknesses between 0.1*1.0 μm, and CuI:Se thin films, with 0.4*3.8 at% Se and ~1.0 μm thickness, were prepared and capped with Al_2O_3 layers to prevent oxidation. X-ray Absorption Spectroscopy (XAS) at low temperatures (~10 K) was conducted at the Cu, Se, and Ni K-edges to study the local structure of Ni and Se in the CuI matrix. The near edge structure and extended fine structure for a pure CuI thin film at the Cu K-edge suggests possible Cu oxidation. For CuI:Ni thin films, an increase in Ni concentration correlates with reduced Cu oxidation because Ni prefers to bond with oxygen rather than iodine, forming disordered NiO as seen from the Ni K-edge spectra. For CuI:Se thin films, the Cu K-edge spectra show small changes but no clear trend with Se content and the Se K-edge spectra indicate a Cu neighborhood similar to Cu_2Se and CuSe. Quantitative analyses are in progress to provide a deeper understanding of how Ni and Se content affects local structural changes.

HL 53: 2D Semiconductors and van der Waals Heterostructures V

The session covers excitonic properties of 2D semiconductors and van der Waals heterostructures.

Time: Thursday 15:00–17:15 Location: H15

HL 53.1 Thu 15:00 H15

1D exciton confinement in monolayer $MoSe_2$ near ferroelectric domain walls in periodically poled $LiNBo_3$ — •Pedro Soubelet, Yao Tong, Asier Astaburuaga Hernandez, Andreas V. Stier, and Jonathan J. Finley — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Monolayer transition metal dichalcogenides are an emergent platform for exploring and engineering quantum phenomena in condensed matter. Due to their atomic thickness, the excitonic response is highly influenced by the dielectric environment. In this work, we explore the optical properties and exciton kinetics of monolayer thick $MoSe_2$ straddling domain wall boundaries in ferroelectric periodically poled $LiNbO_3$ (PPLN). Spatially resolved photoluminescence (PL) experiments reveal sorting of neutral and charged excitons across the boundary. Our results reveal evidence for extremely large in-plane electric fields (≃4000 kV/cm) at the domain wall (DW), whose effect is manifested in the routing of free charges and trions towards oppositely poled domains, resulting in a nonintuitive spatial PL intensity pattern. In a second step, we engineer the PPLN substrate and the 2D heterostructure to exploit the non-uniform in-plane electric field exerted by the DW to confine neutral excitons in a 1D dipolar gas. Reducing the dimensionality holds an excellent potential for unlocking strong exciton-exciton interaction regimes, enabling exploration of exotic quantum phases of matter and designing advanced optoelectronic devices.

HL 53.2 Thu 15:15 H15

Collective charge excitations between moiré minibands in twisted WSe_2 bilayers probed with resonant inelastic light scattering — •Hendrik Lambers[1], Nihit Saigal[1,2], Nicolai-Leonid Bathen[1], Veljko Antić[1], Lennart Klebl[3], Dante M. Kennes[4], Tim O. Wehling[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]EMBL Imaging Centre, Heidelberg, Germany — [3]Institute of Theoretical Physics, University of Hamburg, Germany — [4]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany

The weak van der Waals coupling between monolayers of transitionmetal dichalcogenides (TMDCs) allows the realization of twisted van der Waals structures resulting in precisely tailored 2D quantum systems with superimposed moiré superlattice structures. These are dependent on twist angle and lattice constant mismatch and can cause flat moiré mini bands in the reduced Brillouin zone of the superlattice. Here we study these moiré minibands in $tWSe_2$ homobilayers encapsulated in hBN by low temperature resonant inelastic light scattering (RILS) [1]. Guided by theoretical predications, we identify single particle-like collective inter moiré miniband excitations. Thereby, we establish RILS as a tool to quantitatively probe the formation of moiré minibands. Furthermore, we identify local twist angle variations by lateral force microscopy and correlate these findings with optical (Raman) spectroscopy. [1] N. Saigal et al., Phys. Rev. Lett. 133, 046902 (2024).

HL 53.3 Thu 15:30 H15

Unraveling Rashba spin-orbit coupling in TMDs — •Miguel Morales Cocera[1,2], Marta Prada[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Transition metal dichalcogenides (TMDs) possess unique optical and electronic properties, making them ideal candidates for exploring new physical phenomena. Their significant spin-orbit coupling enables a rich landscape of spin-valley physics within the realm of excitonic effects or topologically non-trivial materials, to name a few. However, there are still unanswered questions concerning the mechanisms that rule Rashba spin-orbit coupling (RSOC), such as the role of the atomic and orbital composition, number of layers, or band character. In this work, we employ ab-initio calculations together with perturbative approaches to unravel the intricacies of bilayer TMDs with an intrinsic dipole, which is far from trivial. We deliver with high numerical precision the Rashba parameters in Rmx (Bernal stacking) bilayers (M= Mo, W. X=S, Se, Te).

HL 53.4 Thu 15:45 H15

Theory of Magnetic Field Dependence of Excitonic Spectra in Atomically Thin Semiconductors — •Michiel Snoeken and Henry Mittenzwey — Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany

The linear absorption spectrum of TMDC monolayers under the influence of an in-plane magnetic field is theoretically studied in an excitonic picture. It is shown that in-plane magnetic fields induce a hybridization between spin-bright and spin-dark exciton transitions, resulting in a brightening of spin-dark excitons in the linear absorption spectrum with increasing in-plane field-strength. Numerical evaluation shows that with increasing field strength, not only the energy splitting between bright and dark excitonic resonances increases, but also an impact on the respective excitonic linewidths can be observed. Some limiting cases are investigated analytically, allowing to discuss a detailed physical picture of the magnetic field-dependent excitonic energies and linewidths.

15 min. break

HL 53.5 Thu 16:15 H15

Spatial mapping of the tunable band gaps of bilayer graphene using a WSe_2 sensor layer — David Tebbe[1], •Alexander Polkowski[1], Sophia Lackhoff[1], Jonas Blum[1], Takashi Taniguchi[2], Kenji Watanabe[2], Bernd Beschoten[1,3], Lutz Waldecker[1], and Christoph Stampfer[1,4] — [1]2nd Institute of Physics A, RWTH Aachen University, Aachen — [2]National Institute for Materials Science, Namiki, Tsukuba, Japan — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [4]Peter Grünberg Institute (PGI-9) Forschungszentrum Jülich, Jülich, Germany

Bernal bilayer graphene (BLG) is a 2D material with promising properties for future quantum technologies, due to its tunable band gap and rich correlated phases, which have been detected by electrical transport measurements. However, due to their nature, these measurements have not been able to spatially resolve the bandgap and other electronic properties of BLG. Here, we show optical sensing can overcome this limitation. To achieve this we place a sensing monolayer of WSe_2 in direct contact to BLG in a double-gated device structure. The sensor layer hosts excitons, with the ability to sense changes in the electronic configuration of the BLG. The WSe_2 hosts Rydberg excitons, which are sensitive to the surrounding dielectric environment and thus sense small changes in carrier density within the BLG, allowing to observe the band gap opening. These excitonic states can be resolved using white light reflection spectroscopy, which allowed us to spatially map the potential landscape in the BLG.

HL 53.6 Thu 16:30 H15

Beyond the K-Valley: Exploring Unique Trion States in Indirect Band Gap Monolayer WSe_2 — •Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Atomically thin layers of transition metal dichalcogenides are of great interest due to their exceptional electronic and optical properties. Their lack of inversion symmetry and strong spin-orbit interaction from heavy metal atoms leads to an additional valley degree of freedom and significant spin splittings in the Brillouin zone. The reduced dimensionality and dielectric screening make these materials ideal for studying Coulomb-bound many-body states, such as excitons and trions.

We will discuss calculations of the optical properties of monolayer WSe_2 using *ab initio* many-body screened configuration interaction. We'll highlight our findings on additional species of negatively charged trions including the **Q**-valley, which we found to be more energetically favorable than those in the **K**-valley. Our results align well with experimental data and provide new insights into previously observed but unexplained optical features. Furthermore, we will analyze the many-body interactions that reveal the mechanisms behind the increased singlet-triplet splitting and the redshifted energies in the **Q**-valley trions compared to those in the **K**-valley.

HL 53.7 Thu 16:45 H15

Trion saturation and trion filtering in MoS_2 and MoS_2/graphene heterostructures — Omid Ghaebi[1], Tarlan Hamzayev[1], •Till Weickhardt[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Abbe Center of Photonics, Friedrich Schiller University Jena

Optical excitation of electron-hole pairs in transition-metal dichalcogenides leads to the formation of excitons, that can join with free carriers to form trions [1]. Since trions display an efficient non-radiative decay, tuning their relative density with respect to neutral excitons by external knobs is fundamental to engineer the light emitting efficiency of TMD opto-electronic devices. In this work, we investigate the interplay of excitons, trions, and free electrons with regards to gating and excitation power. By carrying out these experiments on a pristine MoS_2 monolayer as well as on a MoS_2/graphene heterostructure where the graphene facilitates fast charge transfer from the TMD [2,3], we study the interdependent dynamic of excitons and trions. Most prominently, this effect can be seen in a super-linear power-scaling of the exciton density due to saturation of trions in the monolayer MoS_2 [4]. When the graphene is added to form the heterostructure, this effect vanishes due to the elimination of trions.

[1] Mak et al. Nature Mater 12, 207-211 (2013). [2] Lorchat et al. Nat. Nanotechnol. 15, 283-288 (2020). [3] Küchle et al. Opt. Mater.: X 12, 2590-1478 (2021). [4] Wang et al. ACS Photonics 10 (2), 412-420 (2023).

HL 53.8 Thu 17:00 H15

Engineering carrier density and exciton polarization in WSe2 monolayers via photochlorination — •Eirini Katsipoulaki[1,2], George Vailakis[1,3], Delphine Lagarde[4], Vishwas Jindal[4], Konstantinos Mourtzidis[4], Xavier Marie[4], Ioannis Paradisanos[1], George Kopidakis[1,3], George Kioseoglou[1,3], and Emmanouel Stratakis[1,2] — [1]FORTH/IESL, Heraklion, Greece — [2]Dpt. of Physics, UoC, Heraklion, Greece — [3]Dpt. of Materials Science and Engineering, UoC, Heraklion, Greece — [4]Universite de Toulouze, INSA-CNRS-UPS, LPCNO, Toulouze, France

Transition Metal Dichalcogenides (TMDs) represent a special class of 2D van der Waals materials. Unlike their 3D-counterparts, which are indirect gap semiconductors, the monolayers exhibit a direct bandgap, leading to a significant enhancement in photoluminescence quantum yield. TMDs feature valley dependent optical selection rules, establishing them as promising candidates for atomically thin optoelectronic devices. A key factor influencing the performance of TMDs in these applications is the carrier density. To address this, we demonstrate the modulation of the Fermi level in WSe2 monolayers using an UV-assisted photochlorination method. Systematic shifts and relative intensities between charged and neutral excitons indicate a controllable decrease of the electron density and switch WSe2 from n- to a p-type semiconductor. DFT calculations predict Cl2 adsorption at Se vacancies. Furthermore, this method can strongly impact the circular polarization degree of excitons. These findings indicate that photochlorination can tailor nanopatterned lateral p-n junctions.

HL 54: Ultra-fast Phenomena II

Time: Thursday 15:00–17:15 Location: H17

HL 54.1 Thu 15:00 H17

Effect of the acceptor strength on intermolecular conical intersection dynamics in aggregates of quadrupolar dyes — •Katrin Winte[1], Somayeh Souri[1], Daniel Lünemann[1], Teresa Kraus[2], Elena Mena-Osteritz[2], Peter Bäuerle[2], Sergei Tretiak[3], Antonietta De Sio[1], and Christoph Lienau[1] — [1]Oldenburg University, Germany — [2]Ulm University, Germany — [3]Los Alamos National Laboratory, USA

Aggregated films of quadrupolar acceptor-donor-acceptor (A-D-A) molecules have emerged as promising materials for organic photovoltaics. The optoelectronic properties in the molecule are governed by an interplay between electronic and vibronic couplings in the molecule. In aggregated films, we have uncovered the existence of intermolecular conical intersections (CoIn) occurring on timescales of less than 50 fs, which funnel energy from the photoexcited bright state into the lower-lying dark electronic state of the aggregate [1]. This raises the question whether the quantum dynamics of the aggregates can be altered by modifying the intramolecular charge transfer character of the A-D-A monomers. Chemical intuition suggests that increasing the acceptor strength might accelerate charge transfer and with it the passage through the CoIn. To explore this hypothesis, we synthesize thin films of A-D-A molecules with varying acceptor strengths and study their ultrafast dynamics by femtosecond time-resolved spectroscopy. Our results show only minimal effects on the CoIn dynamics, suggesting that intermolecular vibronic couplings play the dominant role in the quantum dynamics. [1] A. De Sio et al., Nature Nano 16, 63 (2021).

HL 54.2 Thu 15:15 H17

Ultrafast decay of spin-polarization of semiconductor holes measured by attosecond transient absorption spectroscopy — •Lauren Drescher[1,2], Kylie Gannan[1], and Stephen Leone[1] — [1]Department of Chemistry, University of California, Berkeley, California 94720, USA — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

Carrier excitation by light can lead to spin-polarization in semiconductor conduction and valence bands. While the dynamics of the spin-polarization of conduction band electrons are often well characterized, comparably little is known about the counterpart polarization of valence band holes, due to its much shorter lifetime.

Here we introduce circular dichroic attosecond transient absorption spectroscopy which allows to follow the spin-polarization of materials on attosecond timescales through coupling to the angular momentum of light. Corroborated by real-time time-dependent density functional theory calculations, our experimental results reveal the few femtosecond decay of semiconductor hole spin-polarization in germanium. Our method opens the door to measure spin dynamics in non-magnetic materials with extreme temporal resolution, high spectral resolution and core-level specificity.

HL 54.3 Thu 15:30 H17

Picosecond Femtojoule Resistive Switching in Nanoscale VO2 Memristors — •Sebastian Schmid[1,2], Laszlo Posa[1,3], Timea Török[1,3], Botond Santa[1,4], Zsigmond Pollner[1], György Molnar[3], Yannik Horst[5], Janos Volk[3], Juerg Leuthold[5], Andras Halbritter[1,4], and Miklos Csontos[5] — [1]Department of Physics, Institute of Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86159, Germany — [3]Institute of Technical Physics and Materials Science, HUN-REN Centre for Energy Research, 1121 Budapest, Hungary — [4]HUN-REN-BME Condensed Matter Research Group, H-1111 Budapest, Hungary — [5]Institute of Electromagnetic Fields, ETH Zurich, 8092 Zurich, Switzerland

The dynamics of the Mott transition in correlated electron oxides could provide a sustainable alternative to the von Neumann computation by exploiting device-level functional complexity at low energy consumption. We fabricated nanoscale VO2 devices and tested them in our picosecond timeresolution, real-time resistive switching experiments, using 20 ps short and <1.7 V amplitude voltage pulses. There we observed tunable resistance states from insulator-metal transitions with down to 15 ps incubation times and switching energies starting from a few femtojoule. These orders of magnitude improvements from other memristive devices open up new possibilities for neuromorphic computing applications, outperforming the human brain at size and speed, with competitive energy consumption.

HL 54.4 Thu 15:45 H17

Agreement between Theoretically Predicted and Measured Bragg Peak Decay in Bismuth Following Femtosecond Laser Excitation — •Bernd Bauerhenne[1], Jimiben Patel[1], Sahar Bakhshi[1], Sascha Epp[2], and Martin Garcia[1] — [1]Institute of Physics, University of Kassel, Heinrich-Plett-Straße 40, D34132 Kassel, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, 3 Luruper Chaussee 149, 22761 Hamburg, Germany

We investigated the time-resolved Bragg peak decay in bismuth films, 30 nm and 50 nm thick, following excitation with femtosecond (fs) laser pulses. These measurements were conducted using x-ray pulses sourced from a free-electron laser. To explain the observed Bragg peak decay, we developed an electronic temperature (Te) dependent interatomic potential for bismuth, generated using forces and energies from ab initio molecular dynamics (MD) simulations at elevated Te levels. Additionally, we computed the optical properties and the Te-dependent electron-phonon coupling constant for bismuth using ab initio methods. Employing these calculated quantities, we conducted MD simulations on similarly laser-excited antimony films, 30 nm and 50 nm thick. The comparison between our theoretical predictions and experimental measurements of Bragg peak decay exhibited an agreement, affirming the accuracy of our model. This model effectively incorporates the fs-laser induced modifications of the potential energy surface and the dynamic influences of electron-phonon coupling, providing a robust framework for understanding laser-material interactions in ultrafast processes.

15 min. break

HL 54.5 Thu 16:15 H17

Ultrafast Time-Domain Spectroscopy Reveals Coherent Vibronic Couplings Upon Electronic Excitation in Crystalline Organic Thin Films — •Naby Hadilou[1], Somayeh Souri[1], Daniel Timmer[1], Daniel C. Lünemann[1], Katrin Winte[1], Antonietta De Sio[1], Martin Esmann[1], Sebastian Anhäuser[2], Michele Guerrini[1], Ana M. Valencia[1], Caterina Cocchi[1], Gregor Witte[2], and Christoph Lienau[1] — [1]Oldenburg university, Germany — [2]Philipps-Universität Marburg, Germany

Coherent coupling between electronic excitations and molecular vibrations significantly influences the optical and charge transport properties of organic semiconductors and may have profound effect on technologically relevant processes such as excitons fission. Highly ordered crystalline films are ideal for probing such couplings since they enable studies of individual domain. Here, we report first polarization-resolved pump-probe experiments probing the ultrafast dynamics of crystalline perfluoropentacene thin films grown on different substrates with 10-fs time resolution. Coherent oscillations in the spectra reveal vibronic couplings to a high-frequency, 25-fs, in-plane deformation mode that is insensitive to the optical polarization, while the coupling to a lower-frequency, 85-fs, out-of-plane ring bending mode depends significantly on the crystalline and molecular orientation. Raman spectra confirm this interpretation and highlight the dominance of solid-state effects on vibronic couplings. Our results represent a first step toward uncovering the role of anisotropic vibronic couplings for singlet fission processes in crystalline molecular thin films.

HL 54.6 Thu 16:30 H17

Attosecond light-driven charge injection in germanium — •Giacomo Inzani[1,9], Lyudmyla Adamska[2,3], Amir Eskandari-asl[4], Nicola Di Palo[1], Gian Luca Dolso[1], Bruno Moio[1], Luciano Jacopo D'Onofrio[4,5], Alessio Lamperti[6], Alessandro Molle[6], Rocio Borrego-Varillas[7], Mauro Nisoli[1,7], Stefano Pittalis[2], Carlo Andrea Rozzi[2], Adolfo Avella[4,5,8], and Matteo Lucchini[1,7] — [1]Dept. of Physics, Politecnico di Milano, Italy — [2]CNR - Istituto Nanoscienze, Modena, Italy — [3]Dept. of Physics, Mathematics and Informatics, University of Modena & Reggio Emilia, Italy — [4]Dip. di Fisica, Università degli Studi di Salerno, Italy — [5]CNR - SPIN, UoS di Salerno, Italy — [6]CNR - IMM, Unit of Agrate Brianza, Italy — [7]IFN - CNR, Milano, Italy — [8]Unità CNISM di Salerno, Università degli Studi di Salerno, Italy — [9]Present address: Dept. of Physics, University of Regensburg, Germany

The injection of charges from the valence to the conduction band of a semiconductor induced by an ultrashort pulse can tailor its electro-optical properties. This process typically occurs on time scales shorter than the laser period - for visible light, in the order of one femtosecond. Despite its relevance, few experiments studied the charge excitation process with attosecond temporal resolution. In this work, we combine attosecond transient reflection spectroscopy measurements to a dual cutting-edge theoretical approach, demonstrating that photoexcitation in Ge cannot be ascribed to a single physical mechanism. The interplay of multi-photon absorption, light-induced band dressing, and intra-band motion is crucial for determining the overall charge injection.

HL 54.7 Thu 16:45 H17

Dephasing Effects in High-Harmonic Generation from Solids — •Francisco Navarrete and Dieter Bauer — Institut für Physik, Universität Rostock, 18051 Rostock, Deutschland

In the calculation of high-order harmonic generation (HHG) in solids, introducing a dephasing time is often crucial for accurately reproducing the distinct spectral peaks observed experimentally in the first plateau region [1,2]. In this contribution, we present analytical and numerical studies on the non-integer contributions to the interband HHG spectrum and investigate how dephasing affects not only the spectral structure but also the amplitude and wavelength dependence of the harmonics. Using a simplified two-band model, we numerically solve and also approximate the semiconductor Bloch equations via a saddle-point method [3] to elucidate these effects. Our findings provide closed analytical expressions for these contributions, offering insights into the interplay between dephasing and electron dynamics in solids and the mechanisms shaping the HHG spectrum.

References:
[1] Vampa et al., Phys. Rev. Lett. 113, 073901 (2014)
[2] Cavaletto et al., Nat. Rev. Phys. (2024) (accepted)
[3] Navarrete et al., Phys. Rev. A 100, 033405 (2019)

HL 54.8 Thu 17:00 H17

Ultrafast Dynamics of Vanadium Dioxide Phase Transformation — •Liuyue Yang, Daniel Sandner, and Hristo Igle — Laser and X-Ray Physics E11, TUM School of Natural Sciences, TUM, James-Franck-Str. 1 85748 Garching, Germany

Vanadium dioxide has been discovered to have a metal-to-insulator transformation (MIT) at 68 °C. To investigate the dynamics of MIT, we use the pump-probe experiment to obtain the reflective transient mid-infared spectrum of VO2. In the photoinduced VO2 MIT, the phase transformation can occur at high pump power. The reflectivity of VO2 increases significantly at the metal state. At high temperature, the phase transformation occurs at lower pump power. Moreover, we observed a reflectivity oscillation in wavelength around the zeropoint of pump delay. The oscillation frequency decreases rapidly with the delay time

HL 55: Graphene and 2D Materials (joint session TT/HL)

Time: Thursday 15:00–18:30 Location: H33

See TT 49 for details of this session.

HL 56: Members' Assembly

- Bericht
- Wahl der Fachverbandsleitung
- Informationen zur Frühjahrstagung 2026
- Verschiedenes

Time: Thursday 17:30–19:00 Location: H17

All members of the Semiconductor Physics Division are invited to participate.

HL 57: Quantum Dots and Wires: Optics II

Time: Friday 9:30–13:00 Location: H13

HL 57.1 Fri 9:30 H13

Deterministic Generation of Linear Photonic Cluster States with Semiconductor Quantum Dots: A Detailed Comparison of Different Schemes — •Nikolas Köcher, David Bauch, Nils Heinisch, and Stefan Schumacher — Physics Department, CeOPP, and PhoQS, Paderborn University, Germany

Graph and cluster states are types of multipartite entangled states with applications in quantum communication [1] and measurement-based quantum computation [2]. We theoretically investigate and compare different schemes for the deterministic generation of linear photonic cluster states using spins and trions in charged semiconductor quantum dots under strong Purcell enhancement. The schemes differ in the method used for spin control and whether the emitted photonic qubits are polarization or time-bin encoded. We efficiently track the fidelity and the usable length of the cluster states by calculating the expectation values of their stabilizer generators, assessing their fidelity beyond the calculation of gate fidelities [3]. We find that the performance of the different schemes and which scheme is optimal strongly depend on the cavity environment and the coherence time of the spin qubit.

[1] K. Azuma, K. Tamaki, H.-K. Lo, Nat. Commun. 6, 6785 (2015).
[2] R. Raussendorf, H. Briegel, Phys. Rev. Lett. 86, 5188 (2001).
[3] D. Bauch, N. Köcher, N. Heinisch, S. Schumacher, APL Quantum 1, 036110 (2024).

HL 57.2 Fri 9:45 H13

Scalable integration of site-controlled quantum dots into circular Bragg grating resonators — •Kartik Gaur, Avijit Barua, Sarthak Tripathi, Sam Baraz, Lukas Dworaczek, Neha Nitin, Imad Limame, Aris Koulas-Simos, Priyabrata Mudi, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

The buried-stressor approach [1] is one of the pivotal methods for the growth of site-controlled quantum dots (SCQDs). This growth technique makes use of the strain from a partially oxidized AlAs layer to induce site-selective nucleation of InGaAs quantum dots. Here, we report on growth, fabrication, and surface and optical characterizations of such SCQDs. A systematic investigation of the effects of variation of SCQD growth parameters on QDs density, surface morphology, and optical properties is done using atomic force microscopy (AFM), cathodoluminescence (CL), and microphotoluminescence (μPL) spectroscopy. Moreover, these SCQDs are integrated into circular Bragg gratings (CBGs) in a scalable manner highlighting the advantage of our advanced growth approach. Quantum optical characterizations are also performed on these SCQD-CBGs. The comprehensive understanding of the intricacies involved in the growth and characterization of SCQDs and their scalability in device integration offers a roadmap for the advancement of nanophotonic technologies and quantum information.

[1] A. Strittmatter, et. al., Applied Physics Letters, 100(9):093111, 03 2012.

HL 57.3 Fri 10:00 H13

Spectral correlations of dynamical resonance fluorescence — •Santiago Bermúdez Feijóo[1], Eduardo Zubizarreta Casalengua[2], Kai Müller[2], and Klaus D. Jöns[1] — [1]PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany — [2]Walter Schottky Institute, School of Computation, Information and Technology and MCQST, Technische Universität München, Garching, Germany

In this work, we explore the time-dependent, frequency-filtered [1] photon statistics of a two-level system under pulsed excitation, whose dynamical emission spectrum [2] has been recently experimentally measured using semiconductor QDs [3]. Our results show that photon statistics are not fixed [4] but vary between bunching and antibunching, depending on the applied frequency filters. This reveals an intricate interplay between pulse area, photon frequencies, and correlations, extending insights from the CW case [5]. Notably, frequency-filtering enhances time-bin applications: for odd pulses, it suppresses two-photon events by up to two orders of magnitude, while for even pulses, it restores single-photon purity. This approach simplifies entanglement generation by enabling photon-number control [6] via frequency selection, eliminating the need for complex excitation schemes. [1] E. del Valle et al. PRL 109(18):183601 (2012). [2] Moelbjerg, A. et al. PRL.108, 017401 (2012). [3] Boos, K. et al. PRL.132, 053602 (2024). [4] Fischer, K. et al. Nature Phys 13, 649*654 (2017). [5] J.C. Lopez Carreno et al. Laser & Photonics Reviews, 11(5):1700090 (2019). [6] Wein, S.C et al. Nat. Photon. 16, 374*379 (2022).

HL 57.4 Fri 10:15 H13

Resonance fluorescence measurements on rapid thermally annealed self-assembled quantum dots — H. Mannel[1], •F. Rimek[1], M. Zöllner[1], N. Schwarz[1], N. Bart[2], A. Ludwig[2], A. D. Wieck[2], A. Lorke[1], and and M. Geller[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A single self-assembled quantum dots (QD) is one of the promising candidate as a bright (high photon rate) and stable (fourier-limited) linewidth single photon source [1]. They are typically grown by molecular beam epitaxy (MBE) and have photon emission energies in the near-infrared spectrum. There are several techniques to control the size, which shift the emission wavelength. The so-called indium flush is often used, where the tip of the dot is thermally flushed away [2]. Alternatively, the confinement can be altered by rapid thermal annealing (RTA) [3], which lets indium and gallium diffuse. Here, we investigate the optical properties of rapidly thermally annealed quantum dots. In particular, we study the effects of RTA on the resonance fluorescence line width. This is done by three different measurements. First, we scan over the applied gate voltage and calculate the linewidth using the Stark shift of the exciton. Second, we scan the linewidth directly with a tunable laser. In addition, we study the lifetime in pulsed resonant measurements. The change in the confinement potential might also change dephasing processes such as photoemission or the Auger effect. [1] N. Tomm et al., Nat. N. **16**, 399-403 (2021). [2] H. Sasakura et al., JAP **102**, 013515 (2007). [3] N. Perret et al., PRB **62**, 5092 (2000).

HL 57.5 Fri 10:30 H13

Exploring the limits of absolute position accuracy in single emitter localization microscopy — •Maximilian Heller, Chenxi Ma, Timon Handrup, Yiteng Zhang, Xian Zheng, Micheal Zopf, and Fei Ding — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover

Solid-state single photon emitters (SPEs) integrated in photonic nanostructures provide highly efficient light-matter interfaces for quantum information applications. Wide-field optical positioning has shown the potential to be an inexpensive method with high troughput to achieve the desired spatial matching of SPEs to the nanostructure. However, the accuracy of optical positioning setups has been overlooked so far and mainly the fitting uncertainty has been used as figure of merit. Here, we use arrays of gold nanodisks with pre-defined positions to systematically quantify the main sources of error in fabrication and imaging. From this, we develop a comprehensive calibration model to render the systematic errors insignificant compared to the uncertainties. We demonstrate that the careful calibration of the optical positioning process leads to an increased yield of quantum photonic devices by fabricating and characterizing a large number of circular Bragg gratings around epitaxial quantum dots.

HL 57.6 Fri 10:45 H13

On-demand storage and retrieval of single photons from a semiconductor quantum dot in a room-temperature atomic vapor memory — •Avijit Barua[1], Benjamin Maass[1,2], Norman Vincenz Ewald[1,2], Elizabeth Robertson[2], Kartik Gaur[1], Suk In Park[3], Sven Rodt[1], Jin-Dong Song[3], Stephan Reitzenstein[1], and Janik Wolters[2] — [1]Technische Universität Berlin (TUB), Berlin, Germany — [2]German Aerospace Center (DLR), Berlin, Germany — [3]Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea

Interfacing light from solid-state single-photon sources with scalable and robust room-temperature quantum memories has been a long-standing challenge in photonic quantum information technologies due to inherent noise processes and time-scale mismatches between the operating conditions of solid-state and atomic systems. Here, we demonstrate on-demand storage and retrieval of single photons from a semiconductor QD device in a room-temperature atomic vapor memory. A deterministically fabricated InGaAs QD light source emits single photons at the wavelength of the cesium D1 line at 895 nm which exhibit an inhomogeneously broadened linewidth of 5.1(7) GHz and are subsequently stored in a low-noise ladder-type cesium vapor memory. We show control over the interaction between the single photons and the atomic vapor, allowing for variable retrieval times of up to 19.8(3) ns at an internal efficiency of 0.6(1)%. Our results significantly expand the application space of both room-temperature vapor memories and semiconductor QDs in future quantum network architectures.

15 min. break

HL 57.7 Fri 11:15 H13

Effects of atomistic fluctuations on the excitonic fine-structure in alloyed colloidal quantum Dots — •Anne Nadine Tewonoue Djota, Surender Kumar, and Gabriel Bester — Institute of physical chemistry and physics, University of Hamburg

The electron-hole exchange interaction in the presence of spin-orbit coupling leads for an atomistic calculation to a small energy splitting of the excitonic state known in this context as the fine structure splitting (FSS). Although this splitting is typically small, it has large consequences for the optical properties. For instance, the photoluminescence originates from these few states and is governed by the splitting (giving rise to temperature dependence) and polarization of these low energy excitonic states. So far most of the theoretical modeling has assumed that high symmetry structures lead to a simple dark-bright splitting with a large degeneracy of the excitonic states. In this work, we show based on atomistic calculations, that even globally perfectly symmetric structures (i.e., as far as an atomistic construction permits a "spherical" quantum dot) show a qualitatively different FSS as soon as alloying is introduced. The alloying effect is significantly stronger than any global shape anisotropy where the symmetry is broken for instance by geometrical elongation of the quantum dot. On the other hand, alloying a quantum dot through processes such as cation exchange is inherently random. As a result, different random alloy configurations with the same size and composition can exhibit significantly different FSS.

HL 57.8 Fri 11:30 H13

How Surface Defects Shape the Excitons and Photoluminescence of Ultrasmall CdSe Quantum Dots — •Torben Steenbock[1], Emilia Drescher[1], Tobias Dittmann[1], and Gabriel Bester[2,3] — [1]Department of Chemistry, University of Hamburg, HARBOR, Hamburg 22761, Germany. — [2]Department of Chemistry and Physics, University of Hamburg, HARBOR, Hamburg 22761, Germany. — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg 22761, Germany.

Ultrasmall CdSe quantum dots (QDs) with diameters up to 2 nm show broad photoluminescence (PL) spectra presumably due to emission from band-edge excitons and defect states. However, the origin of the defect emission and the effect of defects on the band-edge excitons is not fully understood. Based on spin-orbit density functional theory and screened configuration interaction singles, we show that Cd-dimer and Se defects form in-gap defect states. In comparison with experiment, we discuss the role of deep and shallow defect states for the PL and cover the dependence of their contributions to the PL with respect to the QD size. Further, we observe that these defects lead to a localization of the molecular orbitals (MOs) involved in the band-edge excitons creating large electric dipoles in the MOs. In the excitonic states, these dipoles cause multiexponential PL decay from the band-edge states with a highly anisotropic polarization of the emission. The polarization is found to be very sensitive with respect to the exact composition of the surface.

HL 57.9 Fri 11:45 H13

Room-temperature single photon emitters in hexagonal boron nitrite coupled to an open optical cavitiy — •Anthony Ernzerhof, Lukas Lackner, Martin Esmann, Ivan Solovev, and Christian Schneider — Carl von Ossietzky Universität Oldenburg, Germany

Single photon emitters (SPEs) are a key component in photonic quantum technologies. Potential applications include secure communications and quantum metrology. Here, we present SPEs at room temperature (RT) based on hexagonal boron nitride (hBN) nano crystallites, which exhibit remarkable optical properties[1]. Our work focuses on the integration of these SPEs in an optical cavity with open access and full tunability. The cavity device allows to enhance the emitter performance via the Purcell effect, which significantly improves the emitter emission rate and source collection efficiency[2]. We discuss our technological approach towards engineering the open cavity yielding a flexible, transportable, compact and userfriendly opto-mechanically tunable emitter-cavity device, which, in principle, is of universal use beyond hBN based single photon sources. We further discuss challenges associated to the implementation of hBN nano-crystallites in such a cavity.

[1] Tran, T.et al. Quantum emission from hexagonal boron nitride monolayers. Nature Nanotech 11, 37-41 (2016). [2] Tobias Vogl et al. Compact Cavity-Enhanced Single-Photon Generation with Hexagonal Boron Nitride, ACS Photonics 6 (8), 1955-1962 (2019).

HL 57.10 Fri 12:00 H13

Silicon nitride-based photonic integrated circuit interfaced via photonic wire bonds with InGaAs-QDs emitting at telecom wavelength — •Ulrich Pfister[1], Daniel Wendland[2,3], Florian Hornung[1], Lena Engel[1], Hendrik Hüging[2], Elias Herzog[1], Ponraj Vijayan[1], Raphael Joos[1], Erik Jung[3], Michael Jetter[1], Simone L. Portalupi[1], Wolfram H. P. Pernice[2,3], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [3]Kirchhoff-Institute for Physics, University of Heidelberg, 69120 Heidelberg, Germany

Photonic integrated circuits (PICs) play a crucial role for realizing several quantum technologies in a small footprint. In this regard, hybrid approaches are beneficial for combining the highly developed silicon platform with the on-demand single-photon emission of III-V semiconductor quantum dots (QDs). We employed 3D laser writing technology to realize photonic wire bonds (PWBs) for funnelling single-photons from the III-V-based chip, containing the QDs emitting at 1550nm, into a Si_3N_4-based PIC [1]. An on-chip beamsplitter was used to measure a $g^{(2)}(0) = 0.11 \pm 0.02$, demonstrating the functionality of the hybrid approach on a single-photon level. Additionally, the average efficiency of the PWBs was precisely quantified.

[1] Ulrich Pfister, *et al.*, arXiv:2411.05647

HL 57.11 Fri 12:15 H13

Quantum Communication Protocols Using Polarization-Entangled Photon Emitters — Michele Rota[1], Francesco Basso Basset[1], •Francesco Salusti[2], Alessandro Laneve[1], Mattia Beccaceci[1], Giuseppe Ronco[1], Nicolas Claro Rodriguez[2], Thobias Krieger[3], Quirin Buchinger[4], Saimon Filipe Covre Da Silva[3], Sandra Stroj[5], Sven Höfling[4], Tobias Huber-Loyola[4], Armando Rastelli[3], Klaus Jöns[2], and Rinaldo Trotta[1] — [1]Department of Physics, Sapienza University of Rome, 00185 Rome, Italy — [2]PhoQS, CeOPP and Department of Physics, Paderborn University, 33098 Paderborn, Germany — [3]Institute of Semiconductor and Solid State Physics, JKU University, 4040 Linz, Austria — [4]Julius-Maximilians-Universität Würzburg, Physikalisches Institut, 97074 Würzburg, Germany — [5]Forschungszentrum Mikrotechnik, FH Vorarlberg, 6850 Dornbirn, Austria

We demonstrate entanglement swapping using [1] a quantum dot in a novel cavity with piezoelectric actuators [2]. We use these entan- gled photons after the swapping operation for quantum key distribu- tion with a modified Ekert91 protocol [3], highlighting temporal post- selection's impact on photon indistinguishability and protocol metrics.

[1] J.-W. Pan, et al., Phys. Rev. Lett. 80, 3891 (1998)
[2] M. B. Rota, et al., eLight 4, 13 (2024), ISSN 2662-8643
[3] F. B. Basset, et al., Science Advances 7, eabe6379 (2021)

HL 57.12 Fri 12:30 H13

Efficient fiber coupling of telecom single photons from circular Bragg gratings — •Nam Tran[1], Pavel Ruchka[2], Sara Jakovljevic[2], Benjamin Breiholz[1], Peter Gierss[1], Ponraj Vijayan[1], Carlos Eduardo Jimenez[3], Alois Herkommer[3], Michael Jetter[1], Simone Luca Portalupi[1], Harald Giessen[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart — [2]4. Physikalisches Institut, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart — [3]Institut für Technische Optik, Research Center of Photonic Engineering, SCoPE, University of Stuttgart

This work aims at quantitatively investigating the spatial stability and coupling efficiency of telecom C-band photons, generated by an epitaxial quantum dot embedded in a circular Bragg grating, into single mode optical fibers. These results are then compared to a bare single mode fiber without the 3D printed lens and a collection via a microscope objective. In terms of the total fiber coupling efficiency, the lensed and bare fiber outperform the microscope objective by up to a factor of 2.9 corresponding to a measured count rate at the detectors of 0.44MHz and 1.11MHz, respectively. The lateral (vertical) displacement showed that within a few (a few tenths) of microns the coupling degrades less than a factor of two.

HL 57.13 Fri 12:45 H13

Development of Stark-tuned InGaAs quantum dots emitting in the telecom O-band on silicon substrate — •Sarthak Tripathi, Kartik Gaur, Imad Limame, Priyabrata Mudi, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

Quantum dots (QDs) are promising for single-photon emission, essen tial for quantum technologies like secure communication and quantum key distribution (QKD). In particular, InGaAs QDs that emit photons in the telecom O-band are especially valuable due to their compatibility with current metropolitan fiber-based QKD systems. Additionally, it is interesting to develop Si-compatible device concepts. Achieving High quality QDs on silicon are challenging due to lattice mismatch with III-V materials, leading to defects and performance degradation. To overcome this, we use a GaP buffer layer to reduce strain, improve lat tice matching, enabling high-quality QD growth with low defect den sities.By integrating epitaxial n- and p-doped GaAs layers with ohmic contacts, we apply an electric field to modify the QD energy levels via Stark effect, allowing controlled tuning of the emission wavelength. This tunability is crucial for aligning the QD emission with telecom standards or compensating for fabrication-induced variations. Optical and quantum optical characterizations confirm the effectiveness of this approach, demonstrating excellent quantum optical properties. These results highlight the potential of electrically tunable InGaAs QDs on Si as a scalable platform for quantum communication, compatible with Si-based technologies and fiber-based telecom networks.

HL 58: Nitrides: Preparation and Characterization II

Time: Friday 9:30–10:30 Location: H14

HL 58.1 Fri 9:30 H14

Random Alloy and Ordered Phases of Cubic Indium Gallium Nitride From a First-Principle Perspective — •Jan M. Waack[1,2], Markus Kremer[1,2], Nils Andre Schäfer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Although the miscibility gap in cubic zincblende indium gallium nitride ($In_xGa_{1-x}N$) has been overcome, the specific role of ordered phases in this process remains unclear. First-principle density functional theory calculations provide a reference point for addressing this question. Ordered phases, such as CuPt-type and chalcopyrite-type structures, exhibit unique structural and electronic properties that differentiate them significantly from the random alloy. An understanding of these distinctive features of ordered phases provides a basis for their experimental identification.

We present a comprehensive data set on key structural parameters, including lattice constants and bond lengths, as well as elastic properties such as elastic constants and phonon modes. Furthermore, we explore electronic properties including the band gap and Bloch spectral function using *ab-initio* approaches such as LDA-1/2 and the mBJ functional. The presented insights into the physical properties of ordered phases and the random alloy offer a robust foundation for their experimental detection and further exploration.

HL 58.2 Fri 9:45 H14

Characterization of structural and optical properties of a red InGaN/GaN MQW LED — •Niklas Dreyer[1], F. Bertram[1], G. Schmidt[1], H. Eisele[1], S. Petzold[1], O. August[1], A. Dempewolf[1], K. Wein[1], J. Christen[1], B. Sheng[2], and X. Wang[2] — [1]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [2]Peking University, Beijing 100871, China

An InGaN/GaN LED with an intended red emission (> 600 nm) was grown by MOVPE on a sapphire substrate. On an undoped GaN buffer followed by a doped n-GaN layer, the active region consists of a stack of three identical sequences, each with three quantum wells (QWs). The first two QWs nominally contain 15 % In (blue) and the third 40 % In (red). Each sequence is confined by an $Al_{0.32}Ga_{0.68}N$ layer. Finally, a p-doped $Al_{0.17}Ga_{0.83}N$ EBL is positioned, which is further capped by a dielectric DBR and processed, including metal contacts.

The LED is comprehensively characterized by cross-sectional cathodoluminescence performed in scanning transmission electron microscopy (STEM-CL) and by electroluminescence (EL). The luminescence along the growth direction is directly visualized in CL linescans: in particular, each QW can be spectrally and spatially resolved and shows a distinct emission. A wavelength shift for all QWs is observed. Furthermore, the n-GaN exhibits near-band-edge (NBE) luminescence at 356.7 nm at $T = 16$ K corresponding with a high free carrier concentration due to Burstein-Moss Shift.

The EL spectrum shows intense, broad emission around 650 nm, with a weak shift to shorter wavelengths for higher injection current.

HL 58.3 Fri 10:00 H14

Advanced nano-characterization of doped and undoped InGaN/GaN MQW-LED structures — •Luca Greczmiel, F. Bertram, G. Schmidt, P. Veit, H. Eisele, A. Dempewolf, S. Petzold, J. Christen, C. Berger, A. Dadgar, and A. Strittmatter — Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

In this study, we comprehensively investigate structural and optical properties of InGaN/GaN MQW-LED-structures by cathodoluminescence (CL) directly performed in a scanning transmission electron microscope (STEM). The LEDs are grown by MOVPE on top of an optimized GaN/sapphire template. The first pn-junction is formed by an 1.6 μm thick GaN:Si layer and a 345 nm thick GaN:Mg layer, which are nominally doped with a concentration of $7 * 10^{18}\ cm^{-3}$ and $2 * 10^{19}\ cm^{-3}$, respectively. In between the n- and p-layer a MQW is located, which is composed of a stack of five InGaN QWs being separated by GaN:Si barriers, with a thickness of 3 nm and 7 nm, respectively. The InGaN wells have a nominal In content of 12 %. In STEM-linescans of the active region along the sample cross-section, the first QW shows emission at shorter wavelengths with respect to the subsequent following QWs. For comparison, a second MQW structure was investigated, which was identically grown, but sandwiched between uGaN. In contrast to the first sample, the CL of the 1st QW shifts to longer wavelengths, with respect to the subsequently following QWs. Hence, this spectral shift of the 1st QW is supposed to depend on the electric field in the space charge region.

HL 58.4 Fri 10:15 H14

Physical properties and thermal stability of zirconium platinum nitride thin films — Rebecca Gallivan[1], Ana Michelini[1], Nensi Toncich[1], Nerea Abando Beldarrain[1], Julia Manser[1], Arnold Müller[2], Christof Vockenhuber[2], and •Henning Galinski[1] — [1]Laboratory for Nanometallurgy, Department of Materials, ETH Zurich,8093 Zurich, Zurich, Switzerland — [2]Laboratory of Ion Beam Physics, Department of Physics, ETH Zurich, 8093 Zurich, Zurich, Switzerland

By providing new functionality, ternary transition metal nitrides (TMNs) have the potential to greatly broaden the material design space. Nevertheless, the majority of systems have only been studied computationally, and translation to experimental synthesis is restricted by a lack of knowledge about their stabilizing mechanisms. In this talk, we discuss the fabrication of ternary Zr-Pt-N thin films and examine their physical properties [1]. We show that Pt replaces nitrogen on the nonmetallic sublattice, destabilizing the rock salt structure and forming a complicated cubic phase. Additionally, we observe the exsolution of Pt nano precipitates from the Zr-Pt-N films upon annealing as well as degradation in the nitridic film's thermal stability. Even at low concentrations, Pt facilitates a solid reaction with the Si substrate that is otherwise inaccessible in ZrN films.

[1] Appl. Phys. Lett. 125, 221901 (2024)

HL 59: 2D Semiconductors and van der Waals Heterostructures VI

The sesssion covers the physics of interlayer excitons and allied phenomena in van der Waals heterostructures.

Time: Friday 9:30–11:45 Location: H15

HL 59.1 Fri 9:30 H15

Interlayer excitons in electric and magnetic fields — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Over the past years, more and more two-dimensional (2D) materials have been stacked to heterostructures. Due to the coupling interlayer excitations can form.

Here we report on a trilayer heterostructure of MoS_2 and WS_2. In contrast to bilayers, the coupling may lead to quadrupolar excitons. These can be clearly identified by the quadratic response of the corresponding excitons in our GW/BSE calculations in electric fields. In the second example, we report our studies of bulk CrSBr [1]. In a magnetic field the lowest bright excitations of the antiferromagnetically coupled CrSBr shift quadratically. Our calculations reveal the symmetry forbidden dark excitons and the increasing interlayer character. We develop a minimal model to explains this spin-dependent coupling. Despite its simplicity, the proposed model is generally applicable to any coupled 2D magnet.

[1] https://arxiv.org/abs/2403.20174

HL 59.2 Fri 9:45 H15

Signature of Rydberg-like states of interlayer excitons in MoSe2/WSe2 heterostructures — •Chirag Chandrakant Palekar[1], Paulo E. Faria Junior[2], Tobias Manthai[1], Maximilian Nagel[1], Bhabani Sankar Sahoo[1], Shachi Machchhar[1], Avijit Barua[1], Jaroslav Fabian[2], Barbara Rosa[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The heterostructures of transition metal dichalcogenides (TMDCs), formed by the stacking of different TMDC monolayers (MLs), facilitates the formation of spatially indirect interlayer excitons (IX). Due to the higher binding energy, the excited excitonic states have typically been observed in TMDC monolayers for over a decade. Nevertheless, the Rydberg-like higher-order states of the IX in WSe2/MoSe2 HSs have thus far remained undetected due to their weak oscillator strength. In this work, we employ photoluminescence excitation (PLE) spectroscopy to identify the signatures of Rydberg-like higher order states of IX in WSe2/MoSe2 HSs. By examining HSs with varying twist angles, we are able to gain comprehensive insight into the twist angle dependence of such excited states of IX. We compare experimental and theoretical results on the twist angle-dependent behavior of observed states, providing a systematic investigation that advances current understanding of the optical and electronic properties of TMDC HS systems.

HL 59.3 Fri 10:00 H15

Twisted MoSe2 Homobilayer Behaving as a Heterobilayer — •Arka Karmakar — Institute of Experimental Physics, Faculty of Physics, University of Warsaw, 02-093 Warsaw, Poland

Heterostructures (HSs) formed by the transition-metal dichalcogenides (TMDCs) materials have shown great promise in next-generation (opto)electronic applications. Traditionally, at atomically closed proximity the charge transfer (CT) process dominates due to its fast timescale (< 50 fs). In this talk, I introduce our latest work [1] on the ET process in a twisted molybdenum diselenide (MoSe2) homobilayer without any charge-blocking interlayer, i.e., in atomically closed proximity. We fabricated an unconventional homobilayer (i.e., HS) with a large twist angle (~57°) by combining the chemical vapor deposition (CVD) and mechanical exfoliation (Exf.) techniques to fully exploit the lattice parameters mismatch and indirect/direct (CVD/Exf.) bandgap nature. These result in weakening the CT process and allowing the ET process to take over the carrier recombination channels. We employ a series of optical and electron spectroscopy techniques, complementing by the density functional theory (DFT) calculations, to describe a massive room temperature photoluminescence enhancement from the HS area due to an efficient ET process. Our results show that the electronically decoupled MoSe2 homobilayer is coupled by the ET process, mimicking a 'true' heterobilayer nature.

[1] A. Karmakar et al., "Twisted MoSe2 Homobilayer Behaving as a Heterobilayer", Nano Lett. 2024, 24, 31, 9459-9467.

HL 59.4 Fri 10:15 H15

Tailoring Interlayer Exciton Dyanamics of TMDC Heterostructures: From Bilayers to Trilayers embeded in Broadband DBR Cavities — •Bhabani Sankar Sahoo, Shachi Machchhar, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The photoluminescence yield of interlayer excitons (IX) at room temperature remains limited due to electrons and holes residing in different layers. In this work we propose and implement a novel way to enhance the IX emission in transition metal dichalcogenide (TMDC) heterostructures. We first introduce an additional WSe2 on top of a heterobilayers (HBL) of WSe2/MoSe2 to form a heterotrilayer (HTL) with different twist angles which significantly boost the PL emission upto one order magnitude, attributed to improved overlap of the electronic wavefunctions and additional radiative pathways. Further embedding this HTL within a chirped multiresonant distributed Bragg reflector (DBR) microcavity provides strong exciton confinement, enhancing the radiative recombination rate and modifying the exciton lifetime. Compared to the HBL, the HTL displays a reduced exciton lifetime, indicative of stronger light-matter coupling within the cavity, and a pronounced increase in PL intensity due to enhanced photon density of states. Our study highlights the potential of tailored stacking and cavity integration to manipulate light-matter interactions in advanced TMDC heterostructure devices for next-generation optoelectronic applications.

HL 59.5 Fri 10:30 H15

Effect of the Direct-to-Indirect Bandgap Crossover on the Reverse Energy Transfer — •Gayatri Gayatri[1], Debashish Das[2], Natalia Zawadzka[1], Takashi Taniguchi[3], Kenji Watanabe[3], Adam Babiński[1], Saroj K. Nayak[2], Maciej R. Molas[1], and Arka Karmakr[1] — [1]University of Warsaw, Warsaw, Poland — [2]Indian Institute of Technology Bhubaneswar, Odisha, India — [3]National Institute for Materials Science, Ibaraki, Japan

Heterostructures (HSs) made by the vertical stacking of van der Waals monolayers (1Ls) have shown great potential in (opto)electronic devices. In the type-II transition metal dichalcogenide HSs, long-range energy transfer (ET) happens via the dipole-dipole coupling (Förster type). To investigate this, we studied HS made by the 1L tungsten disulfide (WS2) and 1L-5Ls molybdenum disulfide (MoS2), with hexagonal boron nitride (hBN) as a charge-blocking interlayer, using differential reflection contrast, photoluminescence (PL), and photoluminescence excitation. At room temperature, PL enhancement has been observed in the neutral exciton of WS2 in the WS2-hBN-1L MoS2 and WS2-hBN-2L MoS2 regions as compared to the isolated WS2 emission. This enhancement confirms an efficient ET from MoS2 B excitonic level to WS2 A excitonic level. As the number of MoS2 layers increases, bandgap changes from direct-to-indirect, promoting more immediate carrier scattering from the K-valley. Consequently, carrier population decreases and ET becomes less effective.

HL 59.6 Fri 10:45 H15

Interlayer Exciton Traps in TMD heterobilayers — •Thomas Klokkers[1,2], Mirco Troue[1,2], Johannes Figueiredo[1,2], Andreas Knorr[3], Ursula Wurstbauer[4], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany — [3]Institute for Theoretical Physics, Nonlinear Optics and Quantum Electronics, Technical University of Berlin, 10623 Berlin, Germany — [4]Institute of Physics, Münster University, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Long-lived interlayer excitons in MoSe2/WSe2 heterostructures constitute a promising platform to explore many-body physics in a two-dimensional solid-state system. Introducing a trapping potential facilitates exploring the many-body regime by providing a platform to control the density of the interlayer exciton ensemble. Realizations of such exciton traps range from electrostatic strip gates to strain-induced potentials. In this work, we realize enhanced emission from interlayer excitons based on an optical trap. The laterally changed potential landscape allows the investigation of ensembles at high densities without the direct influence of temperature, excess charge carriers and laser-induced coherence.

15 min. break

HL 59.7 Fri 11:15 H15

Hybridized excitons in 2D van der Waals materials — •Andreas Stier — Walter Schottky Institut und TUM School of Natural Sciences, TU München, Garching, Deutschland

I will review our recent progress on magneto optical spectroscopy of atomically thin materials in magnetic fields up to 91 T with an emphasis on the spin-valley physics of neutral and charged excitons.

In monolayer (ML) semiconductors, magneto-absorption spectroscopy revealed the diamagnetic shifts of the exciton Rydberg states, which allowed the first direct experimental measure of the reduced mass and binding energy. Surprisingly, investigating the photoluminescence, we observe the emergence of a new excitonic peak, which we discuss in the framework of the theoretically predicted linear dispersing exciton branch originating from intervalley exchange interactions.

For heterostructures (HS) of a 2D semiconductor with graphene, we find a new multi-step proximity effect due to band folding in the HS, where we show that the spin-valley physics can be used to quantify interlayer hybridization. In HS from ML MoSe2 and the layered antiferromagnetic (AFM) semiconductor CrSBr, we show the formation of new exciton states depending on the twist angle. These excitons exhibit clear signatures of proximity coupling to the magnetic state of the AFM layer, such as hysteretic response to in- and out of plane B fields. We discuss these results in the framework of Ising-type spin-orbit proximity coupling.

HL 59.8 Fri 11:30 H15

Laterally extended states of interlayer excitons in reconstructed $MoSe_2/WSe_2$ heterostructures — •Johannes Figueiredo[1,2], Marten Richter[3], Mirco Troue[1,2], Jonas Kiemle[1,2], Hendrik Lambers[4], Torsten Stiehm[4], Ursula Wurstbauer[4], Andreas Knorr[3], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]Munich Center for Quantum Science and Technology (MCQST) — [3]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin — [4]Institute of Physics, Münster University

Heterostructures made from 2D transition-metal dichalcogenides are ideal platforms for exploring excitonic phenomena, including correlated moiré excitons and degenerate interlayer exciton ensembles. While atomic reconstruction is often assumed to localize excitons, we demonstrate that excitonic states in reconstructed $MoSe_2/WSe_2$ heterostructures can extend beyond the moiré periodicity [1]. Using real-space calculations, we provide lateral potential maps and corresponding excitonic wavefunctions for interlayer excitons in strain-relaxed heterostructures [2]. Cryogenic photoluminescence experiments corroborate the computed level structure and exciton relaxation dynamics. These findings align with recent coherence measurements on degenerate interlayer excitons and suggest potential many-body phenomena in dense, cold exciton ensembles [3].

[1] J. Figueiredo et al., arXiv:2411.19616 (2024) [2] M. Richter, PRB 109, 125308 (2024) [3] M. Troue and J. Figueiredo et al., PRL 131, 036902 (2023)

HL 60: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)

The joint focus session of the divisions HL and MA presents the latest developments of the rapidly growing community working with the van der Waals magnetic semiconductor CrSBr with distinct excitonic and magnetic properties, and it is organized by Shengqiang Zhou (HZ Dresden-Rossendorf), Farsane Tabata-Vakili (TU Braunschweig), and Florian Dirnberger (TU Munich).

Time: Friday 9:30–13:00 Location: H17

Invited Talk HL 60.1 Fri 9:30 H17

Constructing Artificial Matter in the Electron Microscope - Atomic Fabrication at Scale in CrSBr — •Julian Klein — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

The ability to control the arrangement of individual atoms has transcended naturally occurring configurations of matter, enabling experimental breakthroughs in quantum physics. I will show how we can now use scanning transmission electron microscopy to construct artificial atomic arrangements at scale and demonstrate it with the layered magnetic quasi-1D semiconductor CrSBr. By developing strategies to position the electron beam with picometer precision and perform rapid, targeted beam actions, we achieve deterministic control over the movement of Cr atoms in space and time. With this capability, we selectively steer Cr atoms into interstitial positions, forming localized quantum states while simultaneously monitoring atomic movements in real time with microsecond resolution. Fully automating the electron microscope enables us to construct ordered arrays of Cr interstitial superlattices atom by atom as well as nonperiodic structures, spanning hundreds of locations over tens of nanometers, all within minutes. Our results show that atomic fabrication at scale in the electron microscope is now a reality, unlocking unprecedented opportunities to construct quantum defects and phases, atom by atom, in the solid state, that extend over macroscopic length scales.

Invited Talk HL 60.2 Fri 10:00 H17

Tuning the structure and magnetism in CrSBr via external pressure — •Ece Uykur — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

As one of the two-dimensional (2D) van der Waals (vdW) magnets, CrSBr regained significant attention recently because it is air-stable even in the monolayer form making this compound very attractive. It shows strong coupling between its magnetic, electronic, structural, and optical properties [1]. Several ab initio calculations put forward the importance of the balance between Cr-Cr direct exchange and Cr-anion-Cr superexchange interactions and showed that the A-type antiferromagnetism in this compound is delicately balanced with these short- and long-range magnetic interactions [2]. Therefore, studies exploring the tunability of the inter- and inralayer coupling are important and one plausible experimental strategy is the external pressure.

In this talk, I will summarize our recent efforts on high-pressure single crystal XRD and magnetization studies on CrSBr. We performed single crystal XRD studies up to ~20 GPa, which reveals a non-monotonous behavior of Cr-ion in the structure along with a structural phase transition above 17 GPa. The movement of this Cr-ion has also direct link with the magnetization of the compound that is studied with the high-pressure magnetic susceptibility measurements up to ~8 GPa.

[1] K. Lin et al., ACS Nano 18, 2898 (2024) [2] J. Cenker et al., Nat. Nanotechnol. 17, 256 (2022).

Invited Talk HL 60.3 Fri 10:30 H17

A theoretical perspective on exciton-magnon coupling and its implications — •Akashdeep Kamra — Department of Physics, Rheinland-Pfälzische Technische Universität (RPTU) Kaiserslautern-Landau, Kaiserslautern, Germany

The dependence of exciton energies on the magnetic order in CrSBr has opened avenues for controlling optical properties using magnetic fields. Conversely, it has enabled an optical time-resolved sensing of the magnetic degrees of freedom. This has further been exploited to investigate the interplay between excitons and magnons, the excitations of the magnetic order. We will discuss how excitonic energies offer a convenient access to coherent as well as thermal magnon dynamics. Focusing on transport, we will discuss the recent observation of the magnon-exciton drag effect that makes it feasible to leverage thermal magnon currents for transporting excitons at unexpectedly fast velocities. Finally, we will conclude with a brief discussion of emergent non-linearities in exciton energies mediated by the magnonic modes in the canted magnetic state of CrSBr.

1. F. Dirnberger et al., Magneto-optics in a van der Waals magnet tuned by self-hybridized polaritons, Nature 620, 533 (2023).

2. F. Dirnberger, S. Terres, Z. A. Iakovlev, K. Mosina, Z. Sofer, A. Kamra, M. M. Glazov, and A. Chernikov, Exciton transport driven by spin excitations in an antiferromagnet (unpublished).

3. B. Datta et al., Magnon-mediated exciton-exciton interaction in a van der Waals antiferromagnet, arXiv:2409.18501.

15 min. break

Invited Talk HL 60.4 Fri 11:15 H17

Exciton and valley properties of monolayer transition metal dichalcogenides on the van der Waals magnetic semiconductor CrSBr — •Yara Galvao Gobato — Universidade Federal de Sao Carlos, Sao Carlos, Brazil

Chromium sulfide bromide is a promising van der Waals (vdW) magnetic material, undergoing a magnetic phase transition to an A type antiferromagnetic state below the Neél temperature of about 132K in its bulk form. VdW heterostructures composed of monolayer transition metal dichalcogenides (TMDs) and vdW magnetic materials such as CrSBr are an interesting platform to modify valley and excitonic properties of non-magnetic TMDs. In this talk, we will present our recent results on optical and magneto-optical properties of monolayer TMDs on CrSBr under different magnetic field orientations. Remarkably, we have observed a clear influence of the CrSBr magnetic order on the exciton and valley properties of monolayer TMDs, such as an anomalous linear polarization dependence, unsual temperature dependence of emission energies, magnetic field dependence of the emission intensity, and valley g-factor values with clear signatures of an asymmetric magnetic proximity exchange interaction. Our results are explained by asymmetric magnetic proximity effects, charge transfer and a possible contribution of exciton/trion magnon coupling. Our studies suggest that vdW heterostructures with antiferromagnetic nonmagnetic interfaces are interesting platforms to modify the valley and excitonic properties of TMDs for possible applications in opto-spintronics and quantum technology.

HL 60.5 Fri 11:45 H17

Ab initio studies on the electronic and optical properties of magnetic CrSBr — •Marie-Christin Heissenbüttel[1], Pierre-Maurice Piel[2], Julian Klein[3], Thorsten Deilmann[1], Ursula Wurstbauer[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Physical Institute, University of Münster, Germany — [3]Department of Materials Science and Engineering, MIT, Massachusetts, USA

CrSBr recently emerged as a van der Waals layered material exhibiting intriguing electronic and optical properties arising from the intricate interplay between crystal structure and layered magnetic order. A thorough understanding of these effects is essential to assess its potential for applications in spintronic and quantum devices. Due to the large crystal anisotropy, the monolayer, multilayer, and bulk crystal CrSBr show a quasi-one-dimensional behaviour of effective masses and exciton wavefunctions [1]. The interlayer antiferromagnetic (AFM) coupling suppresses layer to layer interactions in the magnetic ordered low temperature phase, resulting in strong quantum confinement of electrons and excitons within the individual layers [2]. Using ab-initio *GW*/Bethe-Salpeter equation calculations, we analyze electronic and excitonic properties on the same footing and elucidate how the AFM van der Waals stacking, symmetry properties and the large crystal anisotropy govern the electronic and optical properties of this material.

[1] https://doi.org/10.1021/acsnano.2c07316
[2] https://doi.org/10.48550/arXiv.2403.20174

HL 60.6 Fri 12:00 H17

Internal structure and ultrafast dynamics of quasi- 1D excitons controlled by magnetic order — •N. Nilforoushan[1], M. Liebich[1], M. Florian[2], F. Mooshammer[1,3], A. D. Koulouklidis[1,3], L. Wittmann[1], K. Mosina[4], Z. Sofer[4], F. Dirnberger[5], M. Kira[2], and R. Huber[1,3] — [1]Dept. of Physics, University of Regensburg, Germany — [2]Dept. of Electrical Engineering and Computer Science, University of Michigan, USA — [3]RUN, University of Regensburg, Germany — [4]Dept. of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [5]Dept. of Physics, Technical University of Munich, Germany

In van der Waals (vdW) layered crystals, Coulomb correlations are often tuned by structural engineering, giving rise to emergent phenomena such as tightly bound excitons and exotic electronic and magnetic phases. Magnetic vdW materials offer a unique platform for in situ control of Coulomb correlations enabled by their intrinsic magnetic order. Here, we present quantitative experiment-theory proof that excitonic correlations can be tailored through spin order in the vdW magnet CrSBr. By probing internal transitions of excitons with phase-locked mid-infrared pulses, we reveal their binding energy and strong anisotropy of their quasi-1D orbitals resulting in significant fine-structure splitting. We switch excitons from monolayer-localized to interlayer-delocalized species by pushing the system from the antiferromagnetic to the paramagnetic phase. The exciton's ultrafast dynamics further support this scenario. In future applications, excitons may be interfaced with spintronics enabling on-demand phase transitions.

HL 60.7 Fri 12:15 H17

Raman controlled lithium intercalation into CrSBr van der Waals structure — •Kseniia Mosina, Aljoscha Söll, Martin Veselý, Jiří Šturala, and Zdenek Sofer — Department of Inorganic Chemistry, University of Chemistry and Technology Prague, 166 28 Prague 6, Czech Republic.

Lithium intercalation into the van der Waals crystalline structure of layered transition metal dichalcogenides by means of chemical and electrochemical intercalation is a well-known method for studying semiconductor-metallic phase transitions. The layered semiconductor chromium sulphur bromine (CrSBr) in recent years becomes an ultimate playground for the studies of low-dimensional magneto-optical properties. The interlayer distance of CrSBr allows the easy cleavage and intercalation of the guest molecules within the crystalline structure. Conveniently air-stable, this material exhibits a direct band gap of 1.5 eV, an antiferromagnetic state in bulk and ferromagnetism in the monolayer. Here, we present the lithium intercalation method into the CrSBr structure by lithium-solvated electron solution. To monitor the lithiation process in real-time, we investigated the Raman spectra evolution upon lithium ion intercalation into a few-layered CrSBr flake. Our findings suggest that the quasi-one dimensional nature of CrSBr leads to weak interlayer hybridization along the b-direction, which facilitates the diffusion of guest ions by lowering the migration energy barrier and enables anisotropic Li+ diffusion. The reliable intercalation methodology allows tracking the intercalation process directly in the desired area favorable for device fabrication.

Invited Talk HL 60.8 Fri 12:30 H17

Electric field control of intra- and interlayer excitons in CrSBr — •Nathan Wilson[1], Amine Ben Mhenni[1], Ferdinand Menzel[1], Alain Dijkstra[1], Zdenek Sofer[2], and Jonathan Finley[1] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]Institute of Chemistry and Technology, Prague, Czech Republic

In the 2D magnetic semiconductor CrSBr, the interplay between a direct bandgap for all layer thicknesses and layered antiferromagnetism with strong magneto-electronic coupling give rise to rich but poorly understood excitonic physics. So far, the presence of two closely spaced conduction bands and existence of both intra and interlayer excitons in multilayers has complicated interpretation of the optical spectrum of its excitons. Here, we study monolayers and bilayers of CrSBr in dual-gated structures, allowing for independent tuning of electric field and charge doping. Our study reveals the existence of the previously unobserved ground state exciton in monolayers, which is darkened both by charge doping and electric field. We find that both intralayer and hybrid intra/interlayer excitons are highly sensitive to the vertical electric field, implying a reasonably large exciton polarizability and control over wavefunction symmetry. With this information, we are able to form a more complete picture of the real space and band character of the excitons in CrSBr.

HL 61: THz and MIR physics in semiconductors

The session covers the THz and MIR physics in semiconductors.

Time: Friday 10:45–11:45 Location: H14

HL 61.1 Fri 10:45 H14

Multi-photon Stark spectroscopy of ultrafast THz waveforms — •Fabian Brütting, Moritz B. Heindl, and Georg Herink — Experimental Physics VIII, University of Bayreuth, Germany

Microscopic electric waveforms can be encoded into luminescence modulations through the quantum-confined Stark effect, enabling ultrafast "videography" of local electric fields up to THz frequencies. This technique, known as Quantum-probe field microscopy (QFIM), relies on the coupling of momentary electric fields with electronic transitions in colloidal quantum dots, with detection achieved via pump-probe microscopy [1].

Here, we propose two-photon absorption (TPA) as a novel probing regime for accessing the THz-driven Stark effect. Unlike conventional Stark spectroscopy, which relies on linear one-photon absorption, TPA operates under different selection rules, resulting in distinct interaction dynamics. In particular, depending on the specific transitions being probed, we observe a sign flip of the nonlinear electro-absorption contribution relative to the linear signal. Consequently, the overall electro-absorption signal is either enhanced, reduced or even inverted compared to the linear signal.

Therefore, two-photon Stark spectroscopy offers potential for improving QFIM detection sensitivity and provides a novel strategy for the ultrafast manipulation of the optical properties in low-dimensional semiconductors.

[1] Heindl, Moritz B., et al. "Ultrafast imaging of terahertz electric waveforms using quantum dots." *Light Sci. Appl.* 11.1 (2022): 5.

HL 61.2 Fri 11:00 H14

Characterization of SiC epilayers with terahertz time-domain spectroscopy — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Christian Röder[3], Franziska Beyer[3], Kuei-Shen Hsu[4], Jan Beyer[4], Nadine Schüler[5], Nico Vieweg[6], Katja Dutzi[6], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department of Materials Characterization and Testing, Fraunhofer ITWM, Kaiserslautern — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau — [3]Department Energy Materials and Test Devices, Fraunhofer IISB, Erlangen — [4]Institute of Applied Physics, Technische Universität Bergakademie Freiberg — [5]Freiberg Instruments GmbH, Freiberg — [6]TOPTICA Photonics AG, Gräfelfing

Silicon carbide (SiC), being a wide-bandgap and robust, temperature-stable semiconductor, is an up-and-coming material that already has applications in power electronics and in high-temperature environments. While the characterization of the electrical and optical properties of bulk semicondcutors with terahertz time-domain spectroscopy (TDS) has already been demonstrated, many applications make use of thin layers with thicknesses of a few tens of microns. Using the Drude model, we performed simulations with varying thicknesses and charge carrier densities of SiC epilayers showcasing the opportunities and possible limitations of TDS to characterize SiC epilayers. Finally, TDS measurements demonstrating the validity of the simulations were used to determine the charge carrier density of SiC epilayers.

HL 61.3 Fri 11:15 H14

Diminishing topological Faraday effect in thin layer samples — Christian Berger, Florian Bayer, Laurens W. Molenkamp, and •Tobias Kiessling — Physikalisches Institut, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

A striking feature of three-dimensional topological insulators (TIs) is the theoretically expected topological magnetoelectric (TME) effect, which gives rise to additional terms in Maxwell's laws of electromagnetism with an universal quantized coefficient proportional to half-integer multiples of the fine-structure constant. In an ideal scenario one therefore expects also quantized contributions in the magnetooptical response of TIs.

We review this premise by taking into account the trivial dielectric background of the TI bulk and potential host substrates, and the often present contribution of itinerant bulk carriers. We show (i) that one obtains a nonuniversal magnetooptical response whenever there is impedance mismatch between different layers and (ii) that the detectable signals due to the TME rapidly approach vanishingly small values as the impedance mismatch is detuned from zero.

HL 61.4 Fri 11:30 H14

Unraveling the Microscopic Mechanism of Displacive Excitation of Coherent Phonons in a Bulk Rashba Semiconductor — •Peter Fischer[1], Julian Bär[1], Moritz Cimander[1], Volker Wiechert[1], Oleg Tereshchenko[2], and Davide Bossini[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany — [2]Nowosibirsk, Russia

Optically driven lattice excitations have recently been intensively investigated as a means to manipulate the macroscopic properties of quantum materials. In solids with an electronic band gap, it is well-established that coherent phonons can be excited by laser pulses with photon energies exceeding the band-gap energy. However, the dominant microscopic mechanism has still not been pinpointed: Neither experimentally nor theoretically has it been possible to disentangle the effect of a photo-induced change in the charge-carrier density from an increase of the carrier temperature. We perform time-resolved pump-probe spectroscopy on the Rashba semiconductor BiTeI. Tuning the pump-photon energy from the visible to the mid-infrared allows us to excite both interband and barely accessible intraband transitions. As a result, we determine that the lattice modes are mainly driven by the increased carrier temperature. In addition, the phonon coherence time in the intraband regime proves robust against an increase in laser fluence. These findings provide new insights for the development of schemes addressing the coherent structural manipulation of solids.

HL 62: 2D Semiconductors and van der Waals Heterostructures VII

The session covers the physics of quantum emitters and defects in 2D materials and their heterostructures. Note, the session starts directly after the session "2D Semiconductors and van der Waals Heterostructures VI".

Time: Friday 11:45–13:00 Location: H15

HL 62.1 Fri 11:45 H15

Deterministic Purcell enhancement of single photon emission from a WSe_2 monolayer quantum emitter — •Ivan Solovev[1], Victor Mitryakhin[1], Sven Stephan[1,2], Jens-Christian Drawer[1], Lukas Lackner[1], Seth Tongay[3], Kenji Watanabe[4], Takashi Taniguchi[5], Martin Esmann[1], and Christian Schneider[1] — [1]Institute for Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany — [2]University of Applied Sciences Emden/Leer, Emden, Germany — [3]Materials Science and Engineering, School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona, USA — [4]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Bright and easily fabricated quantum emitters in two-dimensional semiconductors have emerged as a promising platform for scalable quantum communication [1,2]. Here, we show, how their performance can be markedly elevated by integrating a monolayer into a versatile open plano-concave Fabry-Pérot microcavity. We managed to modulate radiative decay rate of a zero-phonon line by tuning a high Q-factor cavity. Reached five-fold shortening of the lifetime opens the route towards higher rates of quantum key distribution and generation of indistinguishable single photons in 2D semiconductors.

[1] J.C. Drawer et al., Nano Lett. 23 (18), 8683 (2023). [2] T. Gao et al. npj 2D Mater Appl 7, 4 (2023).

HL 62.2 Fri 12:00 H15

Deterministic generation of single-photon emitters in 2D materials by in-situ electron beam lithography — •Shachi Machchhar, Bhabani Sankar Sahoo, Yuhui Yang, Imad Limame, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The development of on-demand sources of single photons with high indistinguishability represents a crucial step in the creation of photonic quantum systems, such as those required for the construction of large-scale quantum networks for the secure transfer of data. One potential avenue for the realization of such sources in a scalable and cost-effective manner is the exploitation of defect centres in transition metal dichalcogenides (TMDCs). The fabrication of these defect centres in TMDC monolayers can be achieved through the introduction of strain, ion implantation, and the structuring or patterning of the substrate. In this study, we employ cathodoluminescence (CL) spectroscopy at cryogenic temperatures to probe hBN-encapsulated WSe* and utilise in-situ electron beam lithography (iEBL) to structure pre-determined patterns on the emission active region. This nanopatterning of the monolayer facilitates the deterministic gener-

ation of single-photon emitters (SPEs) with distinct quantum optical properties. Furthermore, we demonstrate the single-photon nature of these SPEs through second-order correlation measurements on the MLs. Additionally, we study the temperature dependence of such SPEs generated in various patterned geometries.

HL 62.3 Fri 12:15 H15

Generation of luminescent defects in hBN by focused helium ion beam irradiation — •Amedeo Carbone[1,2], Martijn Wubs[1], Alexander W. Holleitner[2], Christoph Kastl[2], Alexander Huck[3], and Nicolas Stenger[1] — [1]Department of Electrical and Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]Walter Schottky Institute, Physik Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [3]Center for Macroscopic Quantum States (bigQ), Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Among the luminescent centres in hBN, which have recently gained attention because of their brightness and exceptional quantum properties at room temperature, the charged boron vacancy (V_B^-) defect stands out for its magnetic properties, which have significant applications in quantum sensing schemes [1]. In the present work [2] we irradiate hBN flakes with a focused helium ion beam to generate V_B^- defects, conduct optical and magnetically resolved characterization, and apply a theoretical model [3] to infer the generated density of charged emitters. These results are further compared to the estimated vacancy density from Molecular Dynamics simulations. Our work provides a systematic study of the defect generation efficiency by comparing different irradiation doses.

[1] Gottscholl, A. et al., *Nat. Mater.* 19, 540-545 (2020), [2] Carbone, A. et al., *in preparation*, [3] Udvarhelyi, P. et al., *npj Comp. Mat.* 9, 150 (2023).

HL 62.4 Fri 12:30 H15

Impact of low-energy ion-irradiation induced defects on optical and vibrational properties of molybdenum disulfide — •Philipp Kraus, Eileen Schneider, Tobias Dierke, Stefan Wolff, Yuri Koval, and Janina Maultzsch — Chair of Experimental Physics, FAU Erlangen-Nürnberg, Erlangen

We present the controlled creation of vacancies in 2D materials, in particular graphene and molybdenum disulfide (MoS_2), by low-energy ion-irradiation. With Raman spectroscopy on exfoliated graphene flakes before and after irradiation, we determined the defect density to calibrate the ion dose of our setup. Then, we irradiated MoS_2 monolayers, grown via chemical vapor deposition (CVD), and determined the impact of the ion-induced defects on Raman and photoluminescence (PL) spectra. These results are additionally compared with density functional theory (DFT) calculations.

HL 62.5 Fri 12:45 H15

Composition- and strain-dependent quantum dot states in transition metal dichalcogenide nanobubbles — •Stefan Velja, Jannis Krumland, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Mechanical deformations in transition metal dichalcogenide monolayers can appear both spontaneously and artificially, giving rise to peculiar nanostructures, such as nanobubbles, or nanowrinkles. These systems have been observed to harbor localized states in the gap region, a known prerequisite for single-photon emission. While recent theoretical studies have attempted to explain these phenomena on selected systems [1,2], a detailed analysis concomitantly examining the role of the chemical constituents and the amount of applied strain is essential to gain full insight. In this work, we investigate the electronic properties of MX_2 nanobubbles (M=Mo, W and X=S, Se) characterized by varying levels of local strain. For materials composed of lighter elements, localized states appear in the gap region when the deforming force reaches the order of 0.01 a.u./atom. A thorough analysis of these states sets the stage for predicting and interpreting the optical fingerprints of these nanostructures.

[1] Krumland et al., *ACS Photonics* **11**, 586 (2024)
[2] Velja et al., *Nanoscale* **16**, 7134 (2024)

HL 63: Focus Session: Nanoscale Light-matter Interaction II

The focus session highlights recent breakthroughs in resolving the optoelectronic properties of individual nanostructures down to the atomic scale. Moreover, the session introduces the rich field of surface polaritons, confined electromagnetic modes through which light can be guided on subwavelength scales.

The session is the second part of the focus session on nanoscale light-matter interaction.

Time: Friday 12:00–13:15 Location: H14

HL 63.1 Fri 12:00 H14

Super-resolution imaging of nanoscale inhomogeneities in hBN-covered and encapsulated few-layer graphene — •Lina Jäckering, Konstantin G. Wirth, Lukas Conrads, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Encapsulating few-layer graphene (FLG) in hexagonal boron nitride (hBN) can cause nanoscale inhomogeneities in the FLG, including changes in stacking domains and topographic defects.[1] Due to the diffraction limit, characterizing these inhomogeneities is challenging. Recently, the visualization of stacking domains in encapsulated four-layer graphene (4LG) has been demonstrated with phonon polariton (PhP)-assisted near-field imaging.[2] However, the underlying coupling mechanism and ability to image subdiffractional-sized inhomogeneities remain unknown. Here, we retrieve direct replicas and magnified images of subdiffractional-sized inhomogeneities in hBN-covered trilayer graphene (TLG) and encapsulated 4LG, enabled by the hyperlensing effect.[3] This hyperlensing effect is mediated by hBN*s hyperbolic PhP that couple to the FLG*s plasmon polaritons. Using near-field microscopy, we identify the coupling by determining the polariton dispersion in hBN-covered TLG to be stacking-dependent. Our work demonstrates super-resolution and magnified imaging of inhomogeneities, paving the way for the realization of homogeneous encapsulated FLG transport samples to study correlated physics.

[1] Geisenhof et al. ACS Appl. Nano Mater. **2**, 6067 (2019). [2] Liu et al. Nat. nanotech. **19**, 188-195 (2024). [3] Li et al. Nat. Commun. **6**, 7507 (2015).

HL 63.2 Fri 12:15 H14

Optical and Electrical Properties of Copper Oxide * Polyvinyl Alcohol Nanocomposites for Solar Cell Applications — •Ahed AL-Faouri[1,2], Mahmoud Abu-Kharma[1], and Mahmoud Hatem[1] — [1]Department of Physics, Faculty of Science, Al-Balqa Applied University, Al-Salt, Jordan — [2]Basic Sciences Department, Faculty of Arts and Sciences, Al-Ahliyya Amman University, Amman, Jordan

Copper oxide nanoparticles (CuO-NPs) were successfully synthesized at ambient temperature using an easy and eco-friendly method, employing the aqueous extract of bougainvillea leaves as reducing and stabilizing agents. First, a thin film of pure polyvinyl alcohol (PVA) was prepared via solution casting. Subsequently, four CuO-PVA nanocomposites were fabricated through solution casting at concentrations of (13, 30, 40, and 51) wt%. The optical and electrical properties of the synthesized CuO NPs, pure PVA, and CuO-PVA thin films were investigated using a UV-Vis spectrophotometer and a Keithley electrometer.

The band gap (Eg) of prepared CuO-NPs was 2.74 eV. The separation of this band gap renders CuO-NPs a suitable material for solar energy conversion and could potentially be used as an active layer material in solar cells., Furthermore, the four prepared CuO-PVA showed that the optical band gap decreased from 4.42 eV (pure PVA) to 3.34 eV (50%CuO-PVA). Further, increased DC electric conductivity was observed

HL 63.3 Fri 12:30 H14

Accessing phase and group velocities of terahertz surface plasmon polaritons in graphene using near-field spacetime imaging — •Simon Anglhuber[1], Martin Zizlsperger[1], Eva A. A. Pogna[2], Yaroslav A. Gerasimenko[1], Anastasios D. Koulouklidis[1], Imke Gronwald[1], Svenja Nerreter[1], Leonardo Viti[3], Miriam S. Vitiello[3], Rupert Huber[1], and Markus A. Huber[1] — [1]Regensburg Center for Ultrafast Nanoscopy (RUN) and Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerche (CNR-IFN), Milano, I-20133, Italy — [3]NEST, CNR - Istituto Nanoscienze and Scuola Normale Superiore, Piazza San Silvestro 12, 56127, Pisa, Italy

The combination of light and matter properties in surface polaritons offers unprecedented opportunities for controlling energy flow and information processing at the nanoscale. Here, we present a novel THz near-field imaging approach to visualize polariton propagation directly in the time domain. Our method allows for the extraction of phase and group velocities, as well as damping. Thus, it

reveals substantial insights into the polariton dispersion curve, even for strongly damped modes. Additionally, we show that our analysis can be expanded to two dimensions, directly visualizing polariton propagation in arbitrary directions, which is especially valuable for anisotropic materials. Finally, the method offers an intuitive approach to visualize non-equilibrium polariton propagation, e.g. upon photoexcitation. Thereby, we achieve subcycle control over polariton dynamics.

HL 63.4 Fri 12:45 H14

Inelastic electron-light interaction probed by holographic scanning transmission electron microscopy — •Nora Bach[1,2], Tim Dauwe[1,2], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Quantitative phase-contrast imaging of electrostatic potentials is an important application in transmission electron microscopy. Recently developed techniques have overcome the challenge to measure phase profiles inherited from optical fields, but offer only limited variability in tailoring the electron-light interactions and require a highly coherent electron source [1,2]. In this contribution, we introduce scanning transmission electron microscopy with spatially separated coherent electron probes [3] for the full imaging of complex optical near fields at a nanostructure with high spatial resolution. In the far field, these electron probes interfere to form a hologram from which we reconstruct phase shifts induced both by elastic scattering processes and by stimulated inelastic interactions. One particular advantage of STEM holography is the relaxed coherence requirements, which could be central to improving time-resolved imaging of electric and magnetic fields on the nanoscale.

[1] Gaida et al., Nat Commun. 14, (2023)
[2] Gaida et al., Nat. Photon. 18 (2024)
[3] Fehmi et al., J. Phys. D: Appl. Phys. 51 (2018)

HL 63.5 Fri 13:00 H14

Unraveling ultrafast exciton dynamics in a monolayer of the magnetic semiconductor CrSBr — •Jakob Schlosser[1], Christian Meineke[1], Martin Zizlsperger[1], Marlene Liebich[1], Niloufar Nilforoushan[1], Kseniia Mosina[2], Sophia Terres[3], Alexey Chernikov[3], Zdenek Sofer[2], Markus A. Huber[1], Matthias Florian[4], Mack Kira[4], Florian Dirnberger[3], and Rupert Huber[1] — [1]University of Regensburg, Regensburg — [2]University of Chemistry and Technology Prague, Prague — [3]Dresden University of Technology, Dresden — [4]University of Michigan, Ann Arbor

Among van der Waals semiconductors, CrSBr stands out as both its bulk and monolayer forms host tightly bound, quasi-1D excitons in a magnetic environment. Despite the strong attention these quasiparticles have attracted, their lifetimes remained unknown. Terahertz spectroscopy can directly probe the dynamics of all electron-hole pairs, independently of interband selection rules. Yet the corresponding far-field foci substantially exceed the lateral sample dimensions. Here, we combine terahertz polarization spectroscopy with near-field microscopy to study the dynamics of bound and unbound electron-hole pairs in bulk CrSBr and extract the nonequilibrium dielectric function of the monolayer in a model-free manner. Interestingly, the femtosecond decay of paramagnetic excitons in monolayer CrSBr is found to be 30 times shorter than the determined lifetime in bulk material. Our results mark the first direct access to the ultrafast dielectric response of quasi-1D excitons in CrSBr, to advance the development of quantum devices based on ultrathin van der Waals magnets.

Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

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Overview of Invited Talks and Sessions

(Lecture halls H9; Poster P1)

Invited Talks

KFM 1.1	Mon	9:30–10:00	H9	**Epitaxial films of layered perovskite-based ferroelectrics: phase stability, polarization enhancement, and pathways to polar metallicity** — •Elzbieta Gradauskaite
KFM 8.1	Tue	9:30–10:00	H9	**Ferrolectric bubble currents** — •Hugo Aramberri
KFM 11.1	Wed	9:30–10:00	H9	**Towards 3D nanoscale chemical mapping with atom probe tomography** — •Kasper Hunnestad, Constantinos Hatzoglou, Antonius van Helvoort, Dennis Meier
KFM 12.1	Wed	11:00–11:30	H9	**Model-assisted Insight into Degradation of Li-Ion Batteries during Thermal Abuse** — •Ulrike Krewer, Leon Schmidt, Jorge Valenzuela
KFM 15.1	Thu	9:30–10:00	H9	**Is CVD diamond now ready to become an electronic material?** — •Philippe Bergonzo
KFM 18.1	Thu	15:30–16:00	H9	**Domain gratings of sub-micrometer period for quantum technologies** — •Carlota Canalias

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff, Matthias Florian, Frank Jahnke
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger, Julian Wiercinski, Moritz Cygorek

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

KFM 1.1–1.6	Mon	9:30–11:15	H9	**(Multi)ferroic States: From Fundamentals to Applications (I)**
KFM 2.1–2.13	Mon	9:30–13:00	H13	**Perovskite and Photovoltaics I (joint session HL/KFM)**
KFM 3.1–3.10	Mon	9:30–12:15	H16	**Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)**
KFM 4.1–4.6	Mon	11:30–13:00	H9	**(Multi)ferroic States: From Fundamentals to Applications (II)**
KFM 5.1–5.7	Mon	15:00–17:00	H9	**Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons**
KFM 6.1–6.1	Mon	15:00–15:30	H10	**Invited Talk: X. Fang (joint session MM/KFM)**
KFM 7.1–7.5	Mon	17:15–18:30	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
KFM 8.1–8.7	Tue	9:30–11:30	H9	**(Multi)ferroic States: From Fundamentals to Applications (III)**
KFM 9.1–9.5	Tue	11:45–13:00	H9	**(Multi)ferroic States: From Fundamentals to Applications (IV)**
KFM 10.1–10.5	Tue	14:00–15:15	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
KFM 11.1–11.4	Wed	9:30–10:45	H9	**(Multi)ferroic States: From Fundamentals to Applications (V)**
KFM 12.1–12.6	Wed	11:00–12:45	H9	**Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Modelling of Battery Materials and Degradation)**
KFM 13.1–13.7	Wed	15:00–16:45	H9	**Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Experimental Characterisation and Safety Testing)**
KFM 14.1–14.26	Wed	17:00–18:30	P1	**Poster**
KFM 15.1–15.12	Thu	9:30–13:15	H9	**Crystal Structure Defects / Real Structure / Microstructure**
KFM 16.1–16.13	Thu	9:30–13:00	H13	**Perovskite and Photovoltaics II (joint session HL/KFM)**
KFM 17.1–17.5	Thu	11:45–13:00	H23	**Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)**
KFM 18.1–18.7	Thu	15:30–17:45	H9	**Materials Research in Polar Oxides: Perspectives for Optics & Electronics**
KFM 19	Thu	18:00–19:00	H9	**Members' Assembly**

Members' Assembly of the Crystalline Solids and their Microstructure Division

Thursday 18:00–19:00 H9

Sessions

– Invited Talks, Contributed Talks, and Posters –

KFM 1: (Multi)ferroic States: From Fundamentals to Applications (I)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Johanna Nordlander (University of Zurich)

Time: Monday 9:30–11:15 Location: H9

Invited Talk KFM 1.1 Mon 9:30 H9

Epitaxial films of layered perovskite-based ferroelectrics: phase stability, polarization enhancement, and pathways to polar metallicity — •Elzbieta Gradauskaite — Laboratoire Albert Fert, CNRS/Thales, Palaiseau, France

Layered perovskite-based compounds offer a range of unconventional properties stemming from their pronounced unit-cell anisotropy. While most renowned for the superconductivity observed in the Ruddlesden-Popper phases, many of these layered compounds are also ferroelectric and exhibit a sizeable in-plane polarization. In this talk, I will review different classes of layered perovskite-based ferroelectrics and the unique functionalities arising from their structural anisotropy.

In particular, the focus will be placed on Carpy-Galy $A_nB_nO_{3n+2}$ phases characterized by 110-oriented perovskite planes interleaved with additional oxygen layers. These compounds have been proposed as platforms for hosting both metallicity and polar displacements. However, their synthesis challenges have hindered integration into devices. Addressing this, our study focuses on $La_2Ti_2O_7$, an n=4 representative of the Carpy-Galy family, exploring its epitaxial growth and concurrent phase stability. Surprisingly, we find that high tensile strain facilitates a controlled layer-by-layer growth mode, yielding films that are ferroelectric from a single unit cell and exhibit polarization enhanced by a factor of four compared to bulk crystals. Most importantly, we show that metallicity in Carpy-Galy films can be induced via interfacial redox processes with a reactive metal, laying the foundation for exploring them as functional polar metals.

KFM 1.2 Mon 10:00 H9

Tailoring ferroelectric to antipolar phase interconversion in multiferroic thin films — •Bixin Yan[1], Marvin Müller[1], Hyeon Ko[1], Yen-Lin Huang[2,3,4], Haidong Lu[5], Alexei Gruverman[5], Ramamoorthy Ramesh[3,4,6], Marta D. Rossell[7], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich, Switzerland — [2]National Yang Ming Chiao Tung University, Taiwan — [3]University of California, Berkeley, USA. — [4]Lawrence Berkeley Laboratory, USA. — [5]University of Nebraska-Lincoln, USA — [6]Rice University, USA. — [7]Empa, Switzerland.

Inversion-symmetry breaking and the emergence of a polar state are essential for technologically relevant effects such as ferroelectricity and nonlinear optical properties. Hence, the ability to reversibly control the onset of such symmetry breaking can be instrumental in establishing emergent computing schemes. In this work, we present a novel approach for reversible control over the ferroelectric-to-antipolar phase transition in epitaxial multiferroic La-substituted $BiFeO_3$ (LBFO) thin films using local pressure and electric field. Utilizing local stress application via a scanning-probe-microscopy tip, we stabilize the antipolar phase. An electric field restores the original ferroelectric phase. Leveraging these insights, we establish the continuous tuning of the ferroelectric/antipolar phase coexistence and can set the net polarization of LBFO to any desired value between its saturation limits. Finally, using optical second harmonic generation as a non-invasive probe, we control the net polarization of our films in device-compliant capacitor heterostructures.

KFM 1.3 Mon 10:15 H9

Unconventional Polarization Response in Titanite-type Oxides due to Hashed Antiferroelectric Domains — •Hiroki Taniguchi[1], Takumi Watanabe[1], Taro Kuwano[2], Akitoshi Nakano[1], Yukio Sato[3], Manabu Hagiwara[4], Hiroko Yokota[2], and Kazuhiko Deguchi[1] — [1]Department of Physics, Nagoya University, Nagoya, Japan — [2]School of Materials and Chemical Technology, Institute of Science Tokyo, Yokohama, Japan — [3]Research and Education Institute for Semiconductors and Informatics, Kumamoto University, Kumamoto, Japan — [4]Department of Applied Chemistry, Keio University, Yokohama, Japan

$CaTiSiO_5$, a titanite-type oxide, consists of one-dimensional chains of TiO_6 octahedra bridged by SiO_4 tetrahedra and CaO_7 polyhedra. While $CaTiSiO_5$ has potential antiferroelectric properties, these have not been directly verified until now. In this study, we demonstrate the antiferroelectricity of $CaTiSiO_5$ by observing a double $P-E$ hysteresis loop. Moreover, we show an unconventional enhancement of permittivity through partial substitution of Si with Ge, resulting in a doubling of permittivity over a wide temperature range in the antiferroelectric phase. Transmission electron microscopy and second harmonic generation measurements have revealed the formation of microscopic polar regions in the antiferroelectric phase of $CaTi(Si_0.5Ge_0.5)O_5$. Antiphase boundaries are suggested to play a role in the generation of these microscopic polar regions. This study provides new insights into boosting the permittivity of antiferroelectric materials from the perspective of domain engineering.

KFM 1.4 Mon 10:30 H9

Dielectric crossover and its structure-function relationship in pseudo Ruddlesden-Popper-type oxides — •Akitoshi Nakano and Hiroki Taniguchi — Nagoya University, Nagoya, Japan

A phase variation of a pseudo-Roddlesden-Popper-type ferroelectric oxide Li2Sr1-xCax(Nb1-xTax)2O7 is systematically investigated using dielectric measurements, and x-ray diffraction experiments. We find an exotic x-T phase diagram, including paraelectric Cmcm, antiferroelectric Pmcn, and in-plane antiferroelectric and out-of-plane ferroelectric P21cn phases. At low x, we observe large and divergent dielectric anomalies associated with phase transitions from Cmcm to P21cn, whereas it crosses over into a small kink as x increases. Structural analyses reveal an internal distortion, and the rotation of octahedra also strongly depends on x. These results demonstrate the great tunability of dielectric properties in layered perovskite-type oxides by tuning the chemical bonding state in the octahedron.

KFM 1.5 Mon 10:45 H9

Stoichiometry of CoFe2O4 as a key to phase control and improved functional properties of multiferroic BaTiO3-CoFe2O4 bulk composites — •Daniil Lewin, Sofia Shamsulbahrin, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstrasse 15, 45141, Essen, Deutschland

Composite multiferroics have been widely studied as materials with a large magnetoelectric effect at room temperature. Barium titanate – cobalt ferrite composites are among the first and most reliable composite systems of such kind. Unfortunately, high-temperature sintering can result in the formation of secondary phases and undesirable chemical modifications, particularly that of barium hexaferrite (BaFe12O19). We present a method to suppress the formation of this phase both by sintering in nitrogen and by changing the stoichiometry of cobalt ferrite to incorporate more cobalt. The latter restricts the diffusion of the iron cations into the barium titanate during sintering. Moreover, composite samples with non-stoichiometric cobalt ferrite show up to a threefold improvement in magnetoelectric coefficient when compared to samples made with stoichiometric cobalt ferrite.

KFM 1.6 Mon 11:00 H9

Stabilization and Characterization of the LiNbO3-type Phase in NiTiO3 Thin Films: Towards Ferroelectricity — •Meriem Chettab[1], Quentin Simon[1], Mustapha Zaghrioui[1], Oleg I. Lebedev[2], Xavier Rocquefelte[3], Gwenhael Duplaix-Rata[3], Richard Retoux[2], and Patrick Laffez[1] — [1]University of Tours, GREMAN, UMR 7347-CNRS, IUT de Blois 15 Rue de la Chocolaterie, 41029 Blois Cedex, France — [2]University of Caen, CRISMAT, UMR 6508 - CNRS, ENSICAEN 6 Bd Maréchal Juin, 14000 Caen, France — [3]Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226 - F-35000 Rennes, France

Nickel titanate (NiTiO3) exhibits polymorphic structures, including ilmenite (IL), LiNbO3-type (LN), and corundum (CR), with the LN phase being potentially ferroelectric. NiTiO3 thin films were deposited by RF sputtering in an Ar/O2 plasma on Si(100) substrates at temperatures between 400 °C and 650 °C. XRD, Raman spectroscopy, and HRTEM revealed a mixture of IL, LN, and CR

phases at lower temperatures, with pure IL films obtained at 650 ˚C. All films showed a [00W] fiber texture. Post-annealing at 800 ˚C transformed the films into pure IL while preserving the texture. DFT simulations predicted Raman spectra for LN and CR phases, offering insight into phase behavior. This study highlights the potential of the LN phase for ferroelectric applications.

KFM 2: Perovskite and Photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00 Location: H13

See HL 1 for details of this session.

KFM 3: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Monday 9:30–12:15 Location: H16

See MA 2 for details of this session.

KFM 4: (Multi)ferroic States: From Fundamentals to Applications (II)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Nives Strkalj (Institute of Physics, Zagreb)

Time: Monday 11:30–13:00 Location: H9

KFM 4.1 Mon 11:30 H9

Oersted Mapping of Current Flow in Ferrorelectric Domain Walls with a Single-spin Magnetometer — •James Dalzell, Conor McCluskey, Marty Gregg, and Amit Kumar — Queen's University Belfast

Nitrogen vacancy (NV) [1] based magnetometers offer outstanding sensitivity for detecting static or dynamic magnetic fields at the nanoscale. As a result, this technique can be employed to evaluate current flow in materials with complex topologies and microstructures through direct measurement of the Oersted fields generated along any current pathways [2]. This creates an opportunity to evaluate fundamental aspects of electron transport in conducting ferroelectric domain walls, employed recently in lab-level ephemeral transistors and neuromorphic domain-wall based computing. We exploit the capability of the NV-AFM system to measure the current density along conducting domain walls in erbium manganite. By integrating high field sensitivity with exceptional spatial resolution, NV-based Oersted mapping has been shown to potentially offer a non-invasive approach to characterizing current flow in ferroelectrics. This advancement paves the way for a deeper understanding of electron transport phenomena in ferroelectric systems with current densities >1x104A/cm2, with improvements capable of being achieved by following pulse probe methods.

[1] Rondin, L. et al, Rep.Prog.Phys. 77 056503,(2014) [2] Tetienne, Jean-Philippe. et al, Sci. Adv. 3, e1602429 (2017). [3] Broadway,D.A, et al, Physics Review Applied 14(2) (2020).

KFM 4.2 Mon 11:45 H9

Transport behavior at domain walls in a depleted ferroelectric semiconductor — •Jiali He[1], Ruben Dragland[1], Leonie Richarz[1], Zewu Yan[2,3], Edith Bourret[3], Gustau Catalan[4,5], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology — [2]ETH Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, USA — [4]Institut Català de Nanociencia i Nanotecnologia (ICN2), Spain — [5]Institucio Catalana de Recerca i Estudis Avançats (ICREA), Spain

Electronic depletion regions naturally form at metal-semiconductor interface, which enables control of electrical currents in pn-junctions and is widely used in CMOS technology. Here, we expand the research towards ferroelectric domain walls, studying their functional properties under electronic depletion. Using ferroelectric p-type semiconductor $ErMnO_3$ as the model system, we deposit W electrodes and systematically investigate changes in the local transport behavior as the material is thinned down to the sub-10 nm range. Combined imaging experiments in terms of scanning electron microscopy (SEM) and scanning probe microscopy (SPM) reveal that for a critical thickness, t_c, a steplike drop occurs in the electronic conduction, which we associate with the width of the depletion region at the W/$ErMnO_3$ interface. Interestingly, ferroelectric domain walls within the depletion region exhibit qualitatively different transport behavior than in the p-type regions. Our results give new insight into the physics of domain walls and demonstrate additional opportunities for controlling their electronic responses, which is of interest for domain-wall-based electronics.

KFM 4.3 Mon 12:00 H9

Domain and domain wall conductance in the vicinity of metal-semiconductor contacts — •Ruben Dragland[1], Leonie Richarz[1], Ingvild Hansen[1], Manuel Zahn[1], Jiali He[1], Zewu Yan[2], Edith Bourret[2], Mario Hentschel[3], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA,USA — [3]University of Stuttgart, Stuttgart, Germany

Ferroelectric domain walls hold promise as functional quasi-2D systems and are intensively studied as key electronic elements for next-generation nanotechnology. Despite their outstanding application potential, however, little is known about the performance in actual device geometries and the contact phenomena that co-determine the current injection. In this study, we perform a systematic analysis of the local transport behavior of the ferroelectric semiconductor $ErMnO_3$ in the vicinity of different electrode materials. By applying electron beam lithography and evaporation, we design metal-semiconductor contacts with varying work functions and investigate the impact on the electronic conductance and respective barrier formation. Combining conductive atomic force microscopy (cAFM), Kelvin probe force microscopy (KPFM), as well as mesoscopic probe techniques, we correlate the band bending at the interface to the measured conductance of domains and domain walls. Our results are relevant for the integration of ferroelectric domain walls and the understanding of the nanoscale physics at metal-semiconductor junctions in ferroelectrics in general.

KFM 4.4 Mon 12:15 H9

Exploring ferroelectric oxides for reservoir computing — •Yan Meng Chong[1], Atreya Majumdar[2], Ingvild Hansen[1], Karin Everschor-Sitte[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany

In reservoir computing, input data is mapped into higher dimensional space, translating non-linear problems into linearly solvable ones. In general, any physical system that possesses non-linearity, complexity, short-term or fading memory, and reproducibility can serve as reservoir. Here, we investigate ferroelectric semiconductor $ErMnO_3$ as potential candidate material for reservoir computing. We show that the system displays pronounced non-linear changes in photocurrent under varying light intensity. The response can be tuned by changing the metal-semiconductor contacts (Schottky or Ohmic) used for readout, determining the timescale on which photocurrents vanish after illumination. This relaxation behavior in the OFF state gives the fading memory. We perform training for recognition on variations in the output (photocurrent), which allows for reconstructing the sequential input (light pulses). Interestingly, both ferroelectric domains and domain walls can be used as reservoirs with characteristic photocurrent signals, giving new opportunities for downscaling or enhancing the complexity of physical reservoirs.

KFM 4.5 Mon 12:30 H9

Coupling between small polarons and ferroelectricity in $BaTiO_3$ — •Darin Joseph[1] and Cesare Franchini[1,2] — [1]Dipartimento di Fisica e Astronomia, Università di Bologna, 40127 Bologna, Italy — [2]University of Vienna, Faculty of Physics, Center for Computational Materials Science, Vienna, Austria

Ferroelectric properties of materials are found to be modified upon polaron formation. In this study, we investigate the formation of electron and hole small polarons in the prototypical ferroelectric material barium titanate ($BaTiO_3$), with a focus on their interaction with ferroelectric distortive fields. To accurately describe the ferroelectric phase in $BaTiO_3$, we employ the HSE06 hybrid functional, which addresses the limitations of conventional DFT and DFT+U models, providing a more precise depiction of both ferroelectric and polaronic behaviours. Our analysis spans three structural phases of $BaTiO_3$: cubic, tetragonal, and rhombohedral. We uncover a phase-dependent trend in electron polaron stability, which progressively increases across the structural phases, peaking in the rhombohedral phase due to the constructive coupling between the polaron and ferroelectric phonon fields. In contrast, hole polarons exhibit a stability pattern largely unaffected by the phase transitions. Furthermore, we observe that polaron self-trapping significantly alters the local ferroelectric distortive pattern, which propagates to neighbouring sites but has a minimal effect on the long-range macroscopic spontaneous polarization. Charge trapping is also associated with localized spin formation, opening new possibilities for enhanced functionalities in multiferroic materials.

KFM 4.6 Mon 12:45 H9

Energy barriers for small electron polaron hopping in bismuth ferrite from first principles — •Sabine Körbel[1,2] and Harini Priyanka Shanmugasundharam Swaminathan[2,3] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University, Fürstengraben 1, 07743 Jena, Germany — [3]University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 Jena, Germany

Evidence from first-principles calculations indicates that excess electrons in $BiFeO_3$ form small polarons with energy levels deep inside the electronic band gap. Hence, *n*-type transport could occur by hopping of small electron polarons rather than by band-like transport. Here, by means of first-principles calculations, small electron polaron hopping in $BiFeO_3$ was investigated. Both bulk $BiFeO_3$ and a typical ferroelectric domain wall, the neutral 71° domain wall, were considered. The latter was included to account for experimental observations of currents that appear to be localized within domain-wall planes. The object of this study is to shed light on the intrinsic *n*-type conduction mechanism in rhombohedral $BiFeO_3$ and the role of the ferroelectric domain walls in electrical conductivity. Based on the computed energy barriers for small electron polaron hopping, the intrinsic *n*-type mobility in bulk $BiFeO_3$ and at 71° domain walls is estimated.

KFM 5: Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Monday 15:00–17:00 Location: H9

KFM 5.1 Mon 15:00 H9

Simulation study of beam splitting of vortex electron beams inside crystals — •Christian Bick and Dorothee Hüser — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Electron vortex beams have long been of interest for applications such as electron magnetic circular dichroism (EMCD), beam shaping and nanoparticle manipulation. They have attracted new attention with the recent development of an orbital angular momentum (OAM) sorter, theoretical developments in analysis of momentum transfer and as a quantum logic gate.

When propagating through a crystal, the vortex electron wave interacts with the asymmetric crystal potential, causing the wave to split into intensity centres around atomic columns, called channelling. This behaviour gives rise to a total OAM that can no longer be described by an integer vortex quantum number. In this simulation-based study we track the behaviour of electron beams inside different crystals. We show an in-depth analysis of the wave phase propagating through the crystal for different materials, focussing our research on beam splitting into intensity centres with their own OAM. This study was carried out using multislice simulations of the electron beam propagation through the crystal potential together with vector analysis to identify the local vortex centres.

KFM 5.2 Mon 15:15 H9

Single-phase valence band structure of a $Ge_{0.85}Si_{0.15}$ Crystal - Insights by momentum microscopy — •Andreas Fuhrberg[1], Pia M. Düring[1], Kevin Gradwohl[2], Olena Fedchenko[3], Yaryna Lytvynenko[3], Olena Tkach[3], Sergii Chernov[4], Christoph Schlueter[4], Gerd Schönhense[3], Hans-Joachim Elmers[3], and Martina Müller[1] — [1]Universität Konstanz — [2]IKZ, Berlin — [3]Universität Mainz — [4]DESY, Hamburg

Spin qubits are the fundamental components of quantum computing devices. Planar $Ge/Ge_{1-x}Si_x$ heterostructure qubits have proven to be advantageous for upscaling and fabrication. The Si concentration of the $Ge_{1-x}Si_x$ buffer has been shown to be an important parameter for tuning the valence band (VB) electronic structure of $Ge/Ge_{1-x}Si_x$ qubits by homoepitaxial strain, which is difficult to realize experimentally without phase separation.

Synchrotron-based hard X-ray momentum microscopy (MM) is used to study the VB electronic structure of a $Ge_{0.85}Si_{0.15}$ single crystal grown to provide well-defined small strain. Our MM experiments reveal an individual VB structure of $Ge_{0.85}Si_{0.15}$, that is clearly distinct from Si and Ge references. The shape of the heavy/light hole band and split-off band follows that of Ge, but with lower binding energies at Γ, X and L points and a reduced split-off band gap, hence no evidence for phase separation. Additional diffraction experiments, supported by Bloch wave calculations, show that the Si atoms occupy Ge lattice positions within the crystal. This result is very promising for the future experimental realization of single-phase GeSi-based spin qubits.

KFM 5.3 Mon 15:30 H9

Miniature device for in situ application of strain inside Scanning Tunnelling Microscope — •Uladzislau Mikhailau, Rashed Alhamli, and Peter Wahl — University of St Andrews, St Andrews, United Kingdom

Recent studies [1] have demonstrated that uniaxial strain significantly affects the macroscopic properties of strongly correlated electron systems. Scanning Tunneling Microscopy (STM) is a powerful technique for investigating changes in the electronic structure induced by such lattice deformation. Controlled application of strain adds an additional degree of freedom to tune, e.g., Van Hove singularities in quantum materials [2] and thereby control their ground state. To perform such studies, we have developed a specialized STM sample holder capable of applying strain at cryogenic temperatures and in high magnetic fields. Strain is applied by bending a plate beneath the sample, with stress adjustable up to the crystal's buckling limit. The device allows for the application of uniaxial or biaxial strain, depending on the configuration of the bending plate. With these capabilities, the system provides a versatile platform for exploring strain-induced phenomena through a powerful combination of atomic scale imaging in strain tuning.

[1] Clifford W. Hicks et al., Strong Increase of T_c of Sr_2RuO_4, Under Both Tensile and Compressive Strain. Science 344, 283 (2014).

[2] Chandrasekaran, A., Rhodes, L.C., Morales, E.A. et al. On the engineering of higher-order Van Hove singularities in two dimensions. Nat Commun 15, 9521 (2024).

KFM 5.4 Mon 15:45 H9

Defects in Materials: Limitations of the Trapping Model - the Influence of Corrupt Components in Positron Lifetime Spectra — •Torsten Staab, Dominik Boras, and Danny Petschke — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

Since the early days of positron lifetime spectroscopy, the meaningful decomposition of lifetime spectra into two or more components has been highly disputed. This procedure is extremely important to extract correct defect densities. Since the procedure of fitting several exponential decays folded by a mimicked instrumental resolution function to extract positron lifetimes and intensities is an "ill-posed problem", the goodness of the fit relies heavily on the quality of the recorded data. In the past there have been several simulation attempts to create and decompose spectra into two or three components (lifetimes and intensities). However, those attempts always assumed "ideal", random number Monte Carlo simulated data. Hence, the following data analysis has been fairly straight forward. By our recently developed digital twin of a positron lifetime spectrometer we could clearly see the strong influence of back scattered and corrupted coincidences on the lifetime spectrum. Unfortunately, those events cannot be removed by physically filtering digitised pulses. Changes in the geometry of the set-up lead to much more realistic bulk positron lifetimes of light materials (Mg, Al, Si) in accordance with calculations and correct decompositions in accordance with the trapping model, while the efficiency is reduced by 95%.

15 min. break

KFM 5.5 Mon 16:15 H9

Investigating Mechanical Properties of Porous Materials with Brillouin Light Scattering and Machine-Learned Force Fields — •Florian Lindner[1], Nina Strasser[1], Sandro Wieser[2], Egbert Zojer[1], and Caterina Czibula[3] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria — [3]Institute of Bioproducts and Paper Technology, Graz University of Technology, Austria

Brillouin light scattering (BLS) is based on the inelastic scattering of light from thermally activated gigahertz acoustic phonons. As the later are correlated with a material's elastic tensor via the Christoffel dispersion the elastic constants can be determined in a non-destructive and contactless manner. From these, practically relevant mechanical properties like the Young's modulus can be derived. In this contribution we show, how BLS can be used to study the mechanical properties of metal organic frameworks (MOFs), a class of porous crystalline materials with a plethora of possible applications. The measured mechanical properties are then compared to state-of-the-art dispersion corrected DFT calculations and simulations based on machine learned interatomic potentials [1], which speed up simulations by many orders of magnitude [2]. This allows to additionally determine thermoelastic properties of MOFs at elevated temperatures, which in combination with suitable experiments will portray the full potential of the used methodology.

[1] arXiv:2409.07039 (submitted to JPCL, currently under review); [2] npj Comput Mater 10, 18 (2024);

KFM 5.6 Mon 16:30 H9

TwinPALS: A Digital Twin for Laboratory-Based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras — Julius-Maximilians University, Würzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system. This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. The TwinPALS system is designed in a modular structure. The first module is responsible for constructing the digital world, taking into account the influences of position, dimension, and the materials used. The second module combines a customized version of the DLTPulsgenerator with software to process the information from the first module, incorporating considerations of radioactivity, positron lifetime, and PMT blurring. The third and final module serves to visualize the output stream from the second module, utilizing the DDRS4PALS software. In summary, this system is a modular digital twin that can be adapted to the requirements of the system being simulated.

KFM 5.7 Mon 16:45 H9

TwinPALS: A digital Twin for laboratory-based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras, Danny Petschke, and Torsten Staab — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system. This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. Additionally, this approach facilitates the validation of software-based physical filters and provides a unique opportunity to visualize their effects on unwanted components in the spectra. The digital twin represents a comprehensive simulation framework that allows for a multitude of hardware investigations in the digital realm, effectively functioning as a digital mirror of the complete hardware setup. This enables researchers to conduct extensive, risk free experiments and optimize system configurations, ultimately improving the quality and reliability of PALS data.

KFM 6: Invited Talk: X. Fang (joint session MM/KFM)

Time: Monday 15:00–15:30 Location: H10

See MM 5 for details of this session.

KFM 7: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Lithium-based Materials

Time: Monday 17:15–18:30 Location: H22

See MM 8 for details of this session.

KFM 8: (Multi)ferroic States: From Fundamentals to Applications (III)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Morgan Trassin (ETH Zurich)

Time: Tuesday 9:30–11:30 Location: H9

Invited Talk KFM 8.1 Tue 9:30 H9

Ferrolectric bubble currents — •Hugo Aramberri — Luxembourg Institute of Science and Technology

Frustrated ferroelectrics can display complex dipole textures displaying rich physical phenomena. In ferroelectric/paraelectric superlattices, built-in or applied electric fields can result in bubble domains of nanometric size akin to magnetic skyrmions.

Our atomistic calculations predict these bubbles to be quasiparticles that display thermally activated Brownian motion, enabling the conceptualization of some of the all-electric unconventional computing schemes that have already been developed for their magnetic counterparts.

However, control over the bubble motion, which is key for many potential technological applications, is still essentially lacking. In this talk I will present our latest ideas to induce bubble currents. Our simulations indicate that bubbles can be accelerated up to at least 50 m/s in the absence of electric currents, which holds the promise of a competitive alternative to magnetic skyrmion-based technologies.

KFM 8.2 Tue 10:00 H9

Exploring (110) epitaxial strain in ferroelectric films and superlattices — •Lan-Tien Hsu, Chien-Wen Hao, and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

Epitaxial strain in low-symmetry orientations significantly influences the phase stability and polarization orientation of ferroelectric thin films and superlattices,[1] offering the potential for advanced nanoelectronic applications.[2] We

explore the phase diagrams of (110)-oriented $BaTiO_3$, $KNbO_3$, and superlattice $BaTiO_3/SrTiO_3$ under strain and electric field using ab initio based coarse-grained molecular dynamics.[3] We reveal how the epitaxial (110) strain affects polarization, transition temperatures, and the emergence of topological features. Complex multidomain structures appear, particularly in superlattices due to depolarization fields.

[1] Das *et al*, Nature **568**, 368-372 (2019)
[2] Grünebohm *et al*, J.Phys.:Condens.Matter **34**, 073002 (2021)
[3] Nishimatsu *et al*, Phys. Rev. B **78**, 104104 (2008)

KFM 8.3 Tue 10:15 H9

Vortex dynamics in incommensurate 2D and 3D bulk ferroics — •Aaron Merlin Müller[1], Quintin Meier[2], Andrés Cano[2], Manfred Fiebig[1], and Thomas Lottermoser[1] — [1]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 25 Rue des Martyrs, 38042, Grenoble, France

We reveal that in 3D ferroic systems with competing incommensurate stripe phases of ferroic order and topological defects in the form of vortex lines, these vortex lines exhibit fundamentally different dynamics compared to their 2D counterparts. We show that loops of vortex lines can exhibit long relaxation times resulting from their positioning at saddle points in the energy landscape. Using phase-field simulations and analytical approaches, we demonstrate that the distinctive relaxation behavior in 3D systems arises from the interplay between dimensionality and the energy landscape of incommensurate stripe phases. Many ferroically ordered materials, such as hexagonal manganites and planar spin systems, feature periodic order parameters that support such competing orders. Hence, we employ a general model of two-component ferroic order whose findings generalize to all ferroic systems that exhibit vortices and incommensurate stripe phases. We analyze the dynamics of topological defects during the transition from inhomogeneous order without stripes to an incommensurate stripe phase in both 2D and 3D systems. We conclude by discussing the critical role of dimensionality in shaping the system's energy landscape and broader implications for ferroic systems.

KFM 8.4 Tue 10:30 H9

Valence bond solid states in IrTe2 — •Sergey Artyukhin[1], Francesco Foggetti[2], and Daniel Khomskii[3] — [1]Italian Institute of Technology — [2]Uppsala University — [3]University of Cologne

We study the phase diagram of IrTe2. This material manifests, below 280 K, a sequence of states where some Ir-Ir bonds shorten forming dimers, which results in a striped order. Ab-initio calculations suggest that the total energy is decreasing approximately linearly with the dimer fraction for the previously observed phases. The phonon density of states is shifted to higher frequencies, into the dimer-localized phonon bands. We describe the interactions between dimers using the force constant matrix from ab-initio calculations, and find features, similar to those driving striped orders in orthorhombic manganites. The strain texture is consistent with the observed striped orders. A simplified model, based on dimer energetics and phonon entropy, is formulated and the phase diagram of IrTe2 is obtained.

KFM 8.5 Tue 10:45 H9

Ultrafast control of interlayer ferroelectricity in h-BN — •Pooja Rani and Dominik M. Juraschek — Eindhoven University of Technology, Eindhoven, Netherlands

Two-dimensional ferroelectrics in nanoscale systems have received increasing interest due to their potential applications in the areas of memory storage and sensing. Among these materials, bilayer hexagonal boron nitride (h-BN) is a promising material for studying interlayer ferroelectricity because of its out-of-plane polarization that can be reversed by changing the stacking order. Using the first-principles simulation, we investigate the theoretical aspects of ultrafast control of interlayer ferroelectricity in h-BN to determine how the polarization can switch by light-induced shear motion. This phononic sliding mechanism would be particularly favourable since it provides a potential way of modulating ferroelectric behaviour at the nanoscale, creating an entirely novel path for the development of tuneable ferroelectric materials. Specifically, we focus on the excitation of the high-energy degenerate modes by an ultrashort mid-infrared pulse coupled to the low-energy shear and out-of-plane modes. Our findings suggest that the shear modes can significantly enhance the ferroelectric polarisation in h-BN, and we explore whether the ferroelectricity can be switched through this mechanism. With this, observing how out-of-plane modes affect ferroelectric polarization or interlayer ferroelectricity in h-BN will be interesting.

KFM 8.6 Tue 11:00 H9

Phonon-induced multiferroicity — Carolina Paiva[1], Michael Fechner[2], and •Dominik Juraschek[3] — [1]Tel Aviv University, Tel Aviv, Israel — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Eindhoven University of Technology, Eindhoven, Netherlands

A well-known mechanism for multiferroicity involves an electric polarization arising from a spatially varying magnetization, such as a spin spiral or cycloid. Reciprocally, optical phonons can produce a magnetization through a temporally varying electric polarization, an effect also known as dynamical multiferroicity. Here, we go a step beyond this phenomenon and describe a mechanism by which both a ferroelectric polarization and a magnetization can be created in nonpolar, nonmagnetic materials. Using a combination of phenomenological modeling and first-principles calculations, we demonstrate that a ferroelectric polarization, a magnetization, or both simultaneously can be transiently induced by an ultrashort laser pulse upon linearly, circularly, or elliptically polarized excitation of phonon modes in γ-$LiBO_2$. The direction and magnitude of the multiferroic polarization can be controlled by the chirality of the laser pulse and the phonon modes, offering a pathway for controlling multiferroicity and magnetoelectricity on ultrafast timescales.

KFM 8.7 Tue 11:15 H9

Ferroelectric and piezoelectric molecular crystals: From database mining to computational design — •Kristian Berland[1], Elin D. Sødahl[1], Seyedmojtaba Seyedraofi[1], Carl H Gørbitz[2], Ola Nilsen[2], Manjunath Balagopalan[2], Maxi Litterst[3], Martijn Kemerink[3], Jesus Carrete[4], Georg K. H. Madsen[4], Graeme Day[5], and Julian Walker[6] — [1]NMBU, Ås, Norway — [2]U. Oslo, Norway — [3]Heidelberg University, Heidelberg, Germany — [4]TU Wien, Vienna, Austria — [5]U. Southampton, UK — [6]NTNU, Trondheim, Norway

Molecular crystals offer great potential for piezoelectric and ferroelectric devices due to their vast chemical tuneability. Plastic (ionic) crystals hosts malleable orientationally disordered mesophases and their rotational freedom can yield high shear piezoelectric response[CrystGrowthDes. 2023, 23, 729]. Proton-transfer Making new crystals with desired properties, however, is not straightforward. We devised new tools to screen the Cambridge Structural Database (CSD), identifying 60 new potential ferroelectrics[PhysRevMaterials 8, 054413, 2024; CrystGrowthDes 2023, 23, 8607], 5 of which we have experimentally confirmed. Crystal structure prediction (CSP) was used to design additional ones [arXiv:2410.20481]. Finally, machine-learning force fields (MLFFs) can provide insight into dynamical properties of mesopphases [arXiv:2410.15746]. With these examples, I will argue how computational methods can be pivotal in advancing the field of small-molecule ferroic crystals.

KFM 9: (Multi)ferroic States: From Fundamentals to Applications (IV)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Morgan Trassin (ETH Zurich)

Time: Tuesday 11:45–13:00 Location: H9

KFM 9.1 Tue 11:45 H9

Investigating Self-Heating of Conducting Domain Walls Using Scanning Thermal Microscopy — •Lindsey Lynch, Kristina Holsgrove, Marty Gregg, and Raymond McQuaid — Queen's University Belfast

Domain walls (DWs) in ferroelectrics are an exciting category of reconfigurable functional interface, with properties that can differ from bulk. Lab-level transistor [1] and memristor devices [2] have been demonstrated, where functionality is derived entirely from electrically conducting DWs. Here, the DWs perform the equivalent role of conductive nanofilaments in metal-oxide resistive switching memories. While self-heating and local temperature are important factors in oxygen-vacancy based resistive switching [2,3], much less is known about the intrinsic self-heating of domain walls and its influence on device operation. We have been investigating the electrothermal properties of LiNbO3 domain wall devices using Scanning Thermal Microscopy (SThM). This involves using the scanning probe as a mobile nanoscale temperature sensor to map self-heating in

domain wall devices. Temperature hot spots on the order of 10K are detected and PFM corroborates that their origin is due to sub-surface domain wall heating. Since heat spreading occurs within the surrounding ferroelectric film and top electrode, the measured surface temperatures likely represent a lower bound for the intrinsic rise in domain wall temperature.

[1] Nat. Commun. 11, 2811 (2020). [2] Adv. Funct. Mater. 30, 2000109 (2020). [3] Sci. Adv. 8, eabk1514 (2022). [4] ACS Appl. Mater. Interfaces 14, 29025 (2022).

KFM 9.2 Tue 12:00 H9

Thermoelectricity from domain wall formation in a polar metal — •Feifan Wang[1,2], Carl Romao[1], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Institute of Physics, Beijing 100190, China

Simultaneous optimization of the electronic and phononic properties of a thermoelectric material is essential to achieve a high thermoelectric performance. This has been realized in the polar metal compounds by making use of the high configurational entropy, Rashba effect and ferroelectric anharmonicity, tuned at the atomic level. What has been overlooked in this process is the role of macroscopic effect such as the role of domain and domain wall formation in further enhancing the thermoelectric performance. Using GeTe as a prototype, we show that microdomain formation determines the thermal conduction in the polar metal examined by the spatial correlation between the domain structure and the thermal conductivity. In particular, the thermal conductivity decreased by a factor of five following the appearance of the micro-sized antiparallel-aligned domains. Conductive force microscopy shows that the electrical conduction does not change in spite of the presence of domain discontinuities. This is in line with the band gap reduction and the electron–phonon decoupling from density-functional theory calculations. The direct visualization of the association between microdomain formation and thermal/electrical transport suggests the domain and domain wall engineering as a key ingredient in advancing polar-metal-based thermoelectrics.

KFM 9.3 Tue 12:15 H9

Hybrid ferroelectric-antiferroelectric domain walls in noncollinear antipolar oxides — •Ivan N. Ushakov[1], Mats Topstad[1], Muhammad Z. Khalid[1], Niyorjyoti Sharma[2], Christoph Grams[3], Ursula Ludacka[1], Jiali He[1], Kasper A. Hunnestad[1], Mohsen Sadeqi-Moqadam[1], Julia Glaum[1], Sverre M. Selbach[1], Joachim Hemberger[3], Petra Becker[3], Ladislav Bohaty[3], Amit Kumar[2], Antonius T. J. van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology — [2]Queen's University Belfast — [3]University of Cologne

Antiferroelectrics are emerging as advanced functional materials and are fertile ground for unusual electric effects. For example, they enhance the recoverable energy density in energy storage applications and give rise to large electromechanical responses. In my talk, I will present noncollinearity in dipolar order as an additional degree of freedom, unlocking physical properties that are symmetry-forbidden in classical antiferroelectrics. I will show that noncollinear order of electric dipole moments in $K_3[Nb_3O_6|(BO_3)_2]$ leads to a coexistence of ferroelectric and antiferroelectric behaviors. Besides the double-hysteresis loop observed in antiferroelectrics, a pronounced piezoresponse and electrically switchable domains are observed, separated by atomically sharp and micrometer-long charged domain walls. Similar hybrid ferroelectric-antiferroelectric responses are expected in a wide range of noncollinear systems, giving a new dimension to the research on antiferroelectrics and multifunctional oxides in general.

KFM 9.4 Tue 12:30 H9

Step sintering process on sol-gel synthetized Bi0.5Na0.5TiO3 for enhanced temperature stability of relaxor ferroelectric state and energy storage properties — •Thomas Fourgassie[1], Cécile Autret-Lambert[1,2], and Pierre-Eymeric Janolin[2] — [1]Laboratoire GREMAN, UMR 7347 Université de Tours, CNRS, INSA CVL, Université de Tours UFR Sciences & Techniques, 37200 Tours, France — [2]Laboratoire SPMS, UMR 8580 Université Paris-Saclay, CNRS, CentraleSupélec, 91190 Gif-sur-Yvette, France

With the ever-growing need for energy in our society, researchers are striving to obtain new materials with better energy storage properties capable of replacing current lead-based materials. Among all lead-free materials that have been synthesized, Bi0.5Na0.5TiO3 (BNT) has attracted the attention of many. The main reasons are his high temperature of maximum permittivity called Tm at 320°C, a huge maximum polarization and relaxor ferroelectric properties making his phase transition very diffuse in temperature. However, the good energy storage properties only apply at a temperature higher than the depolarization temperature Td (200°C). Usually, to reduce Td, researchers either make solid solutions with other perovskite ceramics or use donor dopants. Here we show the results we obtained while keeping the pristine BNT phase by optimizing the sol-gel synthesis process used. The BNT exhibits sub-micrometric grain size thanks to a multi-step sintering process lowering Td (around 160°C). This BNT has enhanced relaxor ferroelectric at lower temperatures. Results about donor dopants reducing dielectric losses on this BNT will also be shown.

KFM 9.5 Tue 12:45 H9

Composite quadrupole order in ferroic and multiferroic materials — •Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

The formalism of composite and intertwined orders has been remarkably successful in discussing the complex phase diagrams of strongly correlated materials and high-Tc superconductors. Here, we propose that composite orders are also realized in ferroelectric and ferromagnetic materials when lattice anisotropy is taken into account. This composite order emerges above the ferroic phase transition, and its type is determined by the easy axis of magnetization or polarization, respectively. In multiferroic materials, where polarization and magnetization are coupled, composites of both orders are possible. This formalism of composite orders naturally accounts for magnetoelectric monopole, toroidal, and quadrupole orders. More broadly, composite orders may explain precursor phenomena in incipient ferroic materials, arising at temperatures above the ferroic phase transition and potentially contributing to the characterization of currently hidden orders.

[1] R Matthias Geilhufe, J. Phys.: Condens. Matter, 37, 05LT01 (2025)

KFM 10: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 14:00–15:15 Location: H22

See MM 14 for details of this session.

KFM 11: (Multi)ferroic States: From Fundamentals to Applications (V)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Manuel Zahn (University of Augsburg)

Time: Wednesday 9:30–10:45 Location: H9

Invited Talk KFM 11.1 Wed 9:30 H9

Towards 3D nanoscale chemical mapping with atom probe tomography — •Kasper Hunnestad, Constantinos Hatzoglou, Antonius van Helvoort, and Dennis Meier — Norwegian University of Science and Technology, Trondheim, Norway

The discovery of new physical phenomena in materials is closely linked to the progress in characterization, and is propelled by the ability to observe and study physical processes occurring at the atomic level. Nanoscale structural characterization has been a cornerstone for many discoveries related to ferroic phenomena. Chemical characterization at the atomic level, however, remains a major challenge.

In the first part of this talk, I will present how atom probe tomography (APT) can be incorporated into the toolkit of nanoscale research to study ferroic oxide materials. In the second part of this talk, a special emphasis will be put on various ferroic phenomena, such as ferroelectric domain walls and interface effects. The focus will be on understanding their chemical state and the role of defects in controlling their physical properties.

The presentation will demonstrate that correlations between defect chemistry and ferroic phenomena can be experimentally probed with nanoscale spatial resolution using APT, opening an avenue to obtain a deeper understanding of ferroic materials.

KFM 11.2 Wed 10:00 H9

Tuning of ferroelectric polarization by lattice chemistry — •Ipek Efe[1], Alexander Vogel[2], William S. Huxter[1], Elzbieta Gradauskaite[1], Christian L. Degen[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich — [2]Empa, Switzerland

Engineering the lattice chemistry in oxide thin film systems opens up new possibilities for tuning electrostatic boundary conditions beyond the depolarizing-field tuning approaches. Controlling the formation of polarizing charged layers may stabilize highly desired polar textures such as charged domain walls and charge planes, offering great promises for future ultralow-energy-consuming oxide electronics. Here, we demonstrate lattice-chemistry engineering of perovskite oxide ferroelectrics in a heterostructure utilizing Aurivillius-type layering. We insert functional perovskite oxides, including $BiFeO_3$ and $BaTiO_3$, into the layered framework of the Aurivillius phase. By exploiting the characteristic charged interfaces present in the Aurivillius crystal structure and varying the perovskite constituent, we fine-tune the electric-dipole configurations within our composite heterostructures. Using in-situ optical second harmonic generation, we directly resolve the influence of controlled atomic-scale poling of the Aurivillius charged layers on the perovskite constituent. As a result, we achieve new properties while preserving the functionalities of the parent compounds.

KFM 11.3 Wed 10:15 H9

Vector Scanning Electron Microscopy for Domain Imaging in Ferroelectric Polycrystals — •Ellinor Benedikte Anjali Lindström, Ruben Skjelstad Dragland, Jonas Åmli Ingdal, Jan Schultheiss, Jiali He, and Dennis Meier — NTNU Norwegian University of Science and Technology, Norway

Domain imaging in polycrystalline ferroelectrics is challenging due to the non-uniform crystallographic orientation of grains. To gain the full information including the domain polarization and orientational information, imaging techniques such as piezoresponse force microscopy (PFM) and scanning electron microscopy (SEM) are often complimented by electron backscatter diffraction (EBSD) experiments.

Here, we introduce a new SEM-based approach that allows simultaneous mapping of domains and grain orientation information. By performing systematic SEM measurements as a function of the stage rotation angle on the model system $ErMnO_3$, we observe distinct contrast intensity changes within the same grain. Notably, the domain contrasts invert when the stage is rotated by 180°. Complementary PFM and EBSD data confirm that these changes in contrast correlate with both the domain state and the orientation of the polar axis relative to the surface. Our approach offers a contact-free alternative to vector PFM and partially reduces the need for EBSD, giving new opportunities for domain imaging in ferroelectrics.

KFM 11.4 Wed 10:30 H9

Ranges and limits of p-doping in Y:HfO_2 - an electronic structure study by HAXPES — •Oliver Rehm[1], Lutz Baumgarten[2], Florian Wunderwald[3], Andrei Gloskovskii[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[4] — [1]Universität Konstanz — [2]Forschungszentrum Jülich — [3]NaMLab, Dresden — [4]DESY, Hamburg — [5]TU Dresden

Ferroelectric HfO_2-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or FeFET. However, the application of HfO_2-based thin films as active ferroelectrics (FE) in devices still faces reliability issues like wake-up, imprint, and fatigue. A critical concentration of oxygen vacancies (OVs) determines both the stabilization of a FE phase as well as the breakdown during electrical cycling. For p-doped HfO_2, the electronic limits of OV formation remain an experimentally open question.

We investigated Y:HfO_2 samples synthesized via atomic layer deposition (ALD) with Y doping concentrations from 2.1% to 8.6%. TiN/Y:HfO_2 interfaces are investigated regarding the local chemistry and electronic properties by hard X-ray photoelectron spectroscopy (HAXPES). The Hf 4f core level is analyzed to identify Hf^{3+} components and rigid binding energy (BE) shifts, both of which serve as indicators for OVs. We determine the (unexpected) formation of OVs as a function of Y doping, with the conclusion that Y doping above a threshold limit has a detrimental effect on interface stability, thereby promoting increased OV formation at the interface that finally speeds up fatigue and breakdown.

KFM 12: Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Modelling of Battery Materials and Degradation)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterization techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Carlos Ziebert (Karlsruhe Institute of Technology)

Time: Wednesday 11:00–12:45 Location: H9

Invited Talk KFM 12.1 Wed 11:00 H9

Model-assisted Insight into Degradation of Li-Ion Batteries during Thermal Abuse — •Ulrike Krewer, Leon Schmidt, and Jorge Valenzuela — Karlsruhe Institute of Technology, Institute for Applied Materials -Electrochemical Technologies, Karlsruhe, Germany

The electrolyte in Li-ion batteries is inherently thermodynamically instable; this leads to formation of the solid-electrolyte interphase and capacity loss. Exposing batteries to high temperatures above ca. 60°C accelerates interphase growth, but also leads to its dissolution and renewed formation. If the related exothermic heat is not sufficiently fast removed, this leads to self-heating and a thermal runaway of the cell. This talk uses modelling to give a deep insight into the processes and properties causing self-heating and thermal runaway of Li-ion batteries. A complex interaction of exothermic and endothermic reactions is revealed, and the effects of evaporative cooling [1], conditions during battery manufacturing and battery age. [2] Gas analysis with online electrochemical mass spectrometry aids in identifying the network and further sensitivities. [3]

[1] Baakes F. et al., J. Power Sources, 2022, 522, 230881 [2] Baakes, F. et al., Chem. Sci, 2023, 14, 13783 [3] Bläubaum, L. et al., Batter. Supercaps 2024, 7, e20230053.

KFM 12.2 Wed 11:30 H9

Computational investigation of lignin based anode ma- terials for Li- and post-Li ion batteries* — •Jafar Azizi[1], Holger Euchner[2], and Axel Gross[1] — [1]Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany — [2]2 Institute of Physical and Theoretical Chemistry, Tübingen University, 72076 Tübingen, Ger- many

Post-lithium ion batteries have gained a lot of attention as a promising energy storage technology for large-scale grid applications due to their high energy density and low cost. Hard Carbon is one of the most promising anode materials, but is still associated with some performance problems. It is anticipated that improved hard carbon-based cells with a higher energy density and better electrochemical performance will be highly interesting in electrochemical energy storage. Hence, in this work, we propose a novel anode material based on the structure of lignin, one of the most prevalent biomass materials. Based on ab initio molecular dynamic (AIMD) simulations and density functional theory (DFT) calculations we study the formation of lignin-based hard carbon at different temperatures which results show a promising new amorphous structure. We find a noticeable structure stability, and higher energy capacity (AMC_n, $n < 6$) compared to the usual graphite system.

KFM 12.3 Wed 11:45 H9

Stability Enhancement of Cubic $CsSnCl_3$ as Solid Electrolyte - A Computational Approach — •Johannes Döhn[1], Martin Uhrin[2], and Axel Gross[1,3] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Multidisciplinary Institute in Artificial Intelligence, Université Grenoble Alpes, France — [3]Helmholtz Institute Ulm, Germany

For the transition towards renewable energy systems, efficient and reliable technologies for energy storage are needed. Batteries are one of the most widely used

storage devices, but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution, we will present atomic-scale investigations of potential future battery materials carried out using a combination of density functional theory (DFT) and machine learning interatomic potential (MLIP) calculations. We employed a high-throughput approach in order to evaluate potential dopants for the well-known Cl-ion conductor $CsSnCl_3$; a solid electrolyte material for chloride ion batteries (CIBs) which is ascribed the capability to fully exploit the potential of this alternative battery type. The investigated dopants where chosen based on a dual doping strategy: Cation doping aims at enhancing the stability of the material while the introduction of mobile species, i.e., Cl vacancies/interstitials, balances the formal charge of the system and aims at improving the Cl-ion conductivity.

KFM 12.4 Wed 12:00 H9

Stability of $MgSc_2Se_4$ Surfaces — •Sebastian Utz[1] and Axel Gross[1,2] — [1]Ulm University, Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany

Magnesium metal anodes are a promising material for post-lithium battery systems because of their high theoretical gravimetric energy density. One issue that hinders their application is the low ionic conductivity of many magnesium electrolytes. One of the few electrolytes that show good magnesium ion conductivity is the solid electrolyte $MgSc_2Se_4$ with a spinel structure. While the structural and diffusion properties of the bulk material are already well understood, its surfaces and interfaces are hardly explored. To shed some light on the surface properties of this solid-state electrolyte, first principles calculations within the framework of periodic density functional theory were conducted. The stability of low index {100} and high index {222} surfaces are being compared. Additionally, common structural features of the different surfaces that may lead to a stabilisation or destabilisation will be explored.

KFM 12.5 Wed 12:15 H9

Hybrid Interfaces in Focus – Decoding the Berlinite Surface with a Synergetic NMR-DFT Approach — •Javier Valenzuela Reina[1], Vera Barysch[2], Simone Köcher[2,1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH

One of the milestones in the development of the next generation of high-performance lithium batteries is the understanding and improvement of hybrid electrolytes and their interfaces. Nuclear magnetic resonance (NMR) spectroscopy is a non-destructive, powerful technique for unraveling the intricate interface structure and ion dynamics in these materials.

We exploit the synergies between NMR experiments and density-functional theory (DFT) simulations for investigating Berlinite ($AlPO_4$) as a model for the surface of the well-known solid ion conductor $Li_{1+x}Al_xTi_{2-x}P_3O_{12}$ with $0 \leq x \leq 1$ (LATP), a promising candidate for a hybrid electrolyte. By supporting surface-selective NMR techniques such as cross-polarization (CP) and transfer of populations in double resonance (TRAPDOR) on $AlPO_4$ powder with DFT calculations of NMR observables, we study multiple surface models, infere structural characteristics of the sample, and study its interactions with water as well as organic molecules. We demonstrate that the joint experimental-theoretical approach holds future potential for understanding and improving materials whose performance relies on the properties and behavior of complex organic/ceramic interfaces.

KFM 12.6 Wed 12:30 H9

Pits and Traps in the Impedance Analysis of Ionic Conductors — •Janis K. Eckhardt — Center for Materials Research (ZfM), Justus Liebig University, Giessen D-35392, Germany

The development of innovative electrochemical storage systems, such as solid-state batteries, is critical for achieving climate neutrality and sustainability goals. Several hurdles must be overcome before such technologies are ready for the market. Impedance spectroscopy is a powerful method for characterizing the electrical transport properties of new materials and for monitoring systems in operation. Although it is an older measurement technique, the interpretation of data for inhomogeneous solid-state systems lacks established concepts for reliable results. Therefore, we use 3D electrical network models for spatially-resolved transport simulations and systematic investigation of the influence of sample microstructure and solid-solid interface morphology. The material-specific transport quantities derived from 1D models (e.g., brick layer model) sometimes exhibit inaccuracies of several orders of magnitude. In addition, the impedance response of the system exhibits geometric signatures that cannot be adequately represented in physically motivated circuit models, e.g., current constriction phenomena.

KFM 13: Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Experimental Characterisation and Safety Testing)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterization techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Philipp Finster (Karlsruhe Institute of Technology)

Time: Wednesday 15:00–16:45 Location: H9

KFM 13.1 Wed 15:00 H9

Are Li-ion batteries safe for 2nd-life applications? - The case of aged cells with SEI growth — •Thomas Waldmann[1,2,4], Gabriela G. Gerosa[1], Jihed Ayari[2,3], Abdelaziz A. Abd-El-Latif[1], Philipp Moosmann[1,5], Max Feinauer[1], Olaf Böse[1], Markus Hölzle[1], and Margret Wohlfahrt-Mehrens[1,2] — [1]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Helmholtzstrasse 8, Ulm, 89081, Germany — [2]Helmholtz Institute Ulm (HIU), Helmholtzstrasse 11, Ulm, 89081, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, 76021, Germany — [4]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany — [5]Porsche AG, Porschestrasse 911, 71287 Weissach, Germany

Re-using aged Li-ion batteries in 2nd-life applications can increase sustainability. However, there is a lack of knowledge on the safety of aged cells with regard to the underlying aging mechanisms. Room temperature and high temperature aging often lead to growth of the solid electrolyte interphase (SEI) on the surface of graphite or Si/graphite anodes as commonly observed by post-mortem analysis of Li-ion battery cells with physico-chemical analysis methods. We show results on the influence of aging of commercial Li-ion cells in the 1st-life on safety in 2nd-life. Our safety tests (ARC, nail penetration, overcharge, overdischarge) reproducibly show similar or better safety levels for cells with SEI growth in contrast to aged cells with the different mechanism of lithium plating. Possibilities are pointed out to avoid critical mechanisms and for early detection of unsafe behavior.

KFM 13.2 Wed 15:15 H9

Diffraction computed tomography for non-destructive analysis of li-ion batteries — •Vladislav Kochetov — Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

This contribution discusses the application of Diffraction Computed Tomography (DCT), including both X-ray and neutron probes, as a powerful method for non-destructive structural analysis in materials science. DCT uses a pencil-beam scanning technique to yield the reconstructed images of internal structure and chemical gradients of materials, extending the traditional imaging approaches. A notable application of DCT is in the study of commercial lithium-ion batteries, where it has been used to resolve inhomogeneities in lithium distribution and structural evolution during cycling. We apply DCT to various commercial battery types, specifically focusing on cylindrical cells with different diameters, featuring diverse chemistries such as NCA, NMC, and graphite anodes. By employing high-resolution DCT, we map lithiation distributions and investigate electrode degradation mechanisms, providing key insights in battery performance and aging. The efficiency of the method, state-of-the-art resolution capabilities, and technique's extension to neutrons are discussed.

[1] V. Kochetov et al, Powder diffraction computed tomography: a combined synchrotron and neutron study, J Phys Condens Matter 33 (10), 2021. [2] D. Petz et al, Lithium distribution and transfer in high-power 18650-type Li-ion cells at multiple length scales, Energy Storage Materials 41, 2021.

KFM 13.3 Wed 15:30 H9

Optical, structural and electrochemical properties of re-synthesized Graphite powder for Anode battery application — •Slaheddine Jabri[1], Anna Rollin[2], Sukanya Sukanya[3], René Wilhelm[2], Michael Kurrat[3], Uta Schlickum[1], and Markus Etzkorn[1] — [1]Technische Universität Braunschweig, Institute of Applied Physics, Meldensohn Straße2, 38106 Braunschweig, Germany — [2]Mendelssohnstraße 2 — [3]Technische Universität Clausthal, Institute of Organic Chemistry, Leibnitzstraße 6, 38678 Clausthal-Zellerfeld, Germany

By focusing on preserving the components of Li-Ion battery material through cheaper and envi-ronmental friendly methods, recycling process could introduce scavenged impurities into resyn-thesized material and modify its structural and morphological properties. In this work, we investi-gate the optical, structural and electrochemical properties of recycled Graphite compared to the new material. Our findings reveal that a proper recycling process can remove the Solid Electrolyte Interphase (SEI) layer, which is of significant importance in battery performance. The analysis showed that proper cleaning can significant reduce the amounts of organic and inorganic impuri-ties in the graphite, leading to an improvement in material quality. As a result, the battery perfor-mance can even be enhanced by 89% after 200 charge-discharge cycles compared to the commer-cial base material, demonstrating the potential of recycling methods for improving battery life and efficiency.

KFM 13.4 Wed 15:45 H9

Facilitating Sodium-Ion Diffusion in Fe-Doped Co3O4 for High-Rate Performance — •Yonghuan Fu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to its high theoretical capacity, cobalt oxide (Co3O4) has attracted attention to sodium-ion battery (SIB) anodes. However, its low conductivity and poor rate performance have limited its practical application. This work proposes a co-precipitation doping strategy to synthesize iron-doped Co3O4 nanoparticles (FexCo3-xO4 NPs). Both experimental and theoretical results confirm that iron (Fe) doping at octahedral sites within spinel structures is a critical factor in enhancing rate performance. The decreased band gap and enlarged ion transport spacing originate in Fe doping. This effectively facilitates the electron and Na+ transport during discharge/charge processes, delivering an impressive rate capability of 402.9 mA h g-1 at 3 A g-1. The FexCo3-xO4 NPs demonstrate remarkable cycling stability. They maintain a high specific capacity of 786.2 mA h g-1 even after 500 cycles at 0.5 A g-1, with no noticeable capacity fading. This work provides valuable insights into the functional design of high-rate electrodes, offering a promising approach to addressing the critical challenges faced by sodium anodes.

KFM 13.5 Wed 16:00 H9

Reversible Structural Evolution of 3D Vanadium Sulfide Anodes in Sodium-Ion Battery Applications — •Osamah Ali Fayyadh, Yulian Dong, Huaping Zhao, and Yong Lei — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau

Sodium-ion batteries (SIBs) are a promising alternative to lithium-ion batteries due to sodium's abundance and wide distribution. However, SIBs face challenges such as low capacity, poor cycling, and sluggish ion diffusion, due to the large ionic radius of Na+. Thus, extensive research has focused on advanced anode materials, among which vanadium sulfides (VSx) have gained significant attention due to their large interlayer spacing, high theoretical capacities, and versatile electrochemical mechanisms. However,VSx suffer from mechanical pulverization, severe volume changes, and limiting their practical application. Here, we demonstrate a 3D micro/nanostructured VSx anode fabricated, achieving a remarkable reversible capacity of 961.4 mAh g-1 after 1500 cycles at 2 A g-1. The sodiation-driven reconfiguration of 3D-VSx into a stable structure mitigates volume changes, enhances ion diffusion, and improves structural stability.[1] The sodiation-driven reconfiguration enhances ion diffusion, mitigates volume changes, and stabilizes the structure. Electrochemical studies and density functional theory calculations reveal significantly improved Na+ storage capabilities, offering a pioneering strategy for developing high-performance SIB anodes with excellent capacity and stability. [1] Y. Dong, Y. Lei et.al. Adv. Energy Mater. 2023, 13, 2204324.

KFM 13.6 Wed 16:15 H9

synergizing nickel (II) oxide-based catalyst for sodium-carbon dioxide battery — •Tzu-Chin Huang, Changfan Xu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Na-CO2 battery is a novel and environmentally friendly green energy device. Conceptually, it demonstrates excellent capabilities. However, during the operation of batteries, undecomposed discharge products, sodium carbonate, accumulate continuously, which is highly insulating, thermodynamically stable, and difficult to decompose. This increases the ohmic resistance within the battery, resulting in high charging potential and excessive polarization, which leads to serious side reactions, such as the decomposition of the electrolyte and cathode material, reducing the battery's reversibility. Herein three Ni oxide-based catalysts, NiO, NiCoO, and CuNiCoO, attached to carbon clothe cathode were synthesized and employed in Na-CO2 batteries. Electrochemical testing demonstrated that CuNiCoO exhibits the best battery stability and long-term performance. This superior performance is driven by the ability of CuNiCoO catalyst to effectively promote the generation and decomposition of discharge products. Cyclic voltammetry (CV) analysis revealed strong redox peaks, underscoring the outstanding catalytic activity of CuNiCoO catalyst. Furthermore, XRD and Raman characterizations confirmed this by showing the appearance and gradual disappearance of sodium carbonate peaks during charge and discharge cycles, indicating remarkable reversibility.

KFM 13.7 Wed 16:30 H9

A Solar Battolyzer Approach: On-Demand Hydrogen Production and Energy Storage in a 2D Niobium-Tungstate Material — Yang Wang[1], •Yu-Te Chan[2], Takayoshi OshimaViola[1], Viola Duppel[1], Sebastian Bette[1], Kathrin Küster[1], Andreas Gouder[1], Christoph Scheurer[2,3], and Bettina Lotsch[1,4] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Fritz-Haber-Institut der MPG, Berlin — [3]IEK-9 Forschungszentrum, Jülich — [4]Ludwig-Maximilians-Universität, Munich

In the quest to overcome the limitations of solar intermittency, materials that can simultaneously capture and store solar energy offer promising avenues for clean energy solutions. Here, we introduce the 2D niobium-tungstate $TBA^{+}NbWO_{6}^{-}$ as a novel solution capable of harnessing light energy and storing it either for direct grid integration or as fuel through on-demand hydrogen production. This dual-functionality is central to the emerging concept of "battolyzers," devices that combine battery and electrolyzer capabilities to provide both energy storage and fuel generation. Exposure to light triggers ion intercalation and stable polaron formation within the material, reducing resistance and allowing electron storage for extended durations. Introducing Pt as the catalyst allows the stored electrons to be released to generate hydrogen, demonstrating the material's capability for efficient, on-demand solar energy conversion. Our findings on optoionic processes in $NbWO_6$ lay the groundwork for future solar battolyzers, bridging solar energy storage and hydrogen fuel generation in a single system. [1] Y. Wang et al., J. Am. Chem. Soc. **146**, 25467 (2024)

KFM 14: Poster

Chairs: Jan Schultheiß (NTNU, Norway) Anna Grünebohm (RUB)

Time: Wednesday 17:00–18:30 Location: P1

KFM 14.1 Wed 17:00 P1

Stability of Machine-Learned Interatomic Potentials in Molecular Dynamics Simulations for Organic Semiconductors and Metal-Organic Frameworks — •Martin Tritthart and Egbert Zojer — Institute for Solid State Physics, Graz, Austria

Organic semiconductors (OSCs) and metal-organic frameworks (MOFs) are two classes of materials that have garnered significant interest in materials science. To optimize their performance, it is crucial to understand the physical properties of these crystalline polymer materials, such as heat transport and mechanical stability. This understanding can lead to improvements in properties like thermal stability. Molecular dynamics (MD) simulations are commonly used for this purpose, as they are orders of magnitude less computationally expensive than first-principles calculations. While machine learning interatomic potentials (MLIPs) are much faster than ab initio methods, they approximate the true potential energy surface, which can result in significant errors for atomic configurations outside the training data space. Such shortcomings lead to incorrect predictions of forces and energies in MD simulations, potentially causing molecular instability during simulations. To address this issue and improve the robustness of MLIPs, a reliable estimation of their uncertainty is necessary. This enables the identification of uncertain structures, which can then be incorporated into the training set to enhance accuracy. With this iterative approach, larger and more complex molecules can be simulated with relatively efficient computational effort.

KFM 14.2 Wed 17:00 P1

Assessment of new cocrystals of amphotericin B and miltefosine (leishmanicidal pharmaceuticals) via powder X-ray diffraction analysis. — •Memoona Bibi, muhammad Iqbal Choudhary, and Sammer Yousuf — H.E.J. Research Institute of Chemistry, ICCBS, University of Karachi, Pakistan.

Cocrystals and other cutting-edge technologies offer substantial opportunities for patents that present multiple strategies for managing the life cycle of existing and novel drugs. The creation of cocrystals by employing suitable coformers represents a valuable approach toward stability, enhancement, and bio availability of pharmaceutical medications. The focal point of current study was cocrystallization of well-known commercially available anti-leishmanial drugs i.e. Amphotericin B and Miltefosine. Multiple cocrystals of amphotericin B and miltefosine were successfully synthesized. To prepare the co-crystals neat grinding method via mixer mill was applied. The characterization was conducted through powder X-ray diffraction revealing unique crystallinity and significant variation in 2θ values of cocrystals. DSC/TGA, UV, FTIR and melting point were also proceeded for further evaluation. The solubility studies of amphotericin B at pH 6.8, 7.4 and in distilled H2O in comparison with their co-crystals revealed promising results. Invitro testing of all co-crystals against L. major, L. donovani, and L. tropica demonstrated potent anti-leishmanial activity in comparison with reference standard drugs i.e. amphotericin B and miltefosine. However, cytotoxicity results revealed none of them exhibited cytotoxic effect against MTT (3T3) cell line.

KFM 14.3 Wed 17:00 P1

High-temperature properties of $LiNbO_3$ and $LiTaO_3$ — •Eva Westenferlder Gil, Felix Bernhardt, and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, Germany

Lithium niobate (LN) and lithium tantalate (LT) are ferroelectric crystals with a wide range of applications, extending from piezoelectric sensors [1] to integrated photonics [2]. Both, LN and LT, undergo a phase transition towards a paraelectric (PE) phase at around 1400K and 870K, respectively. Since devices employing LN and LT as functional materials are often operated at high temperatures, extensive research has been conducted in order to describe the materials high-temperature properties [3,4]. Here, we show that the high symmetry PE structure for both LN and LT is energetically favoured, which is in contrast to previously suggested models representing the PE phase as a superposition of differently oriented ferroelectric phases [5]. The electronic band structures indicate that both crystals remain electronic insulators in the PE phase. Furthermore, we provide thermal expansion coefficients and elastic constants, calculated from machine-learned potentials. Our results show a good agreement to recent experimental measurements.

[1] M. Xu *et al*, ACS Appl. Mater. Interfaces **9**, 40, (2017)
[2] W. Sohler *et al*, Optics & Photonics News **19**, 1, (2008)
[3] P. Gaczyński *et al*, Phys. Status Solidi A, 2300972, (2024)
[4] C. Kofahl *et al*, Solid State Ionics **409**, 116514 (2024)
[5] F. Bernhardt *et al*, Phys. Rev. Mat. **8**, 054406 (2024).

KFM 14.4 Wed 17:00 P1

Optimizing pre-annealing growth for obtaining pattern fidelity of highly ordered GaAs nanowires — •Juliane Koch[1], Jiajia Qiu[2], Chris Bohlemann[1], David Ostheimer[1], Peter Kleinschmidt[1], Huaping Zhao[2], Yong Lei[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]TU Ilmenau, Institute for Physics, Applied Nanophysics, Ilmenau, Germany

Bottom-up grown III-V semiconductor nanowires (NWs) offer significant potential for advanced electrical and optoelectronic device applications. This study presents a fabrication strategy for highly ordered GaAs NW arrays by combining a non-lithographic nanostructuring technique with metalorganic vapor phase epitaxy (MOVPE). Uniform Au nano-disk arrays, created using anodic aluminum oxide templates, act as catalysts for the subsequent NW growth. The special fabrication process of the Au nano-disks prevents undesired substrate imprinting, which leads to a different behavior than previously utilized methods, namely to an Au particle diffusion during the MOVPE process. The nucleation duration, optimized in terms of the Au particle volume, is crucial for maintaining array uniformity. A short nucleation period fails to anchor particles, resulting in undesired diffusion. To resolve this, pre-annealing nucleation is extended to initiate III-V growth of a pedestal structure that secures the array's highly ordered geometry. A detailed analysis of MOVPE sub-processes supports the development of a refined growth model.

KFM 14.5 Wed 17:00 P1

Synthesis, Properties, and Phase Transitions analysis of ferroelectric TMCM-MnCl3 hybrid halide — •Chithra Kandappanthodi, Sobhan Fathabad, Doru C.Lupascu, and Vladimir V.Shvartsman — Institute for material science, Essen, Germany

Organic-inorganic hybrid halides have gained significant attention in material science due to their environmentally friendly, cost-effective fabrication and exceptional piezoelectric or optoelectronic properties. In this study, we synthesized trimethyl chloromethyl ammonium manganese trichloride (TMCM-MnCl3) and Fe-doped TMCM-MnCl3 crystals. We demonstrate that TMCM-MnCl3 exhibits a monoclinic crystal structure at room temperature, which transforms into a hexagonal structure upon heating, as confirmed by temperature-dependent x-ray diffraction. The phase transitions at 408 K for TMCM-MnCl3 and 404 K for TMCM-Mn0.95Fe0.05Cl3 were further corroborated by differential scanning calorimetry. The step-like anomaly in the temperature dependence of dielectric permittivity observed in TMCM-MnCl3 indicates an improper ferroelectric transition. Piezoresponse force microscopy revealed regular ferroelectric domains. Additionally, Raman spectroscopy identify the vibrational modes of the crystal. Through UV-vis spectroscopy, we observed that the bandgap is tunable through moderate Fe doping. This comprehensive characterization highlights the potential of TMCM-MnCl3 for advanced applications.

KFM 14.6 Wed 17:00 P1

Investigation of hydrogen diffusion in $LiNbO_3$ and $LiTaO_3$ from density-functional theory — •Christa Fink and Simone Sanna — Institute for Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Hydrogen is always present in $LiNbO_3$ and $LiTaO_3$ crystals. Therefore, the lattice locations of hydrogen within the crystal as well as its diffusion and mobility have been a matter of research for many years. While the energetically most favorable positions of hydrogen within the atomic lattice have been investigated intensely, there exist less investigations of diffusion paths and energy barriers. To fully understand the diffusion of hydrogen in $LiNbO_3$, $LiTaO_3$ and their solid solutions, we calculate energy barriers and three-dimensional minimum energy paths for hydrogen diffusion using the nudged elastic band method based on density-functional theory as implemented in VASP [1, 2]. Starting from the energetically most favorable position, we calculate minimum energy paths through the crystal towards the next equivalent position. We extend our calculations from the stoichiometric material to crystals with Lithium vacancies, which are the most common defects in LN and LT, for a better comparison to experimental results [3, 4].

[1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [2] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996). [3] Kofahl, C. et al., Defect and Diffusion Forum, 429, 136-143 (2023). [4] Kofahl, C. et al., Solid State Ionics 403, 116383 (2023).

KFM 14.7 Wed 17:00 P1

Epitaxial Growth of Phase-Pure LiNbO3 Thin Films on LiTaO3 by Pulsed Laser Deposition (PLD) — •Hyeyeon Cho, Steffen Ganschow, René Bararugurika, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Lithium niobate (LiNbO3) is a widely used material in electro-optical and electroacoustic devices due to its outstanding ferroelectric, piezoelectric, electro-optical, and nonlinear optical properties. Thin-film LiNbO3 offers significant advantages, including component miniaturization, broader bandwidths at higher frequencies, and reduced operational voltages. However, achieving these benefits requires the growth of phase-pure films with excellent crystalline quality, stoichiometric composition, and low surface roughness. Pulsed Laser Deposition (PLD) is a reliable method for growing LiNbO3 thin films, providing precise control over stoichiometry and the ability to produce high-quality epitaxial layers. However, high volatility of Li2O at enhanced temperatures during deposition often leads to Li-poor secondary phase formation. In this study, we investigated the effects of various deposition parameters to optimize the growth of phase-pure LiNbO3 films on LiTaO3. Key parameters, including substrate temperature, oxygen partial pressure, laser fluence, laser frequency, and target-substrate distance, were systematically varied. We also explored the use of lithium-rich targets to address lithium loss at high temperatures. X-ray diffraction (XRD) and atomic force microscopy (AFM) analyses confirmed the epitaxial growth of high-quality films with smooth surfaces.

KFM 14.8 Wed 17:00 P1

PALS of Hot-Rolled and Subsequently T4-Treated AlCuMgAg — •Lucian Mathes[1], Leon Heinl[2], Andreas Wagner[3], Maik Butterling[3], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]Institute of Casting Research, Montanuniversität Leoben, Austria — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Positron annihilation lifetime spectroscopy (PALS) is a unique tool for studying the concentration and types of open-volume defects. We performed depth-resolved PALS to investigate such defects and the properties of precipitates in differently (heat) treated AlCuMgAg samples. Alloying AlCu with Ag has been shown to leverage the formation of the so-called $\Omega(Al_2Cu)$ phase, known for its high strength and thermal stability. We present PALS measurements of Al-4Cu-0.3Mg-0.7Ag containing Ω phase precipitation after hot-rolling and subsequent T4-treatment. Our findings showcase the high thermal stability of the Ω phase and that positron annihilation studies help in understading and optimizing the process of strength hardening AlCuMgAg alloys.

KFM 14.9 Wed 17:00 P1

Polycrystalline FeS as ultra-fast charging sodium-ion battery anode — •Zidong Wang and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Fast charging is considered a key development trend and a competitive advantage for sodium-ion battery (SIB) technology. Achieving fast-charging SIBs relies on developing electrode materials that combine high rate performance with excellent capacity retention. While iron sulfide, known for its high theoretical capacity, has shown potential, its fast-charging performance is hindered by poor rate performance due to volume expansion. Conventional approaches, such as compositing with carbon materials or adjusting the cut-off voltage, come with drawbacks*carbon composites reduce volumetric energy density, while cut-off voltage adjustments compromise capacity. Neither approach aligns well with practical applications. To address these challenges, we capitalized on the crystalline structural diversity of iron sulfides and successfully synthesized carbon-free polymorphic FeS. This material achieves high rate performance without relying on carbon additives or cut-off voltage adjustments, marking a significant step forward in SIB development. Impressively, anode demonstrates the best rate performance reported to date at an exceptionally high current density, achieving 236 mAh/g at 50 A/g.

KFM 14.10 Wed 17:00 P1

Nanoscale Thermal Expansion in Crystals Probed by Echo-Resolved Terahertz Spectroscopy — •Nicolas Sylvester Beermann, Andreas Gebauer, Wentao Zhang, Tomoki Hiraoka, Savio Fabretti, Hassan Hafez, and Dmitry Turchinovich — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermal expansion of solids is a ubiquitous phenomenon in condensed matter physics [1]. However, its observation was out of limits for terahertz time-domain spectroscopy (THz-TDS) due to the relatively long sub-millimeter wavelength of THz radiation. To address this, we introduce echo-resolved THz spectroscopy (ERTS) that utilizes THz main and echo pulses in time-domain measurements to simultaneously determine frequency-dependent complex optical constants and material thickness [2]. By numerically solving complex transcendental transmission equations, ERTS allows for sample thickness measurements with deep-subwavelength precision on the order of $\lambda/1000$. We used the ERTS to analyze the THz-TDS data of magnesium oxide, sapphire, and gallium arsenide crystals measured in the temperature range of 10-300 K. The thermal expansion of the crystals on a sub-micrometer scale was measured, and the simple phonon model was applied to determine the material-specific Grüneisen parameters.

[1] K. Takenaka, Sci. Technol. Adv. Mater. 13, 13001 (2012)

[2] N. S. Beermann et al., Terahertz Time-Domain Spectroscopy for Simultaneous Measurement of Optical Constants, and Material Thickness with Deep-Subwavelength Precision, submitted manuscript

KFM 14.11 Wed 17:00 P1

Two Photon Absorption in Lithium niobate tantalate inspected via z-scan technique — •Niklas Dömer[1], Anton Pfannstiel[1], Steffen Ganschow[2], Mike Pionteck[2], Simone Sanna[3], and Mirco Imlau[1] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany — [3]Center for Materials Research J.L.-Univ. Giessen, Heinrich-Buff-Ring 16 , Giessen, Germany

The knowledge of the nonlinear optical properties of polar oxide crystals, such as the two-photon absorption (TPA) coefficient β in lithium niobate (LN), is of significant importance for tailoring technological applications in (integrated) photonics. Here, we present the results of our studies on the dispersion properties $\beta(\lambda)$, i.e. the imaginary part of the third-order susceptibility $\chi^{(3)}_{\mathrm{Im}}$, in the model system lithium niobate tantalate (LNT, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$). Experimentally, an open-aperture z-scan experiment pumped by fs-pulses in the spectral range of 330 - 600 nm from an optical parametric amplifier (OPA) is used. The obtained results are compared with literature data for LN ($x = 0$) and LT ($x = 1$) and the non-vegard-like behavior of the band gap. In extension, the study is applied for the determination of the density of states with LN as an example. We discuss our findings with ab-initio calculations for LN and in the framework of transient absorption phenomena induced by TPA in LNT [N. Dömer, J. Koelmann *et al.*, New J. Phys. **26** (2024) 083027]. This work is financially supported by the DFG (projects IM37/13-1, GA 2403/7-1 and SA1948/3-1 within the research unit FOR 5044, ID: 426703838).

KFM 14.12 Wed 17:00 P1

Refractive Indices and Birefringence Behavior of Lithium Niobate Tantalate Solid Solutions — •Tobias Hehemann[1], Anton Pfannstiel[1], Steffen Ganschow[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrueck University — [2]Leibniz-Institut für Kristallzüchtung, IKZ, Berlin

Lithium niobate tantalate solid solutions (LNT, $LiNb_{1-x}Ta_xO_3$ with $0 \leq x \leq 1$) exhibit a wide range of linear and nonlinear optical properties, that can be tuned by composition x. A unique feature is the disappearance of the birefringence Δn for x between $0.93 \leq x \leq 0.96$ [Wood *et al.*, J. Phys.: Condens. Matter **20** 235237 (2008)] enabling customized applications in photonics. While the dispersive behavior of the ordinary $n_o(\lambda)$ and extra-ordinary $n_e(\lambda)$ indices are well documented for the edge compositions $LiNbO_3$ (LN, x=0) and $LiTaO_3$ (LT, x=1), there remains a lack for LNT along x. In particular, nearly nothing is known about the structural relation between the index of refraction and composition. We here present our results for the dispersion behavior of n_o and n_e of LNT for several x, measured using an interferometric technique at specific wavelengths in the visible spectrum. Our data allow for a more detailed inspection of the birefringence $\Delta n = n_o - n_e$ of LNT at room temperature. The obtained data are analyzed and discussed in the context of existing literature, providing deeper insights into the relation between structure and optical properties of LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.13 Wed 17:00 P1

Surface and near-surface positron annihilation spectroscopy at very low positron energy — •Maximilian Suhr[1], Lucian Mathes[1,2], Vassily V. Burwitz[2], Danny R. Russell[1], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]School of Natural Sciences, Physics Department, TU München

Positron annihilation spectroscopy is a highly sensitive tool for defect characterization in solids. We present the Setup for Low-Energy Positron Experiments (SLOPE) at TUM. This monoenergetic positron beam is realized via a high-activity ^{22}Na source, a W moderator, a sophisticated electromagnetic beam guidance system and two high purity Ge detectors. Our instrument features a state-of-the-art range of implantation energy, namely 3 eV to 40 keV, enabling bulk measurements as well as investigations of surfaces. With three different measurements we showcase the versatile applications of SLOPE: a full range depth profile of a W monocrystal, coincidence ratio curves of H-loaded Ni, and a valley-to-peak (positronium formation) scan of Cu and Kapton at very low implantation energies.

KFM 14.14 Wed 17:00 P1

Microscopic view into non-volatile resistive switching in Au/Prussian blue/Ag layer stacks — •Mohammed Fayis Kalady[1], Daniel Wolf[1], Michael Pohlitz[2], Christian Mueller[2], and Axel Lubk[1,3] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden — [2]University of Applied Sciences Zwickau, 08056 Zwickau, Germany — [3]Institute of Solid State and Materials Physics, TU Dresden, Haeckelstraße 3, 01069 Dresden, Germany

Due to their distinct electrochemical properties, Prussian blue (PB) and its analogs (PBA) are emerging materials for memristor applications. This study uses transmission electron microscopy (TEM) techniques to explore resistive switching in PB-based memristors. Our work will utilize in-situ TEM to apply electrical bias, correlating nanoscale structural changes with electronic properties and employing methods like high-resolution TEM, electron energy-loss spectroscopy, and energy-filtered TEM. By changing the polarity of the external voltage, the Au/PB(A)/Ag is switched between two stable resistance states, the high resistance state and the low resistance state. The experimental technique seeks to elucidate the resistive switching mechanism, contributing to designing efficient and reliable memristor devices for advanced memory applications.

KFM 14.15 Wed 17:00 P1

Phonon Properties of perovskite oxides and halides — •Mwanaidi Mauwa Namisi and Benyao Sun — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

Perovskite materials, which have proven useful in many areas including photovoltaics and ferroelectrics [1], are highly structurally unstable due to the dynamic nature of the metal-halide octahedra and cation off-centering. It is therefore evident that understanding the vibrational properties of these materials is crucial in their modelling and applications. Meanwhile, there is considerable research value in developing high-performance, environmentally friendly, and health-conscious lead-free ferroelectric materials [2, 3]. Particularly, BaTiO3- based lead-free perovskites have become a major research focus. However, systematic studies on BaTiO3-based superlattices combined with BaSnO3 remain scarce. Here, we investigate the phonon properties of perovskite oxides (BaSnO3) and halides (CsPbX3, (X=I, Br, Cl) and discuss the distortions, do- main structures by the anharmonicity. We also investigate how these instabilities couple with an external field and discuss the differences in the ferroelectric nature between perovskite oxides and halides. Additionally, structural optimization was performed on BaTiO3/BaSnO3 superlattices with varying Sn concentration gradients. References (1) Bergenti, I. Appl. Phys. 2022, 55, 033001. (2) Grunebohm, A., Madhura, M., Claude, E. Appl. Phys. Lett. 2015, 107,102901. (3) Grunebohm, A.; Marathe, M. Phys. Rev. Mat. 2020, 4,4417.

KFM 14.16 Wed 17:00 P1

Thermodynamics of Barium Boranate using DFT — •Markus Mehlhorn[1], Konrad Burkmann[2], Angus Demmer[2], Jakob Kraus[1], Franziska Habermann[2], Jürgen Seidel[2], Klaus Bohmhammel[2], Jens Kortus[1], and Florian Mertens[2] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg — [2]Institut für Physikalische Chemie, TU Bergakademie Freiberg

Materials containing high hydrogen content are interesting candidates for solid hydrogen storage. However, there are well-known fundamental challenges to address like the reversibility of the (de)-hydrogenation and sufficiently fast kinetics for these processes before possible applications. Here we present results on thermodynamic properties of $Ba(BH_4)_2$. Unfortunately, the isobaric heat capacity function of this material is not accessible experimentally. $Ba(BH_4)_2$ could not be synthesized in sufficient purity. Therefore we attempt to fill this gap by means of computations based on density functional theory using the PBEsol functional. The quasi harmonic approximation is used to describe volume expansion due to thermal effects assuming that for each fixed volume the harmonic approximation can be employed. For each volume the phonon density of states has been calculated via density functional perturbation theory. This procedure allows to calculate the Gibbs free energy and therefore gives access to thermodynamic properties like entropy and isobaric heat capacity. Comparing the heat capacity to other metal boranates, which have been synthesized and measured, one finds very similar behavior.

KFM 14.17 Wed 17:00 P1

3D nanoscale chemical analysis of WO_3 using Atom Probe Tomography — •Katharina Wolk[1], Jack T. Eckstein[2], Kasper A. Hunnestad[1], Constantinos A. Hatzoglou[1], Gustau Catalán[3], Ekhard K. H. Salje[2], Julia Glaum[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Department of Earth Sciences, University of Cambridge, Cambridge, UK — [3]Institut Català de Nanociència i Nanotecnologia, Campus Universitat Autònoma de Barcelona, Bellaterra, Catalonia

The functional properties of oxides are closely linked to their chemical composition. The transition metal oxide WO_3 is notable for its structural versatility and unusual physical properties, such as the formation of superconducting ferroelastic domain walls. To understand the relation between local variations in chemical composition and material properties, we apply atom probe tomography (APT). APT offers compositional mapping in 3D with sub-nanometer spatial resolution and chemical sensitivity of 100 ppm. Using scanning electron microscopy, we image the ferroelastic domain structure in WO_3 single crystals and extract specimens from different regions of interest with a focused ion beam for the APT analysis. Based on 3D reconstructions, we investigate site-specific variations in chemical composition, exploring the oxidation state and potential formation of oxygen defects. Varying experimental APT parameters, such as laser energy, enables insights into optimizing compositional accuracy.

KFM 14.18 Wed 17:00 P1

Isovalent exchange of Al, Mg and Zr in strontium hexagallate (SrGa12O19) — •Finn. H. Bietz[1], Ch. Rhode[2], and S. Sanna[1,3] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen 35392, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Straße 2, 12489 Berlin — [3]Center for Materials Research (ZfM), Justus Liebig University Gießen, Gießen 35392, Germany

$SrGa_{12}O_{19}$ can be used as a substrate for the growth of barium hexaferrite, a ferrimagnetic and quantum paraelectric material. The lattice parameters of $SrGa_{12}O_{19}$ can be adjusted by substitution of Ga by Al or Mg and Zr respectively for lattice-matched growth and strain engineering of barium hexaferrite. A microscopic picture of the doping mechanisms and their effect on the lattice parameters is missing.

In this contribution, we report on first-principles calculations performed to determine the lattice site of Al, Mg and Zr atoms in the $SrGa_{12}O_{19}$ structure, and support corresponding experiments performed at the IKZ in Berlin. Thereby the defect formation energies of Al, Mg and Zr atoms incorporated in the dilute limit at different lattice sites were calculated within density functional theory.

The atomistic models reveal that Mg populates the so called $Ga^{(3)}$ position, Al prefers the $Ga^{(1)}$ site, but also populates the $Ga^{(4)}$ and $Ga^{(5)}$ sites, and that the Zr is incorporated the $Ga^{(4)}$ site. While the results are in very good agreement with the experimental results in the case of Mg and Al doping, the experimentally determined lattice site of Zr differs from the theoretical predictions, suggesting the formation of defect complexes or co-doping related effects.

KFM 14.19 Wed 17:00 P1

Tailoring ferroelectric and magnetic properties in polycrystalline hexagonal manganites — Jonas Åmli Ingdal[1], •Ruben Skjelstad Dragland[1], Catalina Salazar[2], Ellinor Benedikte Anjali Lindström[1], Katharina Wolk[1], Tino Gottschall[2], Jiali He[1], Jan Schultheiss[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany

Rare-earth hexagonal manganites are extensively studied for their diverse physical phenomena, including tunable electronic behavior at ferroelectric domain walls, pronounced magnetocaloric effects, and significant thermal Hall conductivity, which make them highly interesting as advanced multi-functional materials. The intriguing effects arise from the unique combination of improper ferroelectricity and antiferromagnetic ordering, which are intimately linked to the rare-earth ions.

In this study, we systematically investigate the role of the rare-earth atom on the ferroelectric and magnetic properties of h-RMnO3. Polycrystalline samples with R = Tm, Er, Y, Ho, and Dy are synthesized using a solid-state approach. Ferroelectric order is verified across all compositions using piezoresponse force microscopy. Direct adiabatic temperature change measurements in the cryogenic regime reveal a strong correlation between rare-earth magnetism and the caloric response. Our results highlight the possibility to tune both the ferroelectric order and magnetic responses, offering new opportunities for optimizing the system for envisioned applications.

KFM 14.20 Wed 17:00 P1

Characterizing Domains in GeTe using Atom Probe Tomography — •Jan Köttgen[1], Maria Häser[1], Lina Jäckering[1], Julian Pries[1], Carl-Friedrich Schön[1], Pengfei Cao[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons ER-C, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The thermoelectric GeTe undergoes a solid-state phase transition from its cubic to its rhombohedral crystal structure when cooled from the melt to room temperature. This phase transformation results in domains. In this study a polycrystalline GeTe bulk sample was investigated using atom probe tomography (APT), which enables the determination of the sample*s stoichiometry with atomic resolution. The APT analysis revealed that different domains evaporate with different probabilities of multiple events (PME). Metavalent solids such as GeTe are known generally to exhibit a high PME in APT. Our experiments additionally show an anisotropy between different grains as observed in the PME. Using a correlative approach involving TEM, EBSD, AFM, SNOM, and DFT calculations, this effect can be attributed to an expansion of the unit cell and a concomitant change of the dielectric function. Our experiments open new avenues for atom probe tomography as a tool to investigate domains and the atomic distribution simultaneously crucial to improve the performance of thermoelectrics.

KFM 14.21 Wed 17:00 P1

Long-lived, pulse-induced transient absorption in $LiNb_{1-x}Ta_xO_3$ ($0 \leq x \leq 1$) solid solutions — •Julian Koelmann[1], Niklas Dömer[1], Mira Hesselink[1], Tobias Hehemann[1], Anton Pfannstiel[1], Felix Sauerwein[1,2], Laura Vittadello[1,2], Steffen Ganschow[3], and Mirco Imlau[1] — [1]Institute of Physics, Barbarastr. 7, Osnabrück University, Osnabrück, Germany — [2]Research Center for Cellular Nanoanalytics, Osnabrueck (CellNanOs), Osnabrueck University, Barbarastr. 11, Osnabrueck, 49076, Germany — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

Femto-/nanosecond pulse-induced, red and near-infrared absorption is studied in $LiNb_{1-x}Ta_xO_3$ (LNT) solid solutions with the aim of studying transient optical nonlinearities associated with optically generated small bound electron polarons. As a result, a long-lived transient absorption is uncovered for LNT which exceeds lifetimes and starting amplitudes of $LiNbO_3$ (LN) and $LiTaO_3$ (LT) by a significant factor. The transients provide strong evidence for an underlying hopping transport mechanism of small bound polarons. All findings are discussed in comparison to the model systems LN and LT within the framework of appropriate band models and optical generation of polarons via two-photon excitation. To explain the significant differences, the simultaneous presence of Nb_{Li}^{5+}, Ta_{Li}^{5+} antisites, and Ta_V^{5+} interstitial defects is assumed for LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) * Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.22 Wed 17:00 P1

Investigation of Pressure-Induced Dimerization in a Pyrene-based Dyad Crystal: Associated with Auxiliary exhibition of thermally Induced Intramolecular Charge Transfer — •Argha Barman[1], Agniezska Huć[2], and Krishnayan Basuroy[1] — [1]DESY, Hamburg, Germany — [2]University of Warsaw, Poland

We present the design and photophysical properties of a D-B-A dyad with N, N-dimethylaniline (DMA) as the electron donor and pyrene (Py) as the acceptor, linked by a -CH=CH- chain. The molecule crystallizes in the triclinic space group P-1, undergoing a reversible phase transition with solvent-dependent transition temperatures (e.g., 200K in cyclohexane, 198K in toluene, 209K in dichloromethane). Structural changes include variations in bond lengths and pyramidalization at the tertiary nitrogen atom, with persistent strong $\pi^{***}\pi$ stacking. Photophysical analysis reveals a small HOMO-LUMO gap (3.06 eV) and temperature-dependent dual fluorescence from locally excited (LE) and intramolecular charge transfer/excimer (ICT) states, with ICT emission diminishing above 220K. Under hydrostatic pressure (0.5*2.0 GPa), the crystals exhibit

piezochromic behavior with emission redshift and quenching. These multifunctional properties make Py-CH=CH-DMA crystals promising for optoelectronics and pressure sensors.

KFM 14.23 Wed 17:00 P1

Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[1] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

KFM 14.24 Wed 17:00 P1

Theoretical Investigation of [100] Edge Dislocations in Ferroelectric Perovskites — •Himal Wijekoon[1], Pierre Hirel[2], and Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High-performance Materials (ZGH), Ruhr Universität Bochum, Germany — [2]Université de Lille, CNRS, INRAE, Centrale Lille, UMET, F-59000 Lille, France

Ferroelectric switching is critically influenced by nucleation and pinning at defects within the material. Despite their significance particularly at strained interfaces, the role of dislocations on switching is however largely unexplored. We employ atomistic core-shell potentials [1] to demonstrate that edge dislocations can facilitate domain nucleation and reduce the coercive field. These findings suggest that a more comprehensive understanding of these defects could lead to improved material performance.

[1] M. Sepliarsky, A. Asthagiri, S.R. Phillpot, M.G. Stachiotti, and R.L. Migoni, Atomic-level simulation of ferroelectricity in oxide materials, Current Opinion in Solid State and Materials Science, 9(3):107-113, June 2005.

KFM 14.25 Wed 17:00 P1

Interaction of $NaYF_4$:Yb:Er Upconversion Nanoparticles with ultrashort laser pulses — •Leon Siemon[1], Felix Sauerwein[1], Thibault Mengis[1], Leonie Birk[2], Eike Wienbeuker[2], Markus Haase[2], Jacob Piehler[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrück University, Germany — [2]Dept. of Biology/Chemistry, Osnabrück University

Lanthanide-doped upconversion nanoparticles (ucNP), such as $NaYF_4$:Yb:Er, play a significant role for future all-optical interrogation techniques of cellular systems due to their ability to convert infrared excitation light (980 nm/Yb-absorption) into green/red luminescence (520, 540, 660 nm/Er-emission). The corresponding conversion characteristics and energy transfer mechanisms have been studied extensively under continuous-wave illumination - however, so far, the interaction of ucNPs with ultrashort laser pulses has not been studied. We have adressed this question via diffuse fs-pulse reflectometry [C. Kijatkin *et al.*, Photonics **4** (2017) 11] of $NaYF_4$:Yb:Er nanoparticles ($d \approx 18\,nm$) exposed to 980 nm sub-ps-pulses ($\tau_{pulse} > 40$ fs) at peak intensities up to 10^{14}W/m^2 and repetition rates down to 50 Hz. We observe severe differences in the intensity dependence, quantum yield and average power density that are attributed to modified population pathways in the energy diagram if the pulse duration falls below the resonant energy transfer time between Yb and Er ions. The impact of our findings for ucNP applications in cellular environments, particularly to reduce laser-induced cell damages, is discussed. Financial support DFG/RTG2900, 'nanomaterials@biomembranes'.

KFM 14.26 Wed 17:00 P1

Harmonic Nanoparticles: State-of-the-knowledge and future applications — •Moritz Domack[1], Jan Klenen[1], Mirco Imlau[1], and Laura Vittadello[2] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Laboratoire SYMME, 7 Chemin de Bellevue, Université Savoie Mont Blanc, France

Harmonic nanoparticles (HNPs) are receiving growing attention in anorganic chemistry, nanophotonics and life sciences due to their potential for upcoming imaging techniques. For instance, HNPs are successfully used as nanophotonics markers in the near-infrared (NIR) bio-optical windows (III) and (IV), so-called NIR-to-NIR imaging [L. Vittadello *et al.*, Nanomaterials **11** (2021) 3193], as well as for destruction free in-vivo imaging [L. Vittadello *et al.*, Opt. Mater. Express **11.7** (2021) 1953-1969]. HNPs are based on polar oxide nanocrystals with pronounced nonlinear optical response, such as sodium niobate ($NaNbO_3$) or potassium niobate ($KNbO_3$) and can already be synthesized at the nanometer scale (<100 nm), e.g. via hydrothermal synthesis [N. Kohlenbach *et al.*, Nanoscale **12** (2020) 19223], but also surface-functionalized. Nonlinear Diffuse femtosecond-pulse reflectometry of powder-pressed-HNP-samples has been established as major tool for characterization of the nonlinear optical properties [C. Kijatkin *et al.*, Photonics **4.1** (2017) 11]. We here give insight to the state-of-the-art processing routine of HNPs from synthesis, via characterization to applications and highlight upcoming fields, particularly in the framework of all-optical interrogation of cellular environments. Financial support by the DFG/RTG2900, 'nanomaterials@biomembranes'.

KFM 15: Crystal Structure Defects / Real Structure / Microstructure

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Thursday 9:30–13:15 Location: H9

Invited Talk KFM 15.1 Thu 9:30 H9

Is CVD diamond now ready to become an electronic material? — •Philippe Bergonzo — University College London UK — Seki Diamond System, San Jose CA, USA

CVD Diamond is an exceptional material combining superlative properties like electronic properties, thermal conductivity, biocompatibility, radiation resistance, and optical properties. These advantages make diamond an excellent material for a broad range of applications, including radiation detectors, high transparency windows, electronic devices, quantum devices, sensors, etc. Remarkable devices have been fabricated and are still respected as a reference. But still, can diamond come out of the lab to become a competitive device material? Although diamond synthesis is a pretty well-established technique, there are still more than 80% of the machines growing diamond on the planet that grow it to make gemstones. And this has always inhibited the progress this material deserved. Only very recently, and with the recent huge downturn that affects the gem business, one can consider that we may have reached an inflection point where CVD diamond may soon benefit from being something else than a gemstone. Potentially, innovative developments for physics may not be kept secret because they could be more valuable for the gem market, if this latter one is collapsing. In this context, how can we facilitate this progress? Drawing from typical cases where diamond-based devices are used for specific applications, examples will be used to illustrate material opportunities and challenges towards diamond to become a standard for device applications.

KFM 15.2 Thu 10:00 H9

Numerical analyses and loss tangent measurements for the W7-X ECRH gyrotron diamond output windows — •Gaetano Aiello[1], Andreas Meier[1], Heinrich Peter Laqua[2], Theo Scherer[1], Sabine Schreck[1], and Dirk Strauss[1] — [1]KIT, Karlsruhe, Germany — [2]IPP, Greifswald, Germany

The 140 GHz 1 MW gyrotron for the electron cyclotron resonance heating (ECRH) system at the stellarator Wendelstein 7-X (W7-X) is being upgraded to 1.5 MW continuous wave operation to increase the total heating power for achieving operating regimes with high plasma beta and low collisionality. The gyrotron features a chemical vapor deposition (CVD) polycrystalline diamond window with an aperture of 88 mm and a disk of 1.8 mm thickness and 106 mm diameter. In this work, numerical analyses of the window are shown with loss tangent values provided by experimental measurements on 25 bare diamond disks. Computational fluid dynamics (CFD) conjugated heat transfer and structural analyses were carried out to check the window performance at 1.5 MW operation, when cooled by water and silicon oil Dow Corning 200(R) 5cSt.

KFM 15.3 Thu 10:15 H9

Single- and polycrystalline diamond characterization with superconducting microresonators — •Francesco Mazzocchi[1], Martin Neidig[2], Sebastian Kempf[2], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute Of Technology IAM-AWP — [2]Karlsruhe Institute Of Technology IMS

The development of high optical quality, ultra-low-loss single-crystal diamond windows is essential for the realization of future nuclear fusion facilities, such

as DEMO, due to the anticipated increase in power for microwave ECRH systems. So far, accurate measurement of the dielectric properties (ϵr and $\tan\delta$) of these materials has primarily relied on Fabry-Perot microwave resonators in different setups, with a resolution limit around 1E-5 in the determination of the loss tangent. Superconducting thin-film resonators, capable of reach Q factors in excess of 1E6, have the potential to assess the dielectric characteristics of ultra-low-loss materials like single- and polycrystalline diamond while offering a significant boost in resolution when compared to the state-of-the-art Fabry-Perot resonance cavities. We hereby report measurements performed at low (4 - 9 K) an ultra-low (10 - 700 mK) temperatures of several samples including single and poly-crystalline diamond. The samples have been grown with different techniques, including CVD, cloning and HPHT processes.

KFM 15.4 Thu 10:30 H9

Simulated nano-extrusion of graphene hyperbolic pseudosphere surfaces — •Peter Klaver[1], Alfredo Iorio[2], Ruggero Gabbrielli[3], and Dominik Legut[1] — [1]VSB Technical University of Ostrava, Ostrava, Czech Republic — [2]Charles University, Prague, Czech Republic — [3]Independent researcher

We produce curved graphene hyperbolic pseudosphere surfaces in molecular dynamics (MD) simulation of a nano-scale extrusion process. During the extrusion process the carbon atoms form pentagons, hexagons and heptagons and such a mixture is unrealistically less stable than pure graphite or diamond. During relaxation and lengthy high temperature annealing after the extrusion process, polycrystalline curved graphene with a limited number of point defects is formed. The point defects cause bending of the graphene and the pseudosphere edges even more. When these free edges are removed from the simulations by attaching periodic flat graphene sheets to the pseudosphere edges, the carbon atoms assume positions with a root mean square deviation of some tenths of Å from the mathematical hyperbolic pseudosphere surface. The hyperbolic pseudospheres proved to be mechanically stable against large shearing and elongation deformations as well as against annealing at 1500 K. Our methodology is easy to use, employing the REBO2 carbon interaction potential within the open source MD code LAMMPS. Our method offers a practical way to create simulated stable, curved graphene surfaces with a wide variety of desired shapes. It allows for the testing in advance of the stability of graphene shapes that are to be produced experimentally.

KFM 15.5 Thu 10:45 H9

Inverted Designs of Dielectric Metasurfaces Based on TiO_2.: A Study on Quasi-Bound States in Continuum (qBIC) — •Justin Schulz[1], Jack Dobie[1,2], Oisin McCormack[1,2], Yongliang Zhang[1], Hodjat Hajian[1], Owen Moynihan[2], Brian Corbett[2], and A. Louise Bradley[1,2] — [1]School of Physics, Trinity College Dublin, Dublin 2, Ireland — [2]IPIC, Tyndall, University College Cork, Cork, Ireland

Dielectric metasurfaces, engineered to manipulate light primarily by controlling the phase and amplitude of the scattered light, have garnered significant interest in recent years, particularly due to their ability to support quasi-Bound States in Continuum (qBIC).

Building upon previous work on slotted disk metasurfaces fabricated in Si_3N_4, we investigate inverted TiO_2-based designs. TiO_2, with its high refractive index, offers distinct advantages in enhancing the resonance properties of dielectric metasurfaces, enabling more efficient light-matter interactions. A key objective of this work is to perform a comparative analysis between slotted disk structures and their inverted counterparts, with a focus on their respective lattice and qBIC modes. Future prospects of TiO_2-based dielectric metasurfaces and the potential applications in low-energy switching and polariton lasing are discussed, with a particular focus on their integration with transition-metal dichalcogenide (TMDC) monolayers or quantum dots. This project is funded through; Taighde Éireann/Research Ireland Frontiers for the Future Award - SFI-21/FFP-P/10187, 12/RC/2278_2, and 12/RC/2276_P2.

15 Minutes Break

KFM 15.6 Thu 11:15 H9

Phase modifications in Beta-Gallium Oxide via Focus ion beam irradiations — •Umutcan Bektas, Nico Klingner, Paul Chekhonin, Fabian Ganss, Rene Hübner, Maciej Oskar Liedke, and Gregor Hlawacek — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Gallium oxide (Ga2O3) is a highly versatile material with power electronics, optoelectronics, and battery technologies applications. Among its polymorphs, monoclinic β-Ga2O3 is the most chemically and thermally stable phase. However, managing the metastable polymorph phases remains challenging, and the fabrication technology for nanoscale structures is still under development. We aim better to understand the polymorph conversion mechanisms under ion irradiation. In this study, we investigate the β-Ga2O3 samples irradiated with different ions and fluences, together with α- and κ-Ga2O3 thin films. Focused ion beam (FIB) irradiation was used to locally modify the samples under controlled conditions by varying the ion beam current, size, spacing, scan type, and ion species. The irradiated regions were characterized using electron backscatter diffraction and transmission electron microscopy to analyze structural changes. Broad beam irradiation experiments were complemented by positron annihilation spectroscopy methods to determine defect types and concentrations. Initial results indicate that spatially resolved polymorph transitions can be achieved using FIB irradiation. In addition, the defect size and concentration were found to depend on the polymorph and the implanted ion species, providing critical into defect engineering in Ga2O3.

KFM 15.7 Thu 11:30 H9

An EXAFS analysis of the laser-driven tetragonal to cubic phase-transition in $BaTiO_3$ — •Janosch Tasto[1], Rajdwip Bhar[1], Simon Rauls[1], Marco Reinhard[2], Dimosthenis Sokaras[2], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]SLAC National Accelerator Laboratory, Stanford University

This work aims to establish time-resolved Extended X-ray Absorption Fine Structure (tr-EXAFS) spectroscopy as a methodology for solids where the structural information of the EXAFS is combined with a pump-probe setup to study local dynamic lattice processes in the time domain. As a first step along this road, the information contained in a difference-EXAFS scan between the pumped and unpumped state is analyzed.

As proof of concept, the structural cubic to tetragonal phase transition in ferroelectric $BaTiO_3$ is analyzed. The coexistence of displacive and order-disorder phenomena accompanying this transition is debated in the literature of this widely investigated material. Difference-EXAFS scans at the Ti-K and Ba-L_3 edge between the tetragonal and cubic phase provide a direct way to investigate changes in structure and thermal induced disorder in the vicinity of the absorbing atom. We correlate our spectroscopic findings with *ab initio* multiple-scattering calculations using the FEFF10 code to quantify thermal and structural contributions.

We thank the Deutsche Forschungsgemeinschaft (in the framework of the Collaborative Research Center 1242) for financial support.

KFM 15.8 Thu 11:45 H9

Dislocation correlations in GaN epitaxial films revealed by EBSD and XRD — •Domenik Spallek, Vladimir M. Kaganer, Philipp John, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Threading dislocations in group-III nitrides are omnipresent and are a challenge especially in heteroepitaxial growth for device applications. However, the correlation of individual dislocations with each other and the resulting screening of the strain is often disregarded although it is a necessity to describe elastic energies in an extended crystal.

In this study, two GaN epitaxial layers with threading dislocation densities (TDD) of 5×10^8 cm^{-2} and 1.8×10^{10} cm^{-2} are investigated by x-ray diffraction (XRD) and high-resolution electron backscatter diffraction (HR-EBSD), complemented by Monte Carlo simulations to model and interpret the experimental results.

While the XRD measurement directly gives quantitative results about the average strain in the illuminated area, a cross-correlation analysis of Kikuchi patterns results in spatially-resolved maps for the components of the strain and rotation tensors. Through an analysis of the strain-strain correlation functions for the measured and simulated maps, it is found that the spatial resolution in the HR-EBSD maps is highly anisotropic. Furthermore, we discover that the strain is significantly underestimated for higher dislocation densities. As main result, the screening distances for dislocations were determined as 2 μm and 0.3 μm for the sample with the lower and higher TDD, respectively.

KFM 15.9 Thu 12:00 H9

Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[3] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany — [3]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

15 Minutes Break

KFM 15.10 Thu 12:30 H9

Landau Theory for Quasicrystals at the Mesoscale — •Marcello De Donno[1], Luiza Angheluta[2], Ken R. Elder[3], and Marco Salvalaglio[1,4] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Njord Centre, Department of Physics, University of Oslo, 0371 Oslo, Norway — [3]Department of Physics, Oakland University, Rochester, Michigan 48309, USA — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

Quasicrystals challenge traditional concepts of crystallinity by exhibiting ordered yet aperiodic atomic structures. Their peculiar atomic arrangements give rise to exceptional physical properties, including high hardness, low friction, and remarkable wear resistance, making them worth exploring for high-performance engineering applications. Additionally, their slow dislocation creep leads to high-temperature strength and stability in plastic regimes. We present a mesoscale field theory that unifies the modeling of growth, elasticity, and dislocations in quasicrystals. Using the amplitude formulation of the density-wave representation, our approach models the dynamics of quasicrystals through a free energy functional for complex amplitudes, with non-conserved dissipative dynamics describing their evolution. By specifying only the lattice structure in reciprocal space, our theory self-consistently captures elasticity-including phononic and phasonic deformations-along with defect nucleation and motion. Predictions include the kinematics of dislocations and the formation of semi-coherent interfaces, offering new insights into the mechanics of quasicrystals.

KFM 15.11 Thu 12:45 H9

An all-order phonon approach to thermal diffuse scattering — •Benjamin Fahl and Arkadiy Simonov — ETH,Zurich,Switzerland

Phonons play a role in various phenomena, from superconductivity through phonon-electron coupling and spintronics via phonon-spin interactions, to dynamical stability of solids, and are fundamental to elastic properties. They can be probed by measuring Thermal Diffuse Scattering (TDS) from single crystals. However, modelling of the TDS, is a computational challenge due to the number of intensities in the experiment. With existing software, like AB2TDS, the full experiment can be calculated only in one- or two-phonon approximations. Approximations of higher order are possible, but are computationally expensive and can be performed only on small portions of reciprocal space. In this work, we propose a new method for modeling and fitting TDS signals using joint atomic displacement parameters in YELL. This approach uses the crystal's dynamical matrix as input, which is derived by various methods including universal potentials, DFT, or approximated from elastic constants. By using a Fast-Fourier Transform, our method can quickly calculate large volumes of TDS in infinite phonon approximation. This development will enhance the 3D-ΔPDF suite, enabling extraction of elastic constants from various materials and extending to the analysis of high-amplitude soft phonons, which are relevant in negative thermal expansion materials like ScF_3. The softwares capability to handle higher-order phonon contributions makes it particularly valuable for systems where these effects are significant, addressing a current gap in available tools.

KFM 15.12 Thu 13:00 H9

Solving the phase problem: retrieving complex structure factors using Large-Angle Rocking-Beam Electron Diffraction — •Sam Fairman[1], Grigory Kornilov[2], Benedikt Haas[2], Zbignew Galazka[3], Adnan Hammud[4], Niklas Delby[5], and Christoph T. Koch[2] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [4]Fritz-Haber-Institut, Berlin, Germany — [5]Nion Company, Kirkland, WA, USA

X-ray crystallography phasing methods have previously been successfully applied to electron diffraction experiments. However, dynamical scattering, caused by the electron's much larger scattering cross section, is normally viewed as a hindrance to structural determination and is mitigated, e.g. by continuous rotation or precession. Presented here is an ab-initio method that makes use of dynamical scattering to solve the phase problem directly from experimental data. A custom weighting scheme is combined with the ADAM optimizer to directly fit the complex structure factors in the Bloch-wave formalism to Large-Angle Rocking-Beam Electron Diffraction data. Our method allows for an approximate 5−fold increase in spatial resolution compared to the largest spatial frequency directly measured. This recovery of resolution is ideal for beam sensitive materials where high order diffraction data is impossible to measure. Simulated and experimental results are presented for non-centrosymmetric GaN and centrosymmetric $\beta - Ga_2O_3$.

KFM 16: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:00 Location: H13

See HL 45 for details of this session.

KFM 17: Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: H23

See MM 30 for details of this session.

KFM 18: Materials Research in Polar Oxides: Perspectives for Optics & Electronics

The focus session is dedicated to bridge the gap between materials research in polar oxides and research fields that apply those materials, such as nonlinear and quantum optics, electronics or sensoring. The goal is to improve the mutual understanding of each other research goals and necessities. Examples for topics could be improved or novel techniques for domain engineering, which are relevant for (nonlinear) optical applications, the growth of novel polar oxides with improved properties over traditional materials, such as higher temperature stability or improved nonlinear characteristics, or the discussion of novel emergent properties in this context, like conductive domain walls in opto-electronical applications.

Chairs: Michael Rüsing (Paderborn University), Christof Eigner (Paderborn University)

Time: Thursday 15:30–17:45 Location: H9

Invited Talk KFM 18.1 Thu 15:30 H9

Domain gratings of sub-micrometer period for quantum technologies — •Carlota Canalias — KTH-Royal Institute of Technology, Stockholm Sweden

This talk explores the challenges and advancements in developing sub-micron ferroelectric domain gratings, which are vital for nonlinear optical devices capable of generating counter-propagating photons. Conventional materials and poling methods have proven insufficient to support these cutting-edge optical interactions, thereby constraining their applications in both classical and quantum technologies. The presentation showcases a breakthrough in periodic poling techniques for KTP isomorphs, enabling the fabrication of bulk structures with domain sizes as small as 200 nm. This achievement leverages coercive-field gratings formed via ion exchange, which play a pivotal role in domain formation. Our results demonstrate that the creation of sub-micron domains is governed by the characteristics of the ion-exchanged region, rather than the poling period, opening new possibilities for designing smaller and more intricate domain-engineered devices.

KFM 18.2 Thu 16:00 H9

Gray tracks in $KTiOPO_4$ from DFT calculations — •Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Ferroelectric $KTiOPO_4$ (KTP) is commonly applied in (nonlinear) optical devices. However, the irradiation with high-intensity laser light or the application of strong electric fields triggers the formation of detrimental gray tracks [1], the microscopic origin of which is usually attributed to Ti^{3+} centers (i.e., reduced titanium atoms) charge compensating for oxygen vacancies [2]. In this study, we use DFT routines to further clarify the gray-tracking mechanisms by systematically model oxygen-vacancy related Ti^{3+} centers in application-relevant environments, i.e., potassium vacancies and rubidium dopants. We find that the only thermally stable [2] Ti^{3+} center forms close, but not adjacent the oxygen vacancy itself. In addition, displaced potassium ions provide the stabilizing forces, whereas potassium interstitials rather than oxygen vacancies alone appear to be directly related to gray tracks. For this we suggest that the current gray-tracking model has to be partially revised. [3]

[1] M. Roth, in Springer Handbook of Crystal Growth, Chap 20, 691 (2010, Berlin, Heidelberg)

[2] S. D. Setzler, et al., J. Condens. Matter Phys. 15, 3969 (2003)

[3] A. Bocchini, et al., submitted to Phys. Rev. B

KFM 18.3 Thu 16:15 H9

Interaction between small electron-polaron and neutral domain wall in $PbTiO_3$: A DFT+U study — •Mohammad Amirabbasi, Jochen Rohrer, and Karsten Albe — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt-Straße 3, Darmstadt D-64287, Germany

$PbTiO_3$ is a widely studied ferroelectric material that often requires doping to tailor its electronic structure for specific applications. Understanding charge compensation mechanisms, particularly those mediated by local lattice distortions such as small polarons, is crucial for optimizing these modifications. This research investigates the formation and stability of a small electron polaron in $PbTiO_3$, focusing on its interaction with the neutral 180° Pb-centered domain wall using density functional theory with Hubbard corrections (DFT+U). We begin by calculating the formation energy of the 180° Pb-centered domain wall. Next, we determine the Born effective charges for various ions and compute the polarization profile across the domain wall. Our results show that the polarization in the bulk region reaches a saturation value, which is in good agreement with experimental measurements. Finally, we calculate the trapping energy of a small electron polaron at Ti centers in both bulk and domain wall regions. The results reveal that the trapping energy is negative in both cases, indicating that small electron polaron formation is energetically favorable. Furthermore, the similarity in trapping energy values suggests that the 180° Pb-centered domain wall in $PbTiO_3$ has a minimal impact on this type of small electron polaron formation.

15 min. break

KFM 18.4 Thu 16:45 H9

Atomistic Modelling of Ferroelectric Bonded Structures — •Nils Andre Schäfer and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Direct bonding in ferroelectric materials, such as lithium niobate (LN), provides a method to create both head-to-head (H2H) and tail-to-tail (T2T) domain walls (DWs). These DW configurations are particularly interesting due to their ability to exhibit (semi-)metallic behavior by the formation of a two-dimensional electron or hole gas. This phenomenon enables the creation of localized conducting areas within an otherwise wide-gap semiconductor material.

In this work, we model H2H and T2T bonded structures within DFT. Therefore, we start with the thermodynamically stable z-cut surfaces of LN. Simulations were conducted on slabs with varying film thickness to minimize the surface interactions before constructing the bonded structures. The energy landscape of the interface was mapped by systematically translating the films relative to each other and analyzing various quantities, such as free charge carrier densities, the film distance, and the surface energy. In conclusion, H2H and T2T bonded structures exhibit distinct morphological and electronic interfaces, resulting in variations in their expected conductivities.

KFM 18.5 Thu 17:00 H9

Influence of different organic molecules on dielectric response in halide perovskites — •Doru Lupascu[1], Youn Un Jin[1], Witchitaya Arpavate[1], Andre Karabanov[1], Lars Leander Schaberg[1], Niels Benson[1], Bernd Marler[2], and Andre Salak[3] — [1]Universität Duisburg-Essen — [2]Ruhr-Universität Bochum — [3]Universidade de Aveiro

The charge carrier mobility in halid perovskites is still not fully understood. We have been discussing dielectric effects as one fundamental piece in the explanation of the large screening of defects and the polaron mobility. In this presentation we compare different organic molecules for their influence on the dielectric response. The interrelation of molecule mobility and dielectric screening will be discussed.

KFM 18.6 Thu 17:15 H9

Piezoresponse force microscopy study of local polarization dynamics in uniaxial relaxors — •Vladimir Shvartsman[1], Boris Slautin[1], Jan Dec[2], Sergei Kalinin[3], and Doru Lupascu[1] — [1]Institute for Materials Science, University Duisburg-Essen, Essen, Germany — [2]University of Silesia, Katowice, Poland — [3]University of Tennessee-Knoxville, USA

The unusual properties of relaxor ferroelectrics are related to their particular polar structure. In these materials, the polarization is correlated only on the nanometer scale within the so called polar nanoregions (PNRs). The dynamics of PNRs strongly affects the dielectric properties of relaxors. Here, we report about piezoresponse force microscopy study of local polarization dynamics in SrxBa1-xNb2O6 single crystals. In these materials having uniaxial polarization, the cross-over from ferroelectric to relaxor behavior occurs with increasing Sr content making SBN a good model system. We use time-resolved piezoresponse force spectroscopy. This technique measures temporal decay of the piezoresponse induced by a locally applied electric field over a dense spatial grid. The analysis of the time dependences of the piezoresponse allows to estimate the local relaxation time. Spatial maps of relaxation parameters are constructed, giving information on the spatial heterogeneity of polarization dynamics for different compositions and temperatures. Temperature dependences of local relaxation time are analyzed.

KFM 18.7 Thu 17:30 H9

Surface-near domain engineering in multi-domain x-cut lithium niobate tantalate mixed crystals — Laura Bollmers[1,2], Tobias Babai-Hemati[2], Boris Koppitz[3], Christof Eigner[1], Laura Padberg[1,2], •Michael Rüsing[1,2], Lukas M. Eng[3,4], and Christine Silberhorn[1,2] — [1]Paderborn University, Institute for Photonic Quantum Systems (PhoQS), 33098 Paderborn, Germany — [2]Paderborn University, Integrated Quantum Optics, 33098 Paderborn, Germany — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence|EXC 2147, TU Dresden, 01062 Dresden, Germany

Lithium niobate tantalate mixed crystals present a novel material plattform, which offer new possibilities over pure lithium niobate or lithium tantalate, such as improved thermal stability or the possibility to tune the birefringence. A key requisite for application in nonlinear optics, electronics and piezotronic is the possibility of domain engineering. So far, this proved difficult for mixed crystals due to stoichiometric inhomogeneities, which stabilizes the random as-grown domain structure. In this work, we investigate surface-near periodic poling of x-cut mixed crystals and demonstrate microscopically how the random domain structure in the as-grown crystals can inhibit large scale poling. If monodomain areas are poled, however, periodic poling becomes possible. Our work lays the foundation for future applications of lithium niobate tantalate mixed crystals.

KFM 19: Members' Assembly

We will elect our spokespersons, plan the programme for the next years, and award the poster prize.

Chair: Anna Grünebohm (Ruhr University Bochum), KFM spokesperson

Time: Thursday 18:00–19:00 Location: H9

All members of the Crystalline Solids and their Microstructure Division are invited to participate.

Magnetism Division
Fachverband Magnetismus (MA)

Claudia Felser
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Overview of Invited Talks and Sessions

(Lecture halls H16, H17, H18, H19, H20, and H36; Poster P1 and P3)

Invited Talks

MA 5.1	Mon	9:30–10:00	H20	**Driving Coherent Phonon-Phonon Angular Momentum Transfer via Lattice Anharmonicity** — •Sebastian Maehrlein
MA 5.2	Mon	10:00–10:30	H20	**Chiral phonons, phono-magnetism, and spin-rotation coupling** — •Matthias Geilhufe
MA 5.3	Mon	10:30–11:00	H20	**Geometry of temporal chiral structures and photoinduced chirality-spin coupling** — •Olga Smirnova, Philip Flores, Aycke Roos, David Ayuso, Piero Decleva, Stefanos Carlstroem, Serguei Patchkovskii, Andres Ordonez
MA 5.4	Mon	11:15–11:45	H20	**Phonon thermal Hall effect** — •Kamran Behnia
MA 5.5	Mon	11:45–12:15	H20	**Giant effective magnetic moment of chiral phonons** — •Swati Chaudhary, Dominik Juraschek, Martin Rodriguez-Vega, Gregory A Fiete
MA 6.1	Mon	15:00–15:30	H16	**Magnetization dynamics of chiral helimagnetic insulators** — •Aisha Aqeel
MA 7.1	Mon	15:00–15:20	H18	**Realizing Reservoir Computing with skyrmions in geometrical confinements tuned by ion irradiation** — •Grischa Beneke
MA 7.2	Mon	15:20–15:40	H18	**Low-energy spin excitations of the Kitaev candidate material $Na_2Co_2TeO_6$ probed by high-field/high-frequency electron spin resonance spectroscopy** — •Luca Bischof, Jan Arneth, Kwang-Yong Choi, Raju Kalaivanan, Raman Sankar, Rüdiger Klingeler
MA 7.3	Mon	15:40–16:00	H18	**Tailoring the first-order magnetostructural phase transition in Ni-Mn-Sn for caloric applications by microstructure** — •Johannes Puy, Enrico Bruder, Oliver Gutfleisch, Franziska Scheibel
MA 7.4	Mon	16:15–16:40	H18	**Tuning the properties of two-dimensional magnetic heterostructures via interface engineering with molecular and inorganic van der Waals crystals.** — •Carla Boix-Constant, Samuel Mañas-Valero, Eugenio Coronado
MA 7.5	Mon	16:40–17:05	H18	**Theoretical Prediction for Probing Magnon Topology** — •Robin R. Neumann
MA 7.6	Mon	17:05–17:30	H18	**Multiphysics-Multiscale Simulation of Additively Manufactured Functional Materials** — •Yangyiwei Yang
MA 23.1	Wed	9:30–10:00	H20	**Magneto-transport effects in crystalline magnetic films** — •Sebastian T. B. Goennenwein
MA 23.2	Wed	10:00–10:30	H20	**Cubic magneto-optic Kerr effect in thin films depending on structural domain twinning and crystal orientation** — •Robin Silber, Maik Gaerner, Jaroslav Hamrle, Timo Kuschel
MA 23.5	Wed	11:15–11:45	H20	**electrical and optical detection of the multipolar structure in the magnetization space** — •Dazhi Hou
MA 23.9	Wed	12:30–13:00	H20	**Ultrafast Néel order dynamics detected by time-resolved magneto-optical Voigt effect** — •Haibin Zhao
MA 30.1	Wed	16:00–16:30	H18	**Boosting Coercivity in Additively Manufactured Magnets Through Nano-Functionalization of NdFeB Powder** — •Anna Ziefuss
MA 35.1	Thu	9:35–10:05	H20	**Artificial Intelligence for Materials Science: Critical Importance of Rare Events, Active Learning, and Uncertainties** — •Matthias Scheffler
MA 35.2	Thu	10:05–10:35	H20	**Physics meets data: decoding magnetic inhomogeneities through latent analysis** — •Karin Everschor-Sitte
MA 35.3	Thu	10:35–11:05	H20	**AI used for micromagnetic simulations** — •Thomas Schrefl, Felix Lasthofer, Qais Ali, Heisam Moustafa, Harald Oezelt, Alexander Kovacs, Masao Yano, Noritsugu Sakuma, Akihito Kinoshita, Tetsuya Shoji, Akira Kato

MA 35.4	Thu	11:15–11:45	H20	**Future method for estimating parameters in magnetic films using machine learning** — •Kenji Tanabe
MA 38.1	Thu	15:00–15:30	H18	**Liquid-mediated surface-surface interactions investigated by close-to-surface magnetic particle transport** — •Rico Huhnstock, Yahya Shubbak, Arno Ehresmann
MA 39.1	Thu	15:00–15:30	H19	**Voltage control of magnetism using hydrogen** — •Markus Gössler

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

MA 1.1–1.3	Sun	16:00–18:15	H4	**Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism (joint session MA/TUT)**
MA 2.1–2.10	Mon	9:30–12:15	H16	**Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)**
MA 3.1–3.13	Mon	9:30–13:00	H18	**Magnonics I**
MA 4.1–4.9	Mon	9:30–11:45	H19	**Electron Theory of Magnetism and Correlations**
MA 5.1–5.8	Mon	9:30–13:00	H20	**Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I (joint session MA/TT)**
MA 6.1–6.12	Mon	15:00–18:30	H16	**Skyrmions I**
MA 7.1–7.6	Mon	15:00–18:00	H18	**INNOMAG e.V. Prizes 2025 (Diplom-/Master and Ph.D. Thesis)**
MA 8.1–8.9	Mon	15:00–17:15	H19	**Spin-Dependent Phenomena in 2D (joint session MA/HL)**
MA 9.1–9.13	Mon	15:00–18:30	H20	**Altermagnets I**
MA 10.1–10.12	Tue	9:30–12:45	H16	**Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II (joint session MA/TT)**
MA 11.1–11.14	Tue	9:30–13:15	H18	**Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)**
MA 12.1–12.8	Tue	9:30–11:30	H19	**Magnetization Dynamics and Damping**
MA 13.1–13.13	Tue	9:30–13:00	H20	**Altermagnets II**
MA 14.1–14.9	Tue	9:30–13:15	H36	**Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)**
MA 15.1–15.48	Tue	10:00–12:30	P1	**Poster I**
MA 16.1–16.5	Tue	14:00–15:15	H16	**Topological Insulators (joint session MA/HL)**
MA 17.1–17.4	Tue	14:00–15:00	H18	**Micro- and Nanostructured Magnetic Materials**
MA 18.1–18.6	Tue	14:00–15:30	H19	**Functional Antiferromagnetism**
MA 19.1–19.5	Tue	14:00–15:15	H20	**Magnetic Imaging and Sensors**
MA 20.1–20.14	Wed	9:30–13:15	H16	**Magnonics II**
MA 21.1–21.12	Wed	9:30–12:45	H18	**Frustrated Magnets I**
MA 22.1–22.8	Wed	9:30–11:30	H19	**Caloric Effects in Ferromagnetic Materials**
MA 23.1–23.9	Wed	9:30–13:00	H20	**Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization I**
MA 24.1–24.7	Wed	9:30–12:45	H36	**Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets (joint session TT/MA)**
MA 25.1–25.2	Wed	15:00–15:30	H15	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)**
MA 26.1–26.14	Wed	15:00–18:45	H16	**Ultrafast Magnetization Effects I**
MA 27.1–27.3	Wed	15:00–15:45	H18	**Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization II**
MA 28.1–28.9	Wed	15:00–17:30	H19	**Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions**
MA 29.1–29.14	Wed	15:00–18:45	H20	**Skyrmions II**
MA 30.1–30.7	Wed	16:00–18:00	H18	**Bulk Materials: Soft and Hard Permanent Magnets**
MA 31.1–31.47	Wed	17:00–19:30	P1	**Poster II**
MA 32.1–32.6	Wed	17:30–19:00	H19	**Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)**
MA 33.1–33.13	Thu	9:30–13:00	H16	**Non-Skyrmonic Magnetic Textures I**
MA 34.1–34.12	Thu	9:30–12:45	H18	**Molecular Magnetism**
MA 35.1–35.5	Thu	9:30–13:00	H20	**PhD Focus Session: Using Artificial Intelligence Tools in Magnetism**
MA 36.1–36.7	Thu	9:30–12:45	H36	**Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)**
MA 37.1–37.10	Thu	15:00–17:45	H16	**Magnetic Imaging Techniques**

MA 38.1–38.10	Thu	15:00–18:00	H18	**Magnetic Particles / Clusters & Biomagnetism**
MA 39.1–39.7	Thu	15:00–17:00	H19	**Magnetic Thin Films**
MA 40.1–40.10	Thu	15:00–17:45	H20	**Frustrated Magnets II**
MA 41.1–41.47	Thu	15:00–17:30	P3	**Poster III**
MA 42	Thu	18:00–19:00	H20	**Members' Assembly**
MA 43.1–43.14	Fri	9:30–13:15	H16	**Skyrmions III / Non-Skyrmionic Magnetic Textures II**
MA 44.1–44.8	Fri	9:30–13:00	H17	**Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)**
MA 45.1–45.11	Fri	9:30–12:30	H18	**Computational Magnetism**
MA 46.1–46.11	Fri	9:30–12:30	H19	**Surface Magnetism**
MA 47.1–47.6	Fri	9:30–11:00	H20	**Altermagnets III**
MA 48.1–48.7	Fri	11:15–13:00	H20	**Ultrafast Magnetization Effects II**

Members' Assembly of the Magnetism Division

Thursday 18:00–19:00 H20

- Bericht
- Verschiedenes

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

MA 1: Into the Third (and Fourth) Dimension: Imaging Methods for 3D Nanomagnetism (joint session MA/TUT)

Nanostructured magnetic materials have found several applications in everyday objects, such as data storage devices, sensors, and biomedical devices. When one brings these materials to the third dimension, a variety of new physics, and opportunities for applications appear. However, until recently, the vast majority of experimental investigations have primarily been focused on 2D planar geometries, as 3D systems provide a set of experimental challenges that still needs to be overcome. This tutorial seeks to provide a comprehensive overview for both experts and non-experts in the field of 3D imaging to gain a deeper understanding of the recent advances and experimental challenges connected to the investigation of 3D magnetic systems.

Organized by Claire Donnelly (MPI-CPFS, Dresden, Germany) and Simone Finizio (Paul Scherrer Institut, Villigen, Switzerland).

Time: Sunday 16:00–18:15 Location: H4

Tutorial MA 1.1 Sun 16:00 H4

3D Magnetic Imaging: Utilizing Synchrotron X-Ray Coherence for Nanometric Resolution in Thick Samples — •Marisel Di Pietro Martinez — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — International Institute for Sustainability with Knotted Chiral Meta Matter (WPI-SKCM2)

In recent years, there has been a growing interest from the magnetism community in expanding to three-dimensional magnetic systems - from exploring new geometries to revealing complex magnetic textures arising in micrometer-thick samples. A key aspect of this exploration is the ability to visualize the magnetization vector field at the nanoscale throughout the entire sample, made possible by the development of 3D magnetic imaging. This technique can achieve nanometric spatial resolution in micrometer-thick samples by leveraging the penetration depth and coherence of synchrotron X-rays. Furthermore, the coherence of the X-ray beam provides magnetic contrast not only in the absorption of the transmitted wave, but also in the phase. This phase contrast enables the investigation of micron-sizes magnets, even with soft X-rays, while minimizing the sample damage. In this tutorial, I will introduce how to exploit these advantages using coherence-based techniques, such as Fourier transform holography and ptychography, to perform 3D magnetic imaging. Visualizing the magnetization vector field with nanometer spatial resolution in micrometer thick samples opens the door to studying magnetic textures in higher dimensions, offering insights into fundamental physical phenomena as well as promising new applications in information storage and processing.

Tutorial MA 1.2 Sun 16:45 H4

Nanoscale Mapping of Magnetic Textures in 3D Using Vector Field Electron Tomography — •Axel Lubk[1,2] and Daniel Wolf[1] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany

Vector field Electron Tomography (VFET) combines Electron Holography and Electron Tomography in the Transmission Electron Microscope (TEM) to reconstruct magnetic induction vector fields in 3D down to several nanometer resolution. In this tutorial we discuss the foundations of the technique, the practical workflow including pitfalls, and application to topical examples in nanomagnetism including domain walls in nanowires and skyrmion strings.

Tutorial MA 1.3 Sun 17:30 H4

3D magnetic imaging: an experimental window to study 3D magnetization at the nanoscale — •Aurelio Hierro-Rodriguez — Department of Physics, University of Oviedo,33007, Oviedo, Spain — CINN (CSIC-University of Oviedo) , 33940, El Entrego, Spain

The synergetic confluence of technological and scientific developments in nanofabrication and characterization techniques is paving the way towards the advance in Three-Dimensional Nanomagnetism, fuelled by the richness of phenomena and technological potential of the exploitation of the magnetization vector field in their natural dimensionality: three dimensions. In this lecture, a broad picture of the importance of the topic, in the framework of the novel physics that can be explored and exploited will be given, with a brief description of the methods that allow to fabricate almost any 3D magnetic geometry with nanometer resolution. The core of the lecture will deal with the advanced magnetic imaging techniques, which are opening a window towards the characterization of the full three-dimensional magnetization vector. Specifically, X-ray based magnetic vector tomography will be described and exemplified, showing the capabilities of the technique to volume resolve the magnetization vector field in arbitrary systems with nanometer resolution. These developments in vector magnetic imaging are making possible a change in the actual paradigm on how magnetization is characterized and studied at the nanoscale, by bringing a direct experimental probe to realize experimental micromagnetism.

MA 2: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Monday 9:30–12:15 Location: H16

MA 2.1 Mon 9:30 H16

Trilinear coupling and toroidicity in multiferroics — Andrea Urru[1] and •Vincenzo Fiorentini[2,3] — [1]Dept. of Physics, Rutgers University, USA — [2]Chair of Materials Science and Nanotech, TU Dresden — [3]Dept. Physics, University of Cagliary, Italy

We discuss the properties of the triple-order-parameter (ferromagnet, ferroelectric, ferrotoroid) layered-perovskite metal Bi5Mn5O17, as predicted from first-principles calculations, in the light of a Landau expansion with trilinear coupling, with particular reference to its multiple degenerate ground states with mutually orthogonal vector order parameters, giant cross-coupling magnetoelectricity, and magnetotoroidic effects.

MA 2.2 Mon 9:45 H16

Engineering magnetic domain wall energies in $BiFeO_3$ via epitaxial strain: A route to assess skyrmionic stabilities in multiferroics from first principles — •Sebastian Meyer[1,2], Bin Xu[3,4], Laurent Bellaiche[4], and Bertrand Dupé[1,2] — [1]Université de Liège, Belgium — [2]Fonds de la Recherche Scientifique, Belgium — [3]Soochow University, China — [4]University of Arkansas, USA

Epitaxial strain has emerged as a powerful tool to tune magnetic and ferroelectric properties in functional materials such as in multiferroic perovskite oxides. Here, we use first-principles calculations to explore the evolution of magnetic interactions in the antiferromagnetic multiferroic $BiFeO_3$ (BFO), one of the most promising multiferroics for future technology [1]. The epitaxial strain in BFO is varied between $\varepsilon \in [-2\%, +2\%]$. We find that both strengths of the exchange interaction and Dzyaloshinskii-Moriya interaction decrease linearly from compressive to tensile strain whereas the uniaxial magnetocrystalline anisotropy lifts the energy degeneracy of the (111) easy plane of bulk BFO. From the trends of magnetic interactions we can explain the destruction of cycloidal order in compressive strain as observed in experiments due to the increasing anisotropy energy. For tensile strain, we predict that the ground state remains unchanged as a function of strain. By using the domain wall energy, we envision a region where isolated chiral magnetic textures might occur as a function of strain [2].

[1] R. Ramesh, N. Spaldin, *Nature Mater* **6**, 21-29 (2007)
[2] S. Meyer *et al.*, *Phys. Rev. B* **109**, 184431 (2024)

MA 2.3 Mon 10:00 H16

Hidden order in Cr_2O_3 and α-Fe_2O_3 as a predictor for (anti-)magnetoelectricity — •Xanthe Verbeek[1,2], Andrea Urru[2,3], and Nicola Spaldin[2] — [1]Insitut für Physik, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [2]Materials Department, ETH Zurich, 8093 Zürich, Switzerland — [3]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

With first-principles calculations of Cr_2O_3 and α-Fe_2O_3, we show that the different magnetoelectric effects in these materials result from the ordering of hidden magnetic multipoles. We reveal for the first time anti-ferroically ordered magnetic multipoles in both Cr_2O_3, and isostructural α-Fe_2O_3, in which the global inversion symmetry is preserved by the different magnetic dipolar ordering. We can relate each of these multipoles and their ordering to linear, quadratic, and cubic (anti-) magnetoelectric effects, where in an anti-magnetoelectric effect the induced moments are ordered antiferromagnetically in the unit cell. We confirm the predicted induced moments using first-principles calculations, showing the lowest response in α-Fe_2O_3 a centrosymmetric magnetic material, to be a linear anti-magnetoelectric effect, revealing the presence of the magnetoelectric coupling despite the preserved global inversion symmetry. Our results demonstrate the existence of hidden magnetic multipoles leading to local linear magnetoelectric responses, even in centrosymmetric magnetic materials, and broaden the definition of magnetoelectric materials by including those showing such local magnetoelectric responses.

MA 2.4 Mon 10:15 H16

Non-trivial Spin Structures and Multiferroic Properties of the DMI-Compound $Ba_2CuGe_2O_7$ — •Peter Wild[1], Korbinian Fellner[1], Michał Dembski-Villalta[1], Markus Garst[2], Eric Ressouche[5], Tommy Kotte[3], Bertrand Roessli[4], Alexandra Turrini[4], and Sebastian Mühlbauer[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Karlsruhe Institute of Technology, (KIT), Karlsruhe, Deutschland — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Paul Scherrer Institut (PSI), Villigen, Switzerland — [5]Institut Laue-Langevin (ILL), Grenoble, France

Antiferromagnetic $Ba_2CuGe_2O_7$, characterized by a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a non-centrosymmetric insulator that exhibits spiral spin structures with potential non-trivial topology and a variety of unconventional magnetic phase transitions. Below the Néel temperature T_N = 3.05K, the DMI term leads to a long-range incommensurate, almost AF cycloidal spin spiral in the ground state. Recently, a new phase with a vortex-antivortex magnetic structure has been theoretically described and experimentally confirmed in a pocket in the phase diagram at around 2.4K and an external field along the crystalline c-axis of around 2.2T. A lack of evidence for a thermodynamic phase transition towards the paramagnet in specific heat measurements and a finite linewidth in E and Q of the incommensurate peaks in neutron scattering, as opposed to the cycloidal ground state, seem to mark the vortex phase as a slowly fluctuating structure at the verge of ordering.

MA 2.5 Mon 10:30 H16

A comparison of Γ-point symmetries and phonon selection rules of spin-space and magnetic point group in $Co_2Mo_3O_8$ — •Onur Ercem[1], Felix Schilberth[1,2], Lilian Prodan[1], Vladimir Tsurkan[1], Alexander Tsirlin[3], István Kézsmárki[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary — [3]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

$Co_2Mo_3O_8$, which has recently come into the focus of research, as different magnetically ordered ground states can be formed and tuned by external magnetic fields or doping. $Co_2Mo_3O_8$ has a hexagonal structure, the polarization along the c-axis, and a collinear antiferromagnetic order below T_N = 40 K. Reflectivity measurements were performed using the FTIR spectrometer, in the frequency range from 100 to 8000 cm^{-1}, and the temperature range from 10 to 300 K could be covered. A preliminary analysis of the infrared-active modes for $E \parallel c$ reveals that 8 out of the 9 predicted A_1 modes are observed at the expected eigenfrequencies and the emergence of the mode at around 300 cm^{-1} below T_N. In $E \perp c$ at room temperature 10 modes were observed. Below T_N two new modes at 301 cm^{-1} and at 362 cm^{-1} observed. Comparison was made with lattice dynamical calculations.

MA 2.6 Mon 10:45 H16

Ferroelectric hafnium oxide-based multiferroic bilayers for magnetoelectric spin-orbit devices — •Maximilian Lederer, Johannes Hertel, Christoph Durner, Tatiana Gurieva, and Benjamin Lilienthal-Uhlig — Fraunhofer IPMS, Center Nanoelectronic Technologies, Dresden, Germany

This study investigates multiferroic heterostructures comprising $Hf_{0.5}Zr_{0.5}O_2$ (HZO) with Co/Pt top and TiN bottom electrodes on Si substrates. Using advanced deposition techniques, sub-nanometric thin films were fabricated. The research highlights achieving both ferroelectricity and perpendicular magnetic anisotropy simultaneously through a two-step annealing process. These properties are crucial for magnetoelectric spin-orbit (MESO) devices, which offer significant advantages such as lower power consumption and enhanced data storage capabilities. Insights into crystallization and diffusion processes were gained through various structural investigation methods. Additionally, the study demonstrates the manipulation of magnetic and ferroelectric domains using different microscopy techniques, underscoring the potential of MESO devices in next-generation electronic applications.

15 min. break

MA 2.7 Mon 11:15 H16

Internal fields at the V-sites and magnetic structure of the lacunar spinel GeV_4S_8 — •Thomas Gimpel[1], Norbert Büttgen[1], Hiroyuki Nakamura[2], Vladimir Tsurkan[1], and István Kézsmárki[1] — [1]University of Augsburg — [2]Graduate School of Engineering, Kyoto

GeV_4S_8 is a multiferroic lacunar spinel that undergoes both structural (T_{JT}=30 K) and magnetic (T_N=13 K) transitions upon which the four V-sites of the V_4 tetrahedra that are equivalent in the cubic phase transform into three distinct sets of V-sites with zero-field ^{51}V NMR frequencies of 21.7, 53.6 and 65.6 MHz. This indicates that only two V-sites have the same internal magnetic field, while the other two have different ones. Based on the angular dependence of the resonance field upon the rotation of the field, we conclude that the direction of the internal field is common for the four V-sites and is parallel to one of the cubic [110]-type axes, which indicates that the magnetic space group is $Pmn2_1$.

MA 2.8 Mon 11:30 H16

Fast control of antiferromagnetic domains via pulsed electric fields in Co_3O_4 — •Isabel Täuber, Maximilian Winkler, Somnath Ghara, Lilian Prodan, and Istvan Kezsmarki — Universität Augsburg, Deutschland

Co_3O_4 shows the linear magnetoelectric effect below the Neel-temperature of 30K, with a large magnetoelectric coefficient of 14 ps/m. Besides the typical control of the AFM state by colling with electric and magnetic fields across TN, the domains can be switched by voltage pulses as short as a few ns far below the transition temperature. To improve the application ability, we focus on switching of thin films of Co_3O_4 single crystals, paving the way for the next generation of spintronics.

MA 2.9 Mon 11:45 H16

Anomalously strong magnetoelectric coupling in hexaferrite films — •Jakub Vít[1], Kwang-Tak Kim[2], Hyunju Hwang[2], Radomír Kužel[3], Milan Dopita[3], Darina Smržová[4], Kee Hoon Kim[2], and Josef Buršík[4] — [1]Institute of Physics, Czech Academy of Sciences, Czechia — [2]Center for Novel States of Complex Materials Research, Seoul National University, Korea — [3]Faculty of Mathematics and Physics, Charles University, Czechia — [4]Institute of Inorganic Chemistry, Czech Academy of Sciences, Czechia

Bulk hexaferrites are well known to exhibit strong magnetoelectric (ME) effects, often extending up to room temperature. In contrast, ME properties of hexaferrite films have been investigated only in a single recent study: In Z-hexaferrite films, the ME effect was found significantly stronger than in a crystal. [1] We continued this research by studying Y-hexaferrite films $Ba_{2-x}Sr_xCo_2Fe_{11.1}Al_{0.9}O_{22}$ on $SrTiO_3$ (111), grown by chemical solution deposition. For x=1, the magnetic-field-induced polarization reached 6.5 mC/m^2 at 10 K , i.e. 10x more than in the Z-hexaferrite films [1] and 50x more than in Y-hexaferrite crystals. [2] To elucidate these intriguing observations, microstructure of the films was studied in detail by real (SEM, TEM) and reciprocal (XRD) space techniques. Possible influence of the substrate on ME measurements was also taken into account.

[1] K. Shin et al., *Adv. Electron. Mater.* 2101294, (2022) [2] C. B. Park, et al., *Phys. Rev. Mater.* **5**, 034412 (2021)

MA 2.10 Mon 12:00 H16

Higher-order Magnetizations of Non-centrosymmetric Antiferromagnets — •Michael Paulsen[1], Silvia Knappe-Grüneberg[1], Jens Voigt[1], Allard Schnabel[1], Rainer Körber[1], Michael Fechner[2], Ivan Ushakov[3], and Dennis Meier[3] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany — [3]NTNU Norwegian University of Science and Technology, Trondheim, Norway

Antiferromagnetic materials lack macroscopic magnetic dipole fields, due to their compensated magnetic spin texture. In his seminal work, Dzyaloshinskii predicted that higher-order magnetization contributions arise in non-centrosymmetric antiferromagnets, in particular quadrupolar magnetic field contributions, and first experimental data suggested the presence of such fields in the antiferromagnetic model system Cr_2O_3. Here, we present calculations and measurements gained at cryogenic and room temperature using Superconducting Quantum Interference Devices (SQUIDs) and Optically Pumped Magne-

tometers (OPMs) setups, respectively, in ultra-low magnetic field environments. The results demonstrate the existence of quadrupolar far-fields and characteristic signatures in different classes of antiferromagnets. Importantly, our SQUID-based approaches are universal and can be applied to a wide range of systems, establishing new methods for characterizing materials with ultra-small magnetic remanence in general.

MA 3: Magnonics I

Time: Monday 9:30–13:00 Location: H18

MA 3.1 Mon 9:30 H18

Floquet Magnons in a Periodically-Driven Magnetic Vortex — •Christopher Heins[1,2], Luaks Körber[1,2,3], Joo-Von Kim[4], Thibaut Devolder[4], Johan Mentink[3], Attila Kákay[1], Katirn Schultheiss[1], Jürgen Fassbender[1,2], and Helmut Schultheiss[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Radboud University, Institute of Molecules and Materials, Nijmegen, The Netherlands — [4]Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Saclay, Palaiseau, France

Magnetic vortices are prominent examples of topology in magnetism with a rich set of dynamic properties. They exhibit an intricate magnon spectrum and show an eigen-resonance of the vortex texture itself, the gyration of the vortex core. The fundamental modes of both excitation types are separated in their resonance frequencies. While the vortex typically gyrates at a few hundred MHz, the magnon modes typically have frequencies in the lower GHz range. Under the influence of a periodic driving field, Floquet states emerge due to a temporal periodicity imposed on the system's ground state by the gyration, much like the formation of Bloch states in the periodic potential of a crystal lattice. While Bloch states are shifted in momentum space, Floquet states are shifted in energy by multiples of the drive frequency.

MA 3.2 Mon 9:45 H18

Nanoscale YIG-Based Magnonic Crystals — •Khrystyna Levchenko[1], Kristýna Davídková[1], Mathieu Moalic[2], Carsten Dubs[3], Michal Urbánek[4], Qi Wang[5], Maciej Krawczyk[2], and Andrii Chumak[1] — [1]University of Vienna, Austria — [2]A. Mickiewicz University, Poland — [3]INNOVENT, Germany — [4]CEITEC Nano, Czech Republic — [5]Huazhong University, China

Magnonic crystals (MCs) are a spin-wave (SW) based class of artificial magnetic materials characterised by a spatially periodic variation of their properties. The combination of design flexibility and SW intrinsic advantages makes MCs promising candidates for RF applications, although multi-mode SW propagation disturbs the operating characteristics. To overcome this, it is necessary to work with nanostructures in the single-mode regime. Leveraging recent progress in materials science and fabrication techniques, we have realised 1D MCs from 100 nm thick epitaxial yttrium iron garnet (YIG) films. The MCs were developed using electron beam lithography, ion etching and evaporation, with periodicities of 1 μm and optimised notches (100-250 nm depth) or antidots (100-150 nm diameter). Microstrip antennae were used for SW excitation and detection. Experimental characterisation using micro-focused Brillouin light scattering and propagating spin-wave spectroscopy, supported by simulations (TetraX), confirmed efficient single-mode SW transport over a distance of 10 μm and bandgap formation. These results pave the way for further advances, such as 2D arrays with magnon guidance and topologically protected magnon transport - a milestone yet to be achieved experimentally.

MA 3.3 Mon 10:00 H18

The impact of local exchange bias on the dyanmics in chiral antiferromagnetic Mn_3Ir heterostructures with a $Ni_{80}Fe_{20}$ — •Rouven Dreyer[1], James M. Taylor[1], Stuart Parkin[2], and Georg Woltersdorf[1,2] — [1]Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [2]Max Planck Institute for Microstructure Physics, 06120 Halle, Germany

Non-collinear antiferromagnets (AFs) have been found to exhibit the intrinsic spin Hall effect (SHE) and to provide exchange bias (EB) in multilayer system, rendering these AFs interesting candidates for spintronic applications. However, the role of the chiral domain structure in this process and the transmission of the resulting spin current across interfaces with ferromagnets (FMs), remain open questions. Using a combination of integrative spin-torque ferromagnetic resonance (ST-FMR) and super-Nyquist-sampling magneto-optical Kerr effect (SNS-MOKE) measurements, we investigate the impact of the non-collinear spin texture of the Mn_3Ir on the magnetization dynamics in heterostructures with $Ni_{80}Fe_{20}$. Here, we show a strong discrepancy between local and integrative techniques due to interfacial exchange coupling between the AF and the FM. As a result of this, only SNS-MOKE studies allow for a local detection of the SHE. Furthermore, we obtain modifications of the magnetization dynamics strongly depending on the direction of applied EB. Moreover, we demonstrate that a combination of small bias fields and current-induced heating acts as an efficient control mechanism for setting of the exchange bias und thus for changing the magnetization dynamics during the measurements.

MA 3.4 Mon 10:15 H18

Evoution of coherence in magnonic BECs — •Malte Koster[1], Matthias R. Schweizer[1], Vitaliy Vasyuchka[1], Dmytro Bozhko[2], Burkard Hillebrands[1], Mathias Weiler[1], Alexander A. Serga[1], and Georg von Freymann[1,3] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Department of Physics and Energy Science, University of Colorado Colorado Springs, CO 80918 USA — [3]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany

The process of formation of a coherent magnon-Bose-Einstein condensate (BEC) in an over-populated, hot magnon gas has recently been intensively studied. We have already demonstrated an electromagnetic detection scheme that allows direct evaluation of the phase correlation in the BEC. We have now extended the setup to study the evolution of the phase coherence during and after the formation of a homogeneous excitation of the magnon system - a BEC. In our experiments we use a perpendicularly magnetized yttirumiron-garnet film, which is parametrically pumped. This allows us to further demonstrate that coherence arises even though the magnon gas is still heated by the pumping. Furthermore, due to the phase sensitivity of our technique, we observe the spontaneous emergence of a random phase of the BEC without any influence of external factors.

This research was funded by the Deutsche Forschungsgemeinschaft in frame of TRR 173/2*268565370 Spin+X (Project B04).

MA 3.5 Mon 10:30 H18

Ultra-long magnon lifetime in the quantum limit — •Rostyslav O. Serha[1], Kaitlin H. McAllister[2], Fabian Majcen[1], Sebastian Knauer[1], Timmy Reimann[3], Carsten Dubs[3], Gennadii A. Melkov[4], Alexander A. Serga[5], Vasyl S. Tyberkevych[6], Dmytro A. Bozhko[2], and Andrii V. Chumak[1] — [1]University of Vienna, Vienna, Austria — [2]University of Colorado, Colorado Springs, USA — [3]INNOVENT e. V. technology development, Jena, Germany — [4]National Taras Shevchenko University, Kyiv, Ukraine — [5]RPTU, Kaiserslautern, Germany — [6]Oakland University, Rochester, USA

Quantum magnonics seeks to harness the quantum mechanical properties of magnons for quantum information technologies. A major bottleneck in this field is the limited magnon lifetime, which constrains the performance of quantum magnonic systems. In this study, we investigated yttrium iron garnet (YIG) spheres with varying impurity levels using ferromagnetic resonance (FMR) spectroscopy to examine magnon lifetimes at millikelvin temperatures. For k=0 magnon modes, lifetimes of up to one microsecond were observed. Remarkably, a specialized three-magnon splitting experiment revealed lifetimes of short-wavelength dipole magnons to be up to an order of magnitude longer than their k=0 counterparts. We report a maximum magnon lifetime of 18 microseconds at a frequency of 1.6 GHz. These findings offer crucial insights into the mechanisms influencing magnon lifetimes and pave the way for quantum magnonic devices featuring long-lived propagating magnons.

MA 3.6 Mon 10:45 H18

Exotic Magnon Spectra from Strong Dipolar Interactions and Anisotropy — •Konrad Scharff — KIT, Karlsruhe, Deutschland

Magnetic dipole-dipole interactions on lattices have been known to be the source of non-analytical behaviour of associated spin wave dispersions at and around the Brillouin zone center [1,2]. We investigate the consequences and predicted signatures of said non-analyticity in a 3D hexagonal lattice model that additionally hosts magnetic exchange interaction, as well as an easy-plane on-site anisotropy. Dynamical susceptibilities are theoretically evaluated and compared to available experimental data.

[1] Jensen, J. and Mackintosh, A.R. Rare Earth Magnetism. Clarendon Press - Oxford (1991)

[2] Baehr, M. et al. Effect of magnetic dipolar interactions on the interchain spin-wave dispersion in CsNiF3. Phys. Rev B 54, 12932 (1996)

MA 3.7 Mon 11:00 H18

Machine learning tool for inelastic neutron scattering: The case of CrSBr — •Nihad Abuawwad[1], Yixuan Zhang[2], Hongbin Zhang[2], and Samir Lounis[1,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Jülich, Germany — [2]Institute of Materials Science, Technical University Darmstadt, Darmstadt , Germany — [3]Institute of Physics, University of Halle, Halle, Germany

Spin waves, or magnons, are fundamental excitations in magnetic materials that provide insights into their dynamic properties and interactions. Magnons are the

building blocks of magnonics, which offer promising perspectives for data storage, and quantum computing. These excitations are typically measured through Inelastic Neutron Scattering (INS) techniques, which involve heavy and time-consuming measurements, data processing, and analysis based on various theoretical models. Here, we introduce a machine learning algorithm that integrates adaptive noise reduction and active learning sampling, which enables the restoration from minimal INS point data of spin wave information and the accurate extraction of magnetic parameters, including hidden interactions. Our findings, benchmarked against the magnon spectra of CrSBr, significantly enhance the efficiency and accuracy in addressing complex and noisy experimental measurements. This advancement offers a powerful machine-learning tool for research in magnonics and spintronics, which can also be extended to other characterization techniques at large facilities[1].

[1] Abuawwad N. arxiv:2407.04457 (2024)

15 min. break

MA 3.8 Mon 11:30 H18

Thermally Induced Demagnetizing Fields: Effective Potentials for Magnon Bose–Einstein Condensates — •Matthias R. Schweizer[1], Franziska Kühn[1], Victor S. L'vov[2], Anna Pomyalov[2,3], Georg von Freymann[1,4], Burkard Hillebrands[1], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern — [2]Department of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel — [3]Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [4]Fraunhofer Institute for Industrial Mathematics ITWM, Fraunhofer-Platz 1, 67663 Kaiserslautern

We investigate the control of magnon Bose–Einstein condensates (mBEC) by means of reconfigurable potentials. It is shown that the localized decrease of the saturation magnetization leads to strong demagnetizing fields which elevate the resonance frequency of magnons in the mBEC state at the bottom of the spin-wave spectrum. Consequently, spatially varying magnetization and field profiles act as space-modulated potentials, determining the dynamics of the mBEC. For the experimental observation, we create reconfigurable microscopic magnetization profiles using laser heating controlled by optical wavefront modulation. Electromagnetic parametric pumping is used to increase the magnon gas density and Brillouin light scattering spectroscopy is employed to detect the mBEC dynamics. This research was supported by the DFG–TRR 173-268565370 Spin+X (Project B04).

MA 3.9 Mon 11:45 H18

Fluctuations of the inverted magnetic state and how to sense them — •Anna-Luisa Römling[1], Artim Bassant[2], and Rembert Duine[2] — [1]Condensed Matter Physics Center (IFIMAC) and Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [2]Institute for Theoretical Physics, Utrecht University, Utrecht, The Netherlands

Magnons are the low-energy exciations of magnetically ordered materials. While the magnetic moment of a ferromagnet below Curie tempertature aligns with an applied magnetic field, recent theoretical work has demonstrated that the magnetic order can be inverted by pumping spin orbit torque into the magnet. This results in an energetically unstable but dynamically stabilized state where the magnetic moment is antiparallel to an applied magnetic field. The excitations on such a state have negative energy and are called antimagnons, the antiparticle of the magnon. Here, we theoretically study the quantum and classical fluctuations of the inverted magnetic state and their sigatures in experimental set-ups. Our results advance the understanding of fundamental properties of antimagnons as well as experimental data related to the inverted magnetic state. They pave the way for exciting applications in spintronics and magnonics.

MA 3.10 Mon 12:00 H18

Inductive noise spectroscopy of thermally excited magnons — Luise Holder[1], Richard Schlitz[1], Jamal Ben Youssef[2], Christian Runge[1], Akashdeep Kamra[3,4], William Legrand[5], Hans Huebl[6,7,8], •Michaela Lammel[1], and Sebastian T.B. Goennenwein[1] — [1]Universität Konstanz, Konstanz — [2]LabSTICC-CNRS, Université Bretagne Occidentale, Brest — [3]RPTU Kaiserslautern-Landau, Kaiserslautern — [4]Universidad Autónoma de Madrid, Madrid — [5]CNRS, Institute Néel, Université Grenoble Alps, Grenoble — [6]Walther-Meißner-Institut, Garching — [7]Technische Universität München, Garching — [8]Munich Center for Quantum Science and Technology, Munich

For the identification of non-classical (squeezed) magnon states, quantitative knowledge about thermal or vacuum fluctuations of the magnetization is essential. We show that thermal magnetization fluctuations of a ferromagnetic thin film can be sensitively characterized using inductive magnon noise spectroscopy (iMNS). Our broadband approach based on a coplanar waveguide and a commercial spectrum analyzer allows to detect the microwave emission of the equilibrium magnetization fluctuations relative to a cold microwave background. Modeling the response of the whole microwave system and comparing it quantitatively with low-power broadband ferromagnetic resonance measurements in linear response yields excellent agreement, which verifies the equilibrium character of the iMNS. Thus, our work establishes a purely inductive broadband access to the equilibrium properties of magnetization fluctuations.

MA 3.11 Mon 12:15 H18

Threshold of parametric instability of magnons in different magnetization geometries under quasi-continuous pumping — •Tamara Azevedo[1], Rostyslav O. Serha[2], Matthias R. Schweizer[1], Vitaliy I. Vasyuchka[1], Burkard Hillebrands[1], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Faculty of Physics, University of Vienna, 1090 Vienna, Austria

Parametric electromagnetic pumping of magnons is a key method for exciting and amplifying spin waves. Measuring the threshold of parametric instability, where energy input overcomes magnon damping, is crucial. Using a sensitive, automated technique with a quasi-continuous wave generated by a vector network analyzer, we measured this threshold in tangentially magnetized yttrium iron garnet films. Two geometries were studied: a microstrip pumping resonator aligned parallel and perpendicular to the external magnetization field $\mathbf{H}_0$. The threshold power as a function of $\mathbf{H}_0$ shows a sawtooth structure, likely caused by wave vector quantization of parametric magnons. In the perpendicular geometry, threshold power peaks suggest magnon-phonon hybridization with longitudinal, transverse, and surface acoustic modes. These results underline the role of magnetization geometry in determining parametric instability thresholds, providing guidance for optimizing spintronic and magnonic devices. This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)*TRR 173*268565370 Spin+X (Project B04).

MA 3.12 Mon 12:30 H18

Non-reciprocal phonon-magnon interaction in yttrium-iron-garnet/zinc oxide heterostructures — •Yannik Kunz[1], Julian Schüler[1], Kevin Künstle[1], Finlay Ryburn[2], Yangzhan Zhang[2], Katharina Lasinger[1,2], Philipp Pirro[1], John Gregg[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU in Kaiserslautern, Germany — [2]University of Oxford, United Kingdom

Magnon-based devices provide a promising approach for energy-efficient computation due to low intrinsic losses in materials such as yttrium-iron-garnet (YIG). Here we show that surface acoustic waves (SAWs) can be used for the excitation of spin waves in hybrid ferrimagnetic/piezoelectric devices. The SAW thereby couples to magnons under conservation of energy and momentum [1,2]. We studied the excitation and propagation behavior of surface acoustic waves in GGG/YIG/ZnO-heterostructures [3] by electrical and micro-focused optical techniques. The phonon-magnon coupling in YIG is investigated by performing SAW transmission measurement as a function of the magnetic field and orientation. The observed magnetoelastic coupling of phonons and magnons is non-reciprocal and highly dependent on the angle between the propagation direction of the SAW and the applied magnetic field.

[1] Küß et al., Frontiers in Physics 10, 981257 (2022)
[2] Kunz et al., Appl. Phys. Lett. 124 152403 (2024)
[3] Ryburn et al., arXiv 2403.030006 (2024)

MA 3.13 Mon 12:45 H18

Spatial control of hybridization-induced spin-wave transmission stop band — •Franz Vilsmeier[1,2], Christian Riedel[1], and Christian Back[1] — [1]Technische Universität München — [2]Universität Wien

Spin-wave (SW) propagation close to the hybridization-induced transmission stop band is investigated within a trapezoid-shaped 200 nm thick yttrium iron garnet film using time-resolved magneto-optic Kerr effect microscopy. The gradual reduction of the effective field within the structure leads to local variations of the SW dispersion relation and results in a SW hybridization at a fixed position in the trapezoid, where the propagation vanishes since the SW group velocity approaches zero. By tuning the external field or frequency, spatial control of the spatial stop band position and spin-wave propagation is demonstrated.

MA 4: Electron Theory of Magnetism and Correlations

Time: Monday 9:30–11:45 Location: H19

MA 4.1 Mon 9:30 H19

Tunable Half-Metallicity and Ferromagnetism in Gated single layer g-C3N4 via Nitrogen Lone Pair Depletion. — •Pietro Nicolò Brangi, Francesca Martini, Pier Luigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Graphitic carbon nitride (g-C3N4) is a promising catalyst for water splitting and hydrogen production, with nitrogen lone pairs arising from broken carbon-nitrogen bonds in its heptazine structure. These strongly localized and weakly hybridized lone pairs form ultraflat bands potentially leading to correlated states when doped.

Using first-principles calculations, we show that field-effect hole-doping in single-layer g-C3N4 depletes these lone pairs, generating ultraflat bands at the Fermi level and unveiling a rich phase diagram. At low hole concentrations, a half-metallic state emerges with tunable magnetization, increasing linearly with carrier density and reaching up to 1 Bohr magneton /3 f.u.. At an integer filling of one hole per cell, a band-insulating ferromagnetic state is stabilized, followed by an interplay of metallic and half-magnetic phases with further doping, ultimately leading to a second ferromagnetic insulating state.

Our work highlights nitrogen-based lone-pair systems as a novel platform for strongly correlated states, with implications for magnetism even at small electric fields, hinting at unexplored potential in photocatalysis.

MA 4.2 Mon 9:45 H19

Investigation of crystalline environment for Fe oxides using XAS and XPS:A DFT+MLFT approach — •Hamza Zerdoumi, Ruiwen Xie, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt,Germany

Fe oxides are versatile materials with applications spanning catalysis, memory storage, and photoelectrochemical decomposition of seawater for clean hydrogen production. Taking Fe_2O_3 as an example, there exist five distinct phases, i.e., α-Fe_2O_3, β-Fe_2O_3, γ-Fe_2O_3, ϵ-Fe_2O_3, and ζ-Fe_2O_3, each exhibiting unique properties. Therefore, it is intriguing to clarify how the local crystalline environment can shape the electronic structure and hence tailor the corresponding functionalities. In this study, we simulate X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) spectra using a combination of density functional theory (DFT) and multiplet ligand field theory (MLFT). By analyzing individual spectral bands corresponding to iron sites in various crystal structures, we examine the correlation between local symmetry and the simulated spectra. Our work highlights how variations in local environments influence the spectroscopic features of iron oxide polymorphs, offering valuable insights into their diverse properties.

MA 4.3 Mon 10:00 H19

Domain wall engineering in distorted Kagome magnet — •Avdhesh Kumar Sharma[1], Premakumar Yanda[1], Samuel Harrison Moody[2], Chandra Shekhar[1], and Claudia Felser[1] — [1]Max Planck Institute for chemical physics of solids, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

In condensed matter, Kagome material can host interplay of nontrivial topology, correlations, and magnetism due to their unique lattice and band structure. Recently, RTX series with ZrNiAl structure have gained attention due to possessing kagome lattice continuously breaking translation symmetry i.e., distorted kagome lattice. Intriguingly, HoAgGe has been predicted to have a kagome spin ice state and break the the reversal like symmetry and show two degenerate states in anomalous Hall effect. Along this line, we have synthesized single crystals of TbAgGe to investigate the magnetic and electrical transport properties in detail. It crystallizes in a hexagonal crystal structure with space group P-62m. It exhibits long-range AFM ordering of Tb3+ ions at Néel temperatures 29K, 25K and 20K. Further, it shows metamagnetic transitions when H || c, which might result in a non-coplanar spin structure in the system and goes to ferromagnetic (FM) state at high fields. Moreover, it shows significant anomalous Hall effect near the metamagnetic transitions, which is attributed to originating from the magnetic domain walls. Our findings suggest that RTX family with distorted kagome lattice can be an excellent platform to study the interplay of domain wall magnetism and topology.

MA 4.4 Mon 10:15 H19

Magnetic-circular dichroism on low-lying excitations in antiferromagnetic Fe2Mo3O8 — •Kirill Vasin[1], Istvan Kézsmárki[1], Sándor Bordács[2], and Joachim Deisenhofer[1] — [1]University of Augsburg, Augsburg, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary

We report the observation of a strong magnetic circular dichroism (MCD) and Faraday effect in the polar honeycomb antiferromagnet $Fe_2Mo_3O_8$ in the terahertz (THz) range. Using a common linear detection scheme with polarizers on both the emitter and detector set to the same angle, we observe seemingly thickness-dependent features and broadening in the transmission spectrum near narrow resonances in the Faraday configuration. These features are absent in the Voigt geometry with the same static magnetic field configuration, confirming that they arise from Faraday rotation (or MCD). By analyzing the zero-field spectrum and fitting Lorentz oscillators in the time-domain, we resolved oscillators parameters of the observed strong and narrow THz excitations with high accuracy. Using these parameters, we successfully reconstructed our field- and thickness-dependent transmission spectra, highlighting the role of Faraday rotation in the observed phenomena.

Our findings demonstrate the importance of considering detection schemes in Time-Domain THz spectroscopy and provide insights into methods of measuring MCD and Faraday rotation without ellipsometry techniques in «single-shot» transmission measurements for aniferromagnets.

MA 4.5 Mon 10:30 H19

Pressure-induced effects on the electronic band topology, magnetic order, and transport properties in FeSn — •Artem Chmeruk[1], Lilian Prodan[2], and Liviu Chioncel[3] — [1]University of Augbusrg — [2]University of Augbusrg — [3]University of Augbusrg

The family of kagome metals offers a fruitful platform for investigating the interplay between electronic band structure topology and various properties such as magnetism, electrical and optical response, etc. A rather promising topic of research is to control the positions of various topological features such as band (anti-) crossings of different dimensions (nodal points, lines, etc.) by some external parameters. For example, applying an external magnetic field could lead to band reconsctruction and therefore move the band crossings to different locations in the BZ. In a similar fashion, external pressure provides an opportunity to control these topological features both in terms of their location in the momentum space and on the energy scale. The possibility of moving such crossings closer to the Fermi level would immediately have an effect on the various observable quantities such as anomalous Hall conductivity. In this work, we study the effect of pressure on the magnetic order and the electronic band structure in FeSn up to 10 GPa. Furthermore, we investigate changes in the Berry curvature and its influence on the transport properties.

MA 4.6 Mon 10:45 H19

Emergent Majorana Metal from a Chiral Spin Liquid — •Shi Feng[1,2], Penghao Zhu[2], Kang Wang[3], Tao Xiang[3], and Nandini Trivedi[2] — [1]Technical University of Munich, Garching, Germany — [2]The Ohio State University, Columbus, USA — [3]Institute of Physics, Chinese Academy of Sciences, China

We propose a novel mechanism to explain the emergence of an intermediate gapless spin liquid phase (IGP) in the antiferromagnetic Kitaev model in an externally applied magnetic field, sandwiched between the well-known gapped chiral spin liquid (CSL) and the gapped partially polarized (PP) phase. We propose in moderate fields π-fluxes nucleate in the ground state and trap Majorana zero modes. As these fluxes proliferate with increasing field, the Majorana zero modes overlap creating an emergent Z_2 Majorana metallic state with a 'Fermi surface' at zero energy. We further show that the Majorana spectral function captures the dynamical spin and dimer correlations obtained by the infinite Projected Entangled Pair States (iPEPS) method thereby validating our variational approach. The emergence of the IGP as a Majorana metal at zero temperature indicates a new class of gapless QSLs alongside the commonly recognized Dirac spin liquids and $U(1)$ spinon Fermi surfaces in prevailing theories, bringing new insights into the nature of various candidate QSL phases of matter stabilized by moderate magnetic fields.

MA 4.7 Mon 11:00 H19

Tuning the order of a deconfined quantum critical point — Anika Goetz[2], •Natanael C. Costa[1], and Fakher Assaad[2] — [1]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil — [2]Institut für Theoretische Physik und Astrophysik, Universitat Würzburg, Würzburg, Germany

We consider a Su-Schrieffer-Heeger model in the assisted hopping limit where direct electron hopping is subdominant. At fixed electron-phonon coupling and in the absence of Coulomb interactions the model shows a deconfined quantum critical point between a $(0, \pi)$ valence bond solid in the adiabatic limit and a quantum antiferromagnetic (AFM) at high phonon frequencies. Here we show that by adding terms to the model that reinforce the AFM phase, thereby lowering the critical phonon frequency, the quantum phase transition becomes strongly first order. Our results does not depend on the symmetry of the model. In fact by adding a Hubbard-U term to the model lowers the $O(4)$ symmetry to SU(2), such that the DQCP we observe has the same UV symmetries as other models that account for the same quantum phase transitions.

MA 4.8 Mon 11:15 H19

The Laughlin vortex crystal in ideal Chern bands — •Saranyo Moitra and Inti Sodemann — Leipzig University, Leipzig, Germany

We have uncovered a novel phase transition of the celebrated Laughlin Fractional quantum Hall wave-function from its topologically ordered fluid phase onto a power-law-correlated vortex crystal in flat Chern bands with ideal quantum geometry. We will present a theory of ground state correlations and collective modes of these states across this transition and discuss their potential relevance to anomalous fractional quantum Hall phenomena in platforms such as moiré MoTe2, twisted bilayer graphene and pentalayer graphene.

MA 4.9 Mon 11:30 H19

Forestalled Phase Separation as the Precursor to Stripe Order — •Aritra Sinha and Alexander Wietek — Max Planck Institute for the Physics of Complex Systems, Nothnitzer Strasse 38, Dresden 01187, Germany

Stripe order is a prominent feature in the phase diagram of the high-temperature cuprate superconductors and has been confirmed as the ground state of the two-dimensional Fermi Hubbard model in certain parameter regimes. Upon increasing the temperature, stripes and the superconducting state give way to the enigmatic strange metal and pseudogap regime, whose precise nature poses long-standing, unresolved puzzles. Using modern tensor network techniques, we discover a crucial aspect of these regimes. Infinite projected entangled pair state (iPEPS) simulations in the fully two-dimensional limit reveal a maximum in the charge susceptibility at temperatures above the stripe phase. This maximum is located around hole-doping p=1/8 and intensifies upon cooling. Using minimally entangled typical thermal states (METTS) simulations on finite cylinders, we attribute the enhanced charge susceptibility to the formation of charge clusters, reminiscent of phase separation where the system is partitioned into hole-rich and hole-depleted regions. In contrast to genuine phase separation, the charge cluster sizes fluctuate statistically without a divergent charge susceptibility. Hence, while this precursor state features clustering of charge carriers, true phase separation is ultimately forestalled at lower temperatures by the onset of stripe order.

MA 5: Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I (joint session MA/TT)

The magnetic moment of the electron lies at the heart of magnetism and spintronics. However, recent research has unveiled the angular momentum and magnetic moment of chiral phonons as fundamental quantities in their own right. These chiral phonons give rise to a plethora of novel lattice phenomena analogous to electronic effects, such as the phonon Hall and phonon Zeeman effects. Moreover, they play a critical role in angular momentum transfer on ultrafast timescales, as seen in the Einstein-de Haas effect. Chiral phonons can also generate effective magnetic fields reaching the tesla scale, inducing magnetization in antiferromagnetic, paramagnetic, and even nonmagnetic materials - a phenomenon reminiscent of the Barnett effect. These advancements showcase phonon chirality and angular momentum as powerful emerging tools for generating and controlling magnetism. This focus session aims to highlight the latest breakthroughs in chiral-phonon magnetism and foster connections between the rapidly evolving field of chiral phononics and the broader magnetism research community.

Coordinators: Dominik M.Juraschek, Eindhoven University of Technology, d.m.juraschek@tue.nl; Martina Basini, ETH Zürich, m.basini@ethz.ch

Time: Monday 9:30–13:00 Location: H20

Invited Talk MA 5.1 Mon 9:30 H20

Driving Coherent Phonon-Phonon Angular Momentum Transfer via Lattice Anharmonicity — •Sebastian Maehrlein — Fritz Haber Institute of the Max Planck Society — Helmholtz Zentrum Dresden Rossendorf — TU Dresden

The discrete rotational symmetry of crystal structures leads to the conservation of quantized angular momentum in solids. Whereas the exchange of energy and linear momentum between lattice vibrations (phonons) via anharmonic coupling is a cornerstone of solid-state physics, conservation and transfer of angular momentum within the lattice remained a postulate, yet. Recently, phonon angular momentum, often in the form of chiral phonons, was linked to gigantic magnetic fields, dynamical ferroelectricity, ultrafast demagnetization, or magnetic switching. However, the fundamental process of phonon to phonon angular momentum transfer required for demagnetization and other spin-related relaxation phenomena remained elusive.

Here we drive coherent phonon-phonon angular momentum transfer by establishing helical nonlinear phononics. Thereby, we directly observe phonon helicity-switching dictated by (pseudo) angular momentum conservation and the discrete rotational symmetry of the lattice. Ab-initio modeling in conjunction with classical equations of motion confirm the experimentally observed anharmonic phonon-phonon coupling as the dominating lattice angular momentum transfer channel. Our results thus open the field of helical or chiral nonlinear phononics, turning lattice angular momentum into the long missing tuning knob for ultrafast material control.

Invited Talk MA 5.2 Mon 10:00 H20

Chiral phonons, phono-magnetism, and spin-rotation coupling — •Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

High-intensity THz lasers enable the coherent excitation of individual phonon modes. The ultrafast control of emergent magnetism through phonons and phonon angular momentum opens new avenues for tuning functional materials. Recent experiments suggest a substantial magnetization in various materials [1,2], presenting a challenge for theoretical modeling. I will provide an introduction to magnetization induced by phonon angular momentum via the phonon inverse Faraday effect [3]. Additionally, I will discuss a coupling mechanism based on inertial effects, which facilitates the interaction between rotational degrees of freedom and electron spin [4].

[1] Basini et al., Nature, 628, 534 (2024)
[2] Davies et al., Nature, 628, 540 (2024)
[3] Shabala, Geilhufe, Physical Review Letters, arXiv:2405.09538
[4] Geilhufe, Physical Review Research, 4, L012004 (2022)

Invited Talk MA 5.3 Mon 10:30 H20

Geometry of temporal chiral structures and photoinduced chirality-spin coupling — •Olga Smirnova[1,2,3], Philip Flores[1], Aycke Roos[1], David Ayuso[4], Piero Decleva[5], Stefanos Carlstroem[1], Serguei Patchkovskii[1], and Andres Ordonez[4] — [1]Max-Born Institute, Berlin — [2]Technische Universität Berin — [3]Technion - Israeli Institute of Technology, Haifa, Israel — [4]Imperial College London, UK — [5]CNR IOM and Dipartimento di Scienze Chimiche e Farmaceutiche, Universita degli Studi di Trieste, Italy

In non-relativistic physics the concepts of geometry and topology are usually applied to characterize spatial structures, or structures in momentum space. We introduce the concept of temporal geometry [1], which encompasses geometric and topological properties of temporal shapes, e.g. trajectories traced by a tip of a time-dependent vector on sub-cycle time scale, and apply it to light-driven ultrafast electron currents in chiral molecules. The geometric concepts: curvature and connection emerge as ubiquitous features of photoexcited chiral electron dynamics. To demonstrate the link between the geometric fields and spin, we extend the concept of curvature to spin-resolved photoionization, and show that it is responsible for enantio-sensitive locking of the cation orientation to the photoelectron spin. This translates into chirality induced spin selectivity in photoionization of oriented chiral molecules both in one photon and two-photon processes.

[1] Geometry of temporal chiral structures, A. F. Ordonez, A. Roos, P. Mayer, D.Ayuso, O. Smirnova, arXiv preprint arXiv:2409.02500, 2024

15 min. break

Invited Talk MA 5.4 Mon 11:15 H20

Phonon thermal Hall effect — •Kamran Behnia — Ecole Supérieure de Physique et de Chimie Industrielles, Paris, France

In insulating solids and liquids, heat is carried by phonons. The phonon scattering time is close to the so-called Planckian time near the melting temperature. It increases with cooling, as phonon-phonon Umklapp scattering events rarefy. A rigorous determination of thermal conductivity of insulators from first principles has been a major accomplishment of the quantum theory of solids. In contrast, our understanding of momentum and energy exchange between phonons at low temperatures is imperfect. In this context, the experimental detection of

phonon thermal Hall effect in a growing number of insulators is a challenge to the condensed matter theory. The list now includes elmental insulators, such as black phosphorus, silicon and germanium, in which the spin degree of freedom is irrelevant and the atomic bonds are covalent. We will examine how magnetic field can influence anharmonicity.

Invited Talk MA 5.5 Mon 11:45 H20

Giant effective magnetic moment of chiral phonons — •Swati Chaudhary[1,3], Dominik Juraschek[2], Martin Rodriguez-Vega[3], and Gregory A Fiete[4] — [1]The Institute for Solid State Physics, The University of Tokyo, Japan — [2]Eindhoven University of Technology, Eindhoven, Netherlands — [3]The University of Texas at Austin, Austin, USA — [4]Northeastern University, Boston, USA

Chiral phonons carry angular momentum and lead to magnetic responses in applied magnetic fields or when resonantly driven with ultrashort laser pulses. On the basis of purely circular ionic motion, these phonons are expected to carry a magnetic moment of the order of a few nuclear magnetons. However, some recent experiments have demonstrated a phonon magnetic moment of the order of a few Bohr magnetons. This kind of giant magnetic response points towards the electronic contribution to the magnetic moment of phonons. Many diverse mechanisms have been discovered for this enhanced magnetic response of chiral phonons. The orbital-lattice coupling is one such mechanism where low-energy electronic excitations on a magnetic ion hybridize with phonons and endow a large magnetic moment to phonons. In this talk, I'll present a microscopic model for the effective magnetic moments of chiral phonons based on this mechanism. We apply our model to two types of materials: rare-earth halide paramagnets and transition-metal oxide magnets. In both cases, we find that chiral phonons can carry giant effective magnetic moments of the order of a Bohr magneton, orders of magnitude larger than previous predictions.

MA 5.6 Mon 12:15 H20

Extrinsic Phonon Thermal Hall Effect — •Dimos Chatzichrysafis[1], Robin Richard Neumann[1,2], and Alexander Mook[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Germany

The thermal Hall effect is a developing tool to investigate charge-neutral excitations, exposing the quantum many-body ground state of correlated materials. Since a sense of chirality for the energy carriers is necessary for the generation of a thermal Hall effect, it is natural to expect that quasiparticles of magnetic excitations are responsible for the Hall transport. This conventional wisdom has been recently challenged in experiments [1] which revealed a universal character of the thermal Hall effect independent on the magnetic texture and the lattice structure, even in systems where magnetism is completely absent. This finding asks for the re-investigation of the role of phonons in the thermal Hall effect.

Here, we develop a theory for a phononic thermal Hall effect where the source of chirality is given by the presence of the molecular Berry phase. As a toy model we study a non-magnetic system on a Bravais square lattice. We go beyond the intrinsic mechanism [2] usually studied in literature and consider the contribution of different possible extrinsic sources of phonon Hall transport. Our results demonstrate that phonon thermal Hall effects can be native to very generic systems.

[1] Xiaobo Jin et al, arXiv:2404.02863
[2] Takuma Saito et. al, Phys. Rev. Lett. 123, 255901, December 2019

MA 5.7 Mon 12:30 H20

Signatures of chiral phonons in $MnPS_3$ — •Banhi Chatterjee and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057, Duisburg, Germany

Chiral phonons can exist in two-dimensional transition metal dichalcogenide (TMDC) monolayers without inversion symmetry. They can be observed in the non-equilibrium state triggered by optical excitations using circularly polarized light. In existing literature a detailed theoretical calculation of the circular phonons production rate has already been done for the TMDC MoS_2. We investigate the antiferromagnetic semiconductor $MnPS_3$ with a similar hexagonal crystal structure and band-structure like MoS_2 but a larger unit cell as a novel candidate material that may allow for excitation of circular phonons. In $MnPS_3$, although the total magnetic moment is zero in the ground state, exciting the system using circularly polarized light induces a net magnetic moment. The damping of the magnons observed experimentally points to the transfer of orbital angular moment to combined phonon-magnon excitations. Using DFT+U and density functional perturbation theory (DFPT) we obtain in-plane chiral phonon modes at the valley-points of a monolayer $MnPS_3$ and for these modes the S atoms make circular motions. We further study the electron-phonon coupling between these chiral phonon modes and the excited electronic states carrying orbital angular momentum, particularly the dominant d-electrons, in order to theoretically investigate the experimentally observed damping of magnons.

MA 5.8 Mon 12:45 H20

Elliptically polarized coherent phonons in a degenerate mode — Arne Ungeheuer, Mashood T. Mir, Ahmed Hassanien, Lukas Nöding, Thomas Baumert, and •Arne Senftleben — Institut für Physik, Universität Kassel

Controlled excitation of phonons in crystalline solids is an emerging way to alter the property of a material to create phenomena such as transient magnetic polarization [1,2]. Here, we want to focus on controlling the polarization properties of coherent optical phonons that can be launched by ultrashort laser pulses. we demonstrate the excitation of elliptically polarized coherent optical phonons of the E_{2g} shearing mode in graphite. This is achieved by exciting the superposition of two orthogonally polarized phonon modes using a tailored pair of time-delayed optical pulses with tilted polarization. The elliptically polarized coherent phonons are detected by ultrafast electron diffraction [3], where we determine the amount of ellipticity and the sense of rotation.

[1] D. M. Juraschek, et al. *Phys. Rev. Lett.* **118**, 054101 (2017).
[2] A. S. Disa, et al. *Nature Phys.* **16**, 937–941 (2018).
[3] C. Gerbig, et al. *New J. Phys.* **17**, 043050 (2015).

MA 6: Skyrmions I

Time: Monday 15:00–18:30 Location: H16

Invited Talk MA 6.1 Mon 15:00 H16

Magnetization dynamics of chiral helimagnetic insulators — •Aisha Aqeel — University of Augsburg, Augsburg, Germany — Technical University of Munich, Munich, Germany — Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Nature reveals fascinating patterns, often arising from intricate interactions among individual components. In magnets, remarkable patterns can emerge even in the absence of inversion symmetry. Chiral helimagnets, characterized by their twisted magnetic structures, whether topologically trivial or non-trivial, exhibit collective magnetic excitations ranging from GHz to THz. These exceptional properties make helimagnets highly attractive for spintronic technologies and unconventional computing [1]. However, realizing their full potential demands ultraclean magnetic systems with minimal dissipation and a deep understanding of their magnetization dynamics. In this talk, I will delve into the fundamental properties of chiral helimagnets and their dynamic magnetization behavior, focusing on the insulating material Cu2OSeO3. Our studies reveal evidence for a rare magnetic state in Cu2OSeO3 crystals - elongated skyrmions - observed through magnetic resonance experiments [2]. Additionally, utilizing a surface-sensitive electrical probe - spin Hall magnetoresistance - we discovered that the magnetic configurations at the surfaces of chiral magnets deviate significantly from those in the bulk [3].

[1] O. Lee, et al., Nat. Mater. 23(1), 79-87 (2024). [2] A. Aqeel, et al., Phys. Rev. Lett. 126(1), 017202 (2021). [3] A. Aqeel, et al., Phys. Rev. B 103(10), L100410 (2021).

MA 6.2 Mon 15:30 H16

Skyrmion dynamics in Ta/CoFeB/MgO at room temperature — •Hauke Lars Heyen[1], Malte Römer-Stumm[2], Michael Vogel[2], Florian Gossing[2], Jakob Walowski[1], Ethan Andrew Mullen[3], Christian Denker[1], Karin Dahmen[3], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Institute of Physics, University Greifswald, Germany — [2]Institute of Materials Science, Nanoscale Magnetic Materials and Magnetic Domains, CAU Kiel, Germany — [3]Department of Physics, The Grainger College of Engineering, University of Illinois Urbana-Champaign, USA

Applications in future storage devices, like the conceptual skyrmion race-track memory, require fundamental control over the skyrmion dynamics. We use Ta/CoFeB/MgO layer stacks to generate skyrmions at room temperature. The skyrmions are moved by applying nanosecond electric current pulses with current densities of around $5 \cdot 10^{10} A/m^2$ and are imaged with the magneto optical Kerr effect (MOKE). With a tracking algorithm the trajectories are determined and they hint at two diffusion types and the skyrmion-Hall effect. The latter occurs simultaneously with the topological Hall-effect that can be measured electrically. Combining the electrical measurements with MOKE allows us to separate the anomalous and the weak topological Hall effect. This allows for a differentiation between topological and non-topological stabilized magnetic structures.

MA 6.3 Mon 15:45 H16

Skyrmion Screws: A Novel 3D Topological Spin Texture — •Thorsten Hesjedal[1,2], Gerrit van der Laan[2], Haonan Jin[3,4], Jingyi Chen[3,4], and Shilei Zhang[3,4] — [1]Department of Physics, Clarendon Laboratory, Univer-

sity of Oxford, Oxford OX1 3PU, UK — [2]Diamond Light Source, Harwell Science and Innovation Campus, Didcot OX11 0DE, UK — [3]School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China — [4]ShanghaiTech Laboratory for Topological Physics, ShanghaiTech University, Shanghai 201210, China

Three-dimensional (3D) magnetic skyrmions have attracted increasing interest as topological spin textures capable of hosting emergent electromagnetic properties and unique spin dynamics. In this study, we present the first direct experimental observation of skyrmion screws — a 3D spin crystal featuring modulations along the z-axis. Using state-of-the-art soft x-ray ptycho-tomography, we fully visualize the skyrmion screw lattice in a $Co_8Zn_{10}Mn_2$ thin lamella, fabricated to induce boundary confinement effects. Ferromagnetic resonance spectroscopy and micromagnetic simulations reveal a distinct low-frequency resonance mode, establishing skyrmion screws as a fundamentally new phase. These findings open avenues for studying 3D topological magnetism and its applications in magnonics and spintronics.

MA 6.4 Mon 16:00 H16

Skyrmion bags embedded in the skyrmion lattice — •Nikolai S. Kiselev — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

The micromagnetic model of 2D chiral magnets predicts the existence of skyrmion bags – solitons with arbitrary topological charge [1]. Recent experiments have confirmed the stability of skyrmion bags with positive topological charges [2,3]. Using Lorentz TEM on thin plates of B20-type FeGe, we demonstrate the remarkable stability of skyrmion bags with negative charges embedded within a skyrmion lattice [4]. We outline a robust protocol for nucleating these embedded skyrmion bags, which remain stable even in zero or inverted external magnetic fields. Our findings are in excellent agreement with micromagnetic simulations.

[1] F.N. Rybakov, N.S. Kiselev Phys. Rev. B, 99, 064437 (2019). [2] J. Tang et al., Nature Nanotechnol. 16, 1086 (2021). [3] Y. Zhang et al., Nature Commun. 15, 3391 (2024). [4] L. Yang et al., Adv. Mater. 36, 2403274 (2024).

MA 6.5 Mon 16:15 H16

Skyrmion at finite temperature — •Thorben Pürling[1,2] and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Physics Department, RWTH Aachen University, 52062 Aachen, Germany

In the past decade magnetic skyrmions have been under intense scientific scrutiny. Key properties of magnetic skyrmions such as the radius have been shown to exhibit highly nonlinear behavior as a function of the microscopic interaction parameters representing Heisenberg exchange, Dyzaloshinskii-Moriya interaction (DMI) and magnetic anisotropy [1]. Due to thermal fluctuations in both spin and lattice degrees of freedom, these interaction strengths carry an effective temperature dependence. Hence, temperature should demonstrate a strong effect on quantities like the skyrmion radius. Surprisingly little work has been done in this direction, particularly when it comes to taking lattice vibrations into account. Here we present our first attempts at investigating the role of the lattice dynamics on relevant interaction parameters.

We acknowledge funding from the ERC grant 856538 (project "3D MAGIC") and DFG through SFB-1238 (project C1).

[1] H. Jia *et al.*, Phys. Rev. Materials **4**, 094407 (2020).

MA 6.6 Mon 16:30 H16

Skyrmion lattices emerging from magnetic dipolar interactions — Elizabeth M Jefremovas[1], •Kilian Leutner[1], Miriam G. Fischer[1], Jorge Marqués-Marchán[2], Thomas B. Winkler[1], Agustina Asenjo[2], Jairo Sinova[1,3], Robert Frömter[1], and Mathias Kläui[1,4] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Institute of Material Science of Madrid – CSIC, 28049 Madrid, Spain — [3]Department of Physics, Texas A&M University, College Station, Texas, USA — [4]Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Magnetic skyrmions are well-studied two-dimensional topological spin textures. Surprisingly, little is known about the mutual interactions of dipolar-stabilized skyrmions. By engineering a magnetic multilayer stack, we stabilize for 1 to 30 repetitions skyrmion lattices at room temperature and zero field. Using Kerr microscopy and Magnetic Force Microscopy we observe a drastic decrease in skyrmion size as the number of repetitions is increased. We present an analytical model to describe the skyrmion radius and periodicity from the single-layer to the thick-film limit and complement this with micromagnetic simulations. Additionally, we identify the critical role of the nucleation process in forming the skyrmion lattice. Our work provides a comprehensive understanding of skyrmion-skyrmion interactions, which are driven by dipolar interactions as the multi-layer stack thickness increases.

[1] E. M. Jefremovas et al., arXiv:2407.00539 (2024)

15 min. break

MA 6.7 Mon 17:00 H16

Skyrmion size manipulation by external force — Klaus Raab, Kilian Leutner, •Leonie-Charlotte Dany, Simon Fröhlich, Grischa Beneke, Duc Minh Tranh, Sachin Krishnia, Robert Frömter, Peter Virnau, and Mathias Kläui — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany

Magnetic skyrmions, spin textures with quasi-particle like properties, exhibit highly promising potential as information carriers in applications like storage or non-conventional computing.[1,2]

We experimentally investigate how the size of skyrmions is influenced by a combination of spin-orbit torques and repulsion from a structural barrier in a Ta/CoFeB/MgO based magnetic thin film. By employing Ga^+ ion implantation to modify the effective anisotropy of the magnetic layer, we create artificial barriers that serve as additional tools for manipulating skyrmions. Furthermore, the resulting changes in the formation of skyrmions lattice is characterized.

Based on the experimental finding, we then develop a new theoretical model within the framework of Thiele equation approach to describe the change in the skyrmions' size and their trajectories. Thiele equation accounts for the skyrmion size and skyrmion-skyrmion distance of an ensemble of skyrmions to an external stimulus, such as spin-orbit torques.

1. Raab, K. *et al., Nat. Commun.* **13**, 6982 (2022).
2. Beneke, G. *et al., Nat. Commun.* **15**, 8103 (2024).

MA 6.8 Mon 17:15 H16

Eigenmode following for direct entropy calculation — •Stephan von Malottki[4], Moritz A. Goerzen[1], Hendrik Schrautzer[1,2], Pavel F. Bessarab[2,3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany — [2]cience Institute, University of Iceland, 107 Reykjavík, Iceland — [3]Department of Physics and Electrical Engineering, Linnaeus University, SE-39231 Kalmar, Sweden — [4]MODL, Insititute of Condensed Matter and Nanosciences, UC Louvain, Belgium

We present an eigenmode following method (EMF) to numerically calculate entropy contributions beyond harmonic approximation. In the framework of transition state theory, this increases the accuracy and applicability of transition rate calculations. In EMF, the potential energy landscape is explored along the investigated eigenvectors by iteratively updating a partial Hessian matrix along the way. Numerical integration of the Boltzmann factor over the obtained energy curve yields the contribution of the eigenmode to the partition function and entropy of the analysed state. The EMF method can be combined with other methods such as the harmonic approximation, making it a feasible method to improve the description of individual eigenmodes. The application of the method will be shown on the example of the Chimera skyrmion collapse mechanism and anti-skyrmion rotation modes.

MA 6.9 Mon 17:30 H16

Topological magnetism in diluted artificial adatom lattices — •Amal Aldarawsheh[1,2] and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulations, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]aculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

The ability to control matter at the atomic scale has revolutionized our understanding of the physical world, opening doors to unprecedented technological advancements. Quantum technology, which harnesses the unique principles of quantum mechanics, enables us to construct and manipulate atomic structures with extraordinary precision. Here[1], we propose a bottom-up approach to create topological magnetic textures in diluted adatom lattices on the Nb(110) surface. By fine-tuning adatom spacing, previously inaccessible magnetic phases can emerge. Our findings reveal that interactions between magnetic adatoms, mediated by the Nb substrate, foster the formation of unique topological spin textures, such as skyrmions and anti-skyrmions, both ferromagnetic and antiferromagnetic. Since Nb can be superconducting, our findings present a novel platform with valuable insights into the interplay between topological magnetism and superconductivity, paving the way for broader exploration of topological superconductivity in conjunction with spintronics applications.

[1] A. Aldarawsheh et al., In preparation.

Work funded by the PGSB (BMBF-01DH16027)and DFG (SPP 2137; LO 1659/8-1)

MA 6.10 Mon 17:45 H16

The impact of magnetic anisotropy on the stability of antiskyrmions in schreibersite magnets — •Mamoun Hemmida[1], Jan Masell[2,3], Kosuke Karube[3], Dieter Ehlers[1], Hans-Albrecht Krug von Nidda[1], Vladimir Tsurkan[1,4], Yoshinori Tokura[3,5,6], Yasujiro Taguchi[3], and Istvan Kezsmarki[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]RIKEN Center for Emergent Matter Science, Japan — [4]Institute of Applied Physics, Academy of Sciences of Moldova, Republic of Moldova —

[5]Department of Applied Physics and Quantum-Phase Electronics Center, University of Tokyo, Japan — [6]Tokyo College, University of Tokyo, Japan

Magnetic anisotropy is a fundamental property of magnetic materials that plays an essential role in the stability of magnetic domains and skyrmions. In this ferromagnetic resonance (FMR) study we report the evolution of magnetic anisotropy by substituting various 4*d* metals in the easy-plane schreibersite magnet $(Fe,Ni)_3P$ with S_4 tetragonal symmetry,Hemmida2024. Starting from easy-plane anisotropy, Pd doping turns $(Fe,Ni)_3P$ to an easy-axis-type magnet. As a consequence, antiskyrmions are created. FMR study of the planar anisotropy proofs a fourfold symmetry as expected for the tetragonal crystal structure. The corresponding planar anisotropy parameter is an order of magnitude smaller than the uniaxial one. Hemmida2024 M. Hemmida, *et al.*, Phys. Rev. B 110, 054416 (2024).

MA 6.11 Mon 18:00 H16

The impact of the non-chiral magnetic fan state on the transformation of chiral textures in $Mn_{1.4}PtSn$ — M. Winter[1,2], A. Pignedoli[3], M.C. Rahn[4], A.S. Sukuhanov[4], A. Tahn[2], S. Schneider[2], D. Pohl[2], M. Azhar[3], K. Everschor-Sitte[3], J. Geck[4], G. van der Laan[5], T. Hesjedal[5,6], P. Vir[1], C. Felser[1], and •B. Rellinghaus[2] — [1]MPI CPfS, Dresden, Germany — [2]DCN, TU Dresden, Germany — [3]Univ. Duisburg-Essen, Germany — [4]IFMP, TU Dresden, Germany — [5]Diamond Light Source, UK — [6]Univ. Oxford, UK

The Heusler compound $Mn_{1.4}PtSn$ is a chiral magnet that exhibits a rich of variety non-topological and topologically protected chiral magnetic textures at room temperature. We have used Lorentz transmission electron microscopy (LTEM) supported by resonant elastic x-ray scattering (REXS) and micromagnetic simulations to characterize the emerging magnetic structures as function of the magnitude and orientation of an external magnetic field. We find that in out-of-plane fields, chiral soliton lattices emerge, while in-plane fields promote the formation of non-chiral magnetic fan domains. At fields in the stability range of the latter, the nucleation of non-topological bubbles (ntB's) occurs. Intriguingly, ntB's show combined characteristics of chiral solitons and the fan-type structure and may consequently be interpreted as hybrid structures of the latter. Following a distinct field protocol, ordered lattices of these ntB's then successively transform into anti-skyrmion lattices. Financial support by DFG through SPP 2137, project no. 403503416, is gratefully acknowledged.

MA 6.12 Mon 18:15 H16

Emergence of polar skyrmions in 2D Janus CrInX3 (X=Se, Te) magnets — •Duo Wang[1], Fengyi Zhou[1], Monirul Shaikh[2], and Biplab Sanyal[3] — [1]Macao Polytechnic University — [2]University of Nebraska, Kearney — [3]Uppsala University

In the realm of multiferroicity in 2D magnets, whether magnetic and polar skyrmions can coexist within a single topological entity has emerged as an important question. Here, we study Janus 2D magnets CrInX3 (X=Se, Te) for a comprehensive investigation of the magnetic ground state, magnetic excited state, and corresponding ferroelectric polarization by first-principles electronic structure calculations and Monte Carlo simulations. Specifically, we have thoroughly elucidated the magnetic exchange mechanisms, and have fully exemplified the magnetic field dependence of the magnon spectrum. More importantly, our study reveals a previously unrecognized, remarkably large spin-spiral-induced ferroelectric polarization (up to 194.9 μC/m2) in both compounds. We propose an approach to identify polar skyrmions within magnetic skyrmions, based on the observed direct correlation between spin texture and polarization density. Elucidating this correlation not only deepens our understanding of magnetic skyrmions but also paves the way for innovative research in the realm of multiferroic skyrmions.

MA 7: INNOMAG e.V. Prizes 2025 (Diplom-/Master and Ph.D. Thesis)

Die Arbeitsgemeinschaft Magnetismus der DPG hat einen Dissertationspreis und einen Diplom-/Masterpreis ausgeschrieben, welche auf der Tagung der DPG 2025 in Regensburg vergeben werden. Ziel der Preise ist die Anerkennung herausragender Forschung im Rahmen einer Diplom-/Masterarbeit beziehungsweise einer Promotion und deren exzellente Vermittlung in Wort und Schrift. Im Rahmen dieser Sitzung tragen die besten der für ihre an der Hochschule eines Mitgliedslands der European Physical Society durchgeführten Diplom-/Masterarbeit beziehungsweise Dissertation Nominierten vor. Im direkten Anschluss entscheidet das Preiskomitee über den Gewinner bzw. die Gewinnerin des INNOMAG e.V. Diplom/Master-Preises und des Dissertationspreises 2025. Talks will be given in English!

Time: Monday 15:00–18:00 Location: H18

Invited Talk MA 7.1 Mon 15:00 H18

Realizing Reservoir Computing with skyrmions in geometrical confinements tuned by ion irradiation — •Grischa Beneke — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

Physical reservoir computing (RC) is a beyond von-Neumann computing paradigm that harnesses complex physical systems' dynamics for efficient information processing. Magnetic skyrmions, topological spin textures, show promise for RC systems due to their non-linear interactions and low-power manipulation capabilities. Previous spin-based RC implementations either focused on static detection or required rescaling of real-world data to match intrinsic magnetization dynamics timescales. In this thesis, we demonstrate time-multiplexed skyrmion RC by adjusting the reservoir's intrinsic timescales to match real-world temporal patterns [1]. Using hand gestures recorded via range-Doppler radar in collaboration with industry, we show that our hardware solution outperforms conventional software-based neural networks while consuming less energy. The system's ability to directly integrate sensor data without temporal conversion enables real-time applications. To structure the geometrical confinement, we investigate how high-energy ion irradiation influences magnetic properties in skyrmion-hosting multilayers. By locally modifying the perpendicular magnetic anisotropy, we create attractive and repulsive regions that enable controlled skyrmion nucleation, manipulation and confinement, enabling novel devices and, enhancing device functionality. [1] G. Beneke et al., Nat. Commun. 15, 8103 (2024).

Invited Talk MA 7.2 Mon 15:20 H18

Low-energy spin excitations of the Kitaev candidate material $Na_2Co_2TeO_6$ probed by high-field/high-frequency electron spin resonance spectroscopy — •Luca Bischof[1], Jan Arneth[1], Kwang-Yong Choi[2], Raju Kalaivanan[3], Raman Sankar[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Physics, Sungkyunkwan University, Republic of Korea — [3]Institute of Physics, Academia Sinica, Taiwan

The realization of a Kitaev spin liquid state in the Co-based honeycomb magnet $Na_2Co_2TeO_6$ is circumvented by magnetic ordering due to Heisenberg and off-diagonal interactions. The nature of these interactions and the magnetic ground state in $Na_2Co_2TeO_6$ are still under debate. We report high-frequency/high-field electron spin resonance (ESR) measurements of single-crystal $Na_2Co_2TeO_6$ probing the low-energy spin excitations of the ordered phase below $T_N \simeq 27$ K. A complex magnon spectrum for in-plane magnetic fields $B \parallel a^*$ indicates field-induced phase transitions. For out-of-plane magnetic fields $B \parallel c$, we observe one softening and two hardening magnon modes. They share a magnon excitation gap of $\Delta = 219(13)$ GHz. We performed spin wave calculations for the extended Heisenberg-Kitaev model to compare the observed magnon modes to the low-energy excitations expected for zigzag and triple-q ground states in an applied magnetic field.

Invited Talk MA 7.3 Mon 15:40 H18

Tailoring the first-order magnetostructural phase transition in Ni-Mn-Sn for caloric applications by microstructure — •Johannes Puy, Enrico Bruder, Oliver Gutfleisch, and Franziska Scheibel — TU Darmstadt, Darmstadt, Germany

Ni-Mn-Sn Heusler alloys show a large inverse magnetocaloric (MCE) and conventional elastocaloric effect (ECE), making them a promising candidate for multicaloric cooling. The caloric effects arise from a first-order magnetostructural phase transition (FOMST) from high-magnetic austenite to low-magnetic martensite, driven by a nucleation and growth process. Optimizing the multicaloric performance of these materials requires tailoring the FOMST, which implies a comprehensive understanding of the role of microstructure and coupling factors, such as atomic, magnetostatic, and stress coupling. In this study, the influence of microstructure and defects (grain boundaries, pores, sintering necks) on the temperature-driven FOMST is investigated in single- and polycrystalline particles, as well as in spark-plasma-sintered Ni-Mn-Sn. By adjusting the relative density, the effect of porosity on the FOMST is studied. Temperature-dependent magnetometry reveals that an increase of the relative density from 88 % to 99 % narrows the transition ranges from 18 K to 9 K and decreases

the transition temperature from 263 K to 254 K. Temperature-dependent in-situ optical and in-situ scanning electron microscopy reveal preferential martensite nucleation at free particle surfaces in powder and sintered, 88% dense Ni-Mn-Sn, while nucleation in 99 % dense Ni-Mn-Sn is favored at sintering necks. We thank the CRC/TRR 270 'HoMMage' for funding.

15 min. break

Invited Talk MA 7.4 Mon 16:15 H18

Tuning the properties of two-dimensional magnetic heterostructures via interface engineering with molecular and inorganic van der Waals crystals. — •Carla Boix-Constant[1], Samuel Mañas-Valero[2], and Eugenio Coronado[1] — [1]Institute of Molecular Science, 46980 Paterna (Valencia), Spain. — [2]Kavli Institute of Nanoscience - TU Delft, Delft 2628 CJ, The Netherlands.

Two-dimensional (2D) materials offer unprecedented opportunities for fundamental and applied research in several condensed matter physics areas. For this purpose, state-of-the-art techniques were employed in this thesis (divided in two blocks) to fabricate van der Waals heterostructures based on mainly 2D magnets (both inorganic and molecular systems) and to characterize the resulting devices by magneto-transport techniques. On the one hand, new chemically designed molecular building blocks were combined with 2D materials to afford hybrid devices offering a new playground for exploiting the potential of spin transition molecular systems to control the properties of the 2D material. On the other hand, we focused on purely 2D magnetic materials: the quantum spin liquid candidate 1T-TaS2 - where our results throw some light in the debate about the exotic behaviour of the material - and the metamagnet CrSBr - results that afford a new generation of van der Waals heterostructures with programmable properties.

Invited Talk MA 7.5 Mon 16:40 H18

Theoretical Prediction for Probing Magnon Topology — •Robin R. Neumann — Johannes Gutenberg University Mainz — Martin Luther University Halle-Wittenberg

Magnons, the bosonic quasiparticles of collective spin excitations, hold potential as information and energy carriers in spintronic devices. Although the magnonic counterpart of the electronic quantum Hall states was predicted over a decade ago [1, 2], experimental evidence remains absent because established methods fail to probe them [3].

In my thesis I have studied the signatures of topological magnons in transport and spectroscopic observables. While I demonstrated that the thermal Hall effect can be sensitive to topological phase transitions in the magnon band structure [4], magnon-phonon hybridization may obscure their contributions [5]. I present a specific proposal for using electrical probes to detect topological magnons [6]. Despite their charge neutrality, magnetoelectric effects grant magnons an electrical dipole moment. Consequently, edge magnons give rise to an electric polarization at the edges driven by thermal spin fluctuations. Furthermore, magnons are predicted to interact with alternating electric fields, opening up the possibility of resonantly exciting topological magnons. The resulting absorption spectrum encodes footprints of topological magnons that might assist in their detection.

[1] Zhang *et al.*, PRB **87**, 144101 (2013), [2] Shindou *et al.*, PRB **87**, 174427 (2013), [3] Malz *et al.*, Nat. Commun. **10**, 3937 (2019), [4] **RRN** *et al.*, PRL **128**, 117201 (2022), [5] **RRN** *et al.*, PRB **108**, L140402 (2023), [6] **RRN** *et al.*, PRB **109**, L180412 (2024)

Invited Talk MA 7.6 Mon 17:05 H18

Multiphysics-Multiscale Simulation of Additively Manufactured Functional Materials — •Yangyiwei Yang — Technische Universität Darmstadt, Darmstadt, Germany

The progress of additive manufacturing (AM) technologies has led to a growing interest in AM-produced magnetic functional materials with tailored properties, including magnetic coercivity, remanence and saturation magnetization. However, the lack of comprehensive research on the process-microstructure-property (PMP) relationship poses a significant challenge to the production of magnetic materials with designed properties by AM. In this work, a multiphysics-multiscale simulation framework has been developed to thoroughly investigate the PMP relationships in magnetic functional materials and to further facilitate simulation-driven property tailoring. The framework is methodically structured to ensure clarity and depth, with emphasis on key concepts with corresponding physical backgrounds. By employing the established framework, phenomenological relationships between AM processing parameters and the resulting material properties are obtained, notably magnetic hysteresis. The sensitivity of the local magnetic coercivity to residual stress states in AM-produced Fe-Ni permalloy is also revealed. In particular, the relationship between the average residual stress and the magnetic coercivity within the melt zone are shown to obey an exponential growth law, suggesting a strategy for tailoring the magnetic coercivity by controlling the residual stress within an AM-produced permalloy.

30 min. discussion break and bestowal of INNOMAG e.V. Diplom-/Master Prize and Ph.D. Thesis Prize

MA 8: Spin-Dependent Phenomena in 2D (joint session MA/HL)

Time: Monday 15:00–17:15 Location: H19

MA 8.1 Mon 15:00 H19

Magnetoelectric behavior of breathing kagomé monolayers of Nb3(Cl,Br,I)8 from first-principles calculations — •John Mangeri — Technical University of Denmark, Kongens Lyngby, Denmark

We apply density functional theory to explore the magnetoelectric (ME) properties of two-dimensional Nb3(Cl,Br,I)8. These compounds have recently been proposed to exhibit coupled ferroelectric and ferromagnetic order leading to a switchable anomalous valley Hall effect (AVHE). Using both spin-spiral and self-consistent spin-orbit coupled calculations, we predict an in-plane 120 degree cycloid of trimerized spins as the ground state for Nb3Cl8. For Nb3Br8 and Nb3I8 we find long period incommensurate helical order. We calculate a number of magnetic properties such as the exchange constants, orbital magnetization, and Weiss temperatures. It is then shown that, despite having both broken inversion and time-reversal symmetry, the proposed AVHE and linear ME response are forbidden by the presence of helical order in the ground state. In addition, the computed switching trajectory demonstrates that it is unlikely that the polar state of the monolayers can be switched with a homogeneous electric field due to an unusual equation of state of the out-of-plane dipole moment. Nevertheless, we highlight that in the presence of a strong electric field, the trimerized spins in Nb3Cl8 will exhibit a magnetic phase transition from the 120 degree cycloid to out-of-plane ferromagnetic order, which restores the symmetry required for both AVHE and linear ME effects.

MA 8.2 Mon 15:15 H19

Ab-initio Investigation of two-dimensional Fe-Sn Kagome lattice with Nb doping — •Gérald Kämmerer[1,2] and Sinéad Griffin[2] — [1]Faculty of Physics, University of Duisburg-Essen — [2]Lawrence Berkeley National Laboratory (LBNL), Berkeley

This research investigates Fe-Sn-based kagome compounds for green energy applications, focusing on their magnetic and electronic properties, particularly in spintronics and phononics. We are investigating tunable properties in Fe_3Sn. We aim to control spin states in 2D magnetic systems by studying doped variants (Nb) in Kagome lattices to uncover topological electronic states, including Dirac fermions and flat bands.

Using first-principles calculations, we analyse impurity interactions in 2D lattices using VASP. By comparing experimental data with our computational results, this study aims to provide insights into dopant-controlled quantum states and improve material performance in electronic applications.

The financial support of the DFG within the SFB 1242 and the computational time on the LBNL supercomputer system are gratefully acknowledged.

MA 8.3 Mon 15:30 H19

Spin polarization of the two-dimensional electron gas at the EuO/$SrTiO_3$ interface — •Paul Rosenberger[1,2], Andri Darmawan[3], Olena Fedchenko[1], Olena Tkach[1], Serhii V. Chernov[4], Dmitro Kutnyakhov[4], Moritz Hoesch[4], Markus Scholz[4], Kai Rossnagel[4,5], Rossitza Pentcheva[3], Gerd Schönhense[1], Hans-Joachim Elmers[1], and Martina Müller[2] — [1]JGU Mainz, Germany — [2]Uni Konstanz, Germany — [3]UDE, Duisburg, Germany — [4]DESY, Hamburg, Germany — [5]CAU Kiel, Germany

Spin-polarized two-dimensional electron gases (2DEGs) are of particular interest for functional oxide electronics applications. Here, we use magnetic circular dichroism in the angular distribution (MCDAD) of photoemitted electrons to investigate whether and how the induced spin polarization of the redox-created 2DEG at the EuO/$SrTiO_3$ (001) interface depends on the dimensionality of the strongly ferromagnetic (7 $\mu_B/f.u.$) EuO layer [1]. Samples with EuO thicknesses ranging from one to four monolayers were studied. We show that the EuO/STO interfacial 2DEG becomes spin-polarized starting from a threshold EuO thickness of only two monolayers. Experimental data are complemented by DFT+U calculations. Our results, and the potential to enhance the magnetic order of EuO by other proximity effects [2], indicate that the EuO/STO interface is an ideal template for creating functional spin-polarized 2DEGs for application in oxide electronics.

[1] Rosenberger *et al.*, arXiv:2410.23804 (2024).
[2] Rosenberger *et al.*, Sci. Rep. **14**, 21586 (2024).

MA 8.4 Mon 15:45 H19

***Ab initio* calculation of Spin-Orbit torques in 2D magnets** — •Gusthavo Brizolla and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The interplay of spin-orbit coupling and magnetism in two-dimensional materials and their heterostructures presents exciting opportunities for advancing next-generation spintronic devices. In this work, we investigate the role of proximity effects in generating spin-orbit torques (SOTs) in Fe_3GeTe_2 (FGT) and FGT-based van der Waals heterostructures. Using a tight-binding Hamiltonian derived from first-principles calculations via the Wannierization procedure, we evaluate the torkances within the linear response regime using the Kubo formalism. Our results reveal key mechanisms underlying the generation of torques driven by spin accumulation, elucidating the fundamental physics of SOTs in these systems.

This research has been supported by 2D SPIN-TECH.

MA 8.5 Mon 16:00 H19

Unveiling Long-range Magnetic Textures in Twisted Moiré Antiferromagnets — •King Cho Wong[1], Ruoming Peng[1], Xiaodong Xu[3], Elton Santo[2], Adam Wei Tsen[4], Rainer Stoehr[1], and Joerg Wrachtrup[1] — [1]3rd Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]University of Edinburgh, United Kingdom — [3]University of Washington, USA — [4]University of Waterloo, Canada

Stacking two-dimensional (2D) materials offers a controllable and versatile platform to engineer interlayer interactions, unveiling numerous intriguing correlated and topological states. Recent progresses in twisted 2D magnets have revealed periodic ferromagnetic domains due to the local Moiré stacking. In this study, we employed scanning quantum microscopy to investigate local magnetic responses of twisted double bilayer chromium triiodide (tDB CrI3). We observed unexpected antiferromagnetic textures with periods more than 300 nm at the 1.1° twisted devices, which are significantly exceeding the corresponded Moiré size of about 30 nm. These periodic magnetic textures are setting atop randomly distributed ferromagnetic domains with net two-layer magnetization of 30 uB/nm^2 and antiferromagnetic domains with magnetization of 0 uB/nm^2. Our findings suggest that strong magnetic competition at small twisted angles (<2°) can extend magnetic textures beyond the Moiré size, leading to the emergence of Néel skyrmions after field cooling.

MA 8.6 Mon 16:15 H19

Spin model of graphene triangulenes embedded in hexagonal boron nitride — •Dániel Tibor Pozsár[1,3,4,5], László Oroszlány[1,2,3], and Viktor Ivády[1,4,5,6] — [1]Department of Physics of Complex Systems, Eötvös Loránd University, Egyetem tér 1-3, H-1053 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]TRILMAX Consortium, Twinning, Horizon Europe, Budapest, Hungary — [4]QUEST projec, Twinning, Horizon Europe, Budapest, Hungary — [5]MTA*ELTE Lendület "Momentum" NewQubit Research Group, Pázmány Péter, Sétány 1/A, 1117 Budapest, Hungary — [6]Department of Physics, Chemistry and Biology, Linköping University, SE-581 83 Linköping, Sweden

We are investigating triangulene shaped substitutional defects in hexagonal boron nitride filled with carbon atoms. We show how the triangulene shaped defects encompass magnetic moments and with ab initio methods we build Heisenberg like classical spin models representing their interactions. We show how different lattice terminations and sizes impact the magnetic properties of the system.

MA 8.7 Mon 16:30 H19

Realizing Spin-3/2 AKLT State for Quantum Computation with Tetrapod Architectures — •Claire Benjamin[1], László Oroszlány[1,2], Dániel Varjas[3], and Gábor Széchenyi[1] — [1]Department of Physics of Complex Systems, Eötvös University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary — [2]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary

Using a novel tetrapod (5-site cluster) architecture, we implement spin-3/2 degrees of freedom in a semiconductor quantum bit platform. This framework enables us to construct a tunable artificial spin system that can realize the two-dimensional Affleck-Kennedy-Lieb-Tasaki (AKLT) state on a honeycomb lattice, known to be a universal resource for measurement-based quantum computation. We assess the model's robustness and feasibility for measurement based quantum computing using semi-analytic perturbation theory and numerical calculations.

MA 8.8 Mon 16:45 H19

Anomalous quantum oscillations from boson-mediated interband scattering — •Léo Mangeolle[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Quantum oscillations (QO) in metals refer to the periodic variation of thermodynamic and transport properties as a function of inverse applied magnetic field. QO frequencies are normally associated with semi-classical trajectories of Fermi surface orbits but recent experiments challenge the canonical description. We develop a theory of composite frequency quantum oscillations (CFQO) in two-dimensional Fermi liquids with several Fermi surfaces and interband scattering mediated by a dynamical boson, e.g. phonons or spin fluctuations. Specifically, we show that CFQO arise from oscillations in the fermionic self-energy with anomalous frequency splitting and distinct strongly non-Lifshitz-Kosevich temperature dependencies. Our theory goes beyond the framework of semi-classical Fermi surface trajectories highlighting the role of many-body effects. We provide experimental predictions and discuss the effect of non-equilibrium boson occupation in driven systems.

MA 8.9 Mon 17:00 H19

Identifying the Origin of Thermal Modulation of Exchange Bias in $Fe_3GeTe_2/MnPS_3$ van der Waals Heterostructures — Aravind Puthirath Balan[1], •Aditya Kumar[1], Patrick Reiser[2], Joseph Vimal Vas[3], Thibaud Denneulin[3], Rafal E. Dunin-Borkowski[3], Patrick Maletinsky[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

This study investigates the origin of exchange bias in $Fe_3GeTe_2/MnPS_3$ vdW heterostructures. A substantial 170 mT exchange bias is observed at 5 K, one of the largest values reported for vdW heterostructures, despite the compensated interfacial spin configuration of $MnPS_3$. This exchange bias is linked to unexpected weak ferromagnetic ordering in $MnPS_3$ below 40 K that we reveal by NV center imaging. A 1000% variation in the magnitude of exchange bias is obtained through thermal cycling linked to changes in the vdW gap during field cooling. Detailed interface analysis reveals atom migration between layers, forming amorphous regions on either side of the vdW gap. These findings underscore the robust and tunable nature of exchange bias in vdW heterostructures but also challenge the often assumed pristine nature of vdW interfaces calling for in-depth interface characterization.

[1] A. P. Balan et al., Advanced Materials 36, 2403685 (2024).

MA 9: Altermagnets I

Time: Monday 15:00–18:30 Location: H20

MA 9.1 Mon 15:00 H20

Tuning the Octupolar Degrees of Freedom in the Altermagnetic Candidate MnF_2 by Strain and Magnetic Field — •Rahel Ohlendorf[1,2], Hilary M. L. Noad[1], Jörg Schmalian[3], Elena Hassinger[2], Andrew P. Mackenzie[1,4], and Elena Gati[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Technical University, Dresden, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]University of St Andrews, UK

Altermagnetism can unambiguously be differentiated from the known ferro- and antiferromagnetic phases within the framework of spin-group symmetry [1]. In centrosymmetric altermagnets the ordered state can be described in terms of ferroically ordered magnetic octupoles [2]. The experimental conjugate field that is predicted to couple to this order parameter is a combination of strain and magnetic field. Consequently the application of strain and magnetic field should enable the exploration of the physics near the ferrooctupolar critical point, including its associated crossover lines.

We discuss experimental phase diagrams on the centrosymmetric altermagnetic candidate MnF_2 in magnetic field and strain, mapped out by means of elastocaloric measurements and compare our results to theoretical predictions based on a Landau free energy [3].

[1]L. Smejkal et al., Phys. Rev. X 12, 031042 (2022)
[2]S. Bhowal et al., Phys. Rev. X 14, 011019 (2024)

[3]P. McClarty et al., Phys. Rev Lett. 132, 176702 (2024)
*Work is supported by the DFG through TRR288 (Elasto-Q-Mat).

MA 9.2 Mon 15:15 H20

Tuning the magnetic anisotropy of the altermagnet CrSb — •Miriam Fischer[1], Lukas Odenbreit[1], Sonka Reimers[1], Toni Helm[2], Mathias Kläui[1], and Martin Jourdan[1] — [1]Johannes Gutenberg Universität, Mainz — [2]Helmholtz-Zentrum Dresden-Rossendorf

CrSb is an altermagnetic compound, whose band structure we recently investigated by SX-ARPES [Rei24]. For the utilization of this compound in spintronics, a rotation of the magnetic easy axis is required. Thus, we study the tunability of the magnetic anisotropy of CrSb and related compounds by measurements of the spin-flop field.

[Rei24] S. Reimers et al., Nat Commun. 15, 2116 (2024)

MA 9.3 Mon 15:30 H20

Local signatures of altermagnetic order — •Jannik Gondolf[1], Andreas Kreisel[1], Mercè Roig[1], Daniel F. Agterberg[2], and Brian M. Andersen[1] — [1]Niels Bohr Institute, University of Copenhagen, DK-2200 Copenhagen, Denmark — [2]Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201, USA

Altermagnets are known to share properties of ferromagnets and antiferromagnets. They feature time-reversal symmetry breaking, non-relativistic anisotropic band splitting and compensated net magnetization. Fundamental properties of altermagnetism include the anomalous Hall effect, a spin-polarized band structure in angle-resolved photoemission spectroscopy and spin-polarized currents. We employ a minimal model to investigate the local signatures of altermagnetism in the vicinity of impurities using T-matrix theory and exact diagonalization. Our findings suggest that the altermagnetic symmetry breaking is directly imprinted in the local density of states. These signatures can be quantified by scanning tunnel microscopy, offering a new approach for identifying and characterizing potential altermagnetic materials experimentally. Further, we explore potential interplay between altermagnetism and superconductivity.

MA 9.4 Mon 15:45 H20

Spin-wave theory and magnon transport properties of altermagnetic hematite (α-Fe2O3) — •Rhea Hoyer[1], P. Peter Stavropoulos[2], Libor Šmejkal[1,3,4], and Alexander Mook[1] — [1]Department of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Str. 38, 01187 Dresden, Germany — [4]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czech Republic

We develop a four-sublattice spin-wave theory for the g-wave altermagnet hematite (α-Fe2O3) in its two magnetic phases: the easy-axis phase below, and the weak ferromagnetic phase above the Morin temperature. We estimate the Morin temperature with a free energy calculation. The relativistic magnon dispersion relation in the easy-axis phase shows the spin (or chirality) splitting typical of altermagnets. We investigate magnon transport properties with a particular focus on the crystal thermal Hall effect.

MA 9.5 Mon 16:00 H20

Giant spatial anisotropy of magnon lifetime in altermagnets — •António Costa[1,2], João Henriques[1,3], and Joaquín Fernández-Rossier[1] — [1]International Iberian Nanotechnology Laboratory, Braga, Portugal — [2]Physics Center of Minho and Porto Universities (CF-UM-UP), Braga, Portugal — [3]Universidade de Santiago de Compostela, Santiago de Compostela, Spain

Altermagnets are a new class of magnetic materials with zero net magnetization (like antiferromagnets) but spin-split electronic bands (like ferromagnets) over a fraction of reciprocal space. As in antiferromagnets, magnons in altermagnets come in two flavours, that either add one or remove one unit of spin to the $S = 0$ ground state. However, in altermagnets these two magnon modes are non-degenerate along some directions in reciprocal space. Here we show that the lifetime of altermagnetic magnons has a very strong dependence on both flavour and direction. Strikingly, coupling to Stoner modes leads to a complete suppression of magnon propagation along selected spatial directions. This giant anisotropy will impact electronic, spin, and energy transport properties and may be exploited in spintronic applications.

MA 9.6 Mon 16:15 H20

Chiral spin-flip magnons in metallic altermagnets from many-body perturbation theory — •Wejdan Beida[1], Ersoy Sasioglu[2], Gustav Bihlmayer[1], Christoph Friedrich[1], Yuiry Mokrousov[1], Ingrid Mertig[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany

Altermagnets represent a novel class of magnetic materials that bridge the gap between conventional ferro- and antiferromagnets. A unique feature of altermagnets is the lifting of degeneracy of their spin-wave modes (magnons) along the same crystallographic directions in which electronic bands also exhibit spin splitting. This non-degeneracy leads to chirality and directional anisotropy in spin-wave dispersions. In this presentation, we present the spin splitting of electronic bands and chiral spin-wave excitations in a series of metallic altermagnets, which have NiAs-type crystal structure, using DFT and many-body perturbation theory [1]. Our findings reveal a pronounced anisotropic splitting in chiral magnon bands, a small chiral asymmetry in the magnon lifetime, and demonstrate that magnon damping due to Stoner excitations is minimal. This results in long-lived magnons with efficient propagation, underscoring the potential of altermagnets for advanced spintronic and magnonic applications.

W.B. acknowledges support by the Palestinian-German Science Bridge.

[1] E. Sasioglu et al., Phys. Rev. B 81,054434 (2010).

MA 9.7 Mon 16:30 H20

Fingerprints of altermagnetism in the optical properties of MnTe — •Luca Felipe Haag[1], Marius Weber[1,2], Jairo Sinova[2], and Hans Christian Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany — [2]Institut für Physik, Johannes Gutenberg University Mainz, Germany

It has recently been demonstrated by magneto-optical Kerr effect (MOKE) measurements that the spin system in planar d-wave altermagnets can be controlled by linearly polarized optical excitation [2] as one can selectively address spin-up or spin-down electrons by choosing the polarization of the optical pulse. The objective of this study is to investigate whether similar optical effects can be observed in bulk g-wave altermagnets. To this end, we focus on MnTe, which has been demonstrated to be altermagnetic by ARPES measurements [3]. Using ab-initio techniques together with a time-dependent calculation of the absorption process, we study theoretically the optically induced spin polarization for all polarization angles. Our results show an intriguing interplay between the complex nodal-plane structure in bulk g-wave altermagnets and the anisotropic excitation due to the polarized pulses, causing planar d-wave or g-wave signatures depending on the laser's incident direction.

References: [1] L. Šmejkal et al., Phys. Rev. X 12, 040501 (2022) [2] M. Weber et al., arXiv:2408.05187 (2024) [3] Krempaský et al., Nature 626, 517-522 (2024)

15 min. break

MA 9.8 Mon 17:00 H20

Optical Excitation of Spin Polarization in the Altermagnet RuO_2 — •Marius Weber[1], Stephan Wust[1], Luca Haag[1], Akashdeep Akashdeep[2], Kai Leckron[1], Christin Schmitt[2], Rafael Ramos[3], Takashi Kikkawa[4], Eiji Saitoh[4], Mathias Kläui[2], Libor Šmejkal[2], Jairo Sinova[2], Martin Aeschlimann[1], Gerhard Jakob[2], Benjamin Stadtmüller[5], and Hans Christian Schneider[1] — [1]University of Kaiserslautern-Landau, Germany — [2]Johannes Gutenberg University Mainz, Germany — [3]CIQUS, Universidade de Santiago de Compostela, Spain — [4]The University of Tokyo, Japan — [5]Augsburg University, Germany

We explore the ultrafast response of altermagnetic materials after optical excitation with femtosecond light pulses. For the case of RuO_2, we employ ab-initio based dynamical calculations to predict the spin polarization of the optically excited carriers. Our theoretical results are confirmed by time-resolved MOKE experiments[1], which demonstrate that highly spin-polarized carrier distributions can be generated in ultrathin, strained RuO_2 by tuning the excitation conditions, in particular the orientation of the light polarization vector.

[1] M. Weber et al., arXiv:2408.05187 (2024)

MA 9.9 Mon 17:15 H20

Magnetotransport in altermagnetic CrSb — •Christoph Müller — FZU Prague

Altermagnets (AMs) constitute a recently established category of magnetically ordered materials distinguished by an antiparallel alignment of identical magnetic moments, however with an alternating spin polarization in the electronic band structure. This unique attribute has ignited considerable interest in exploring novel applications within the realm of spintronics. Furthermore, AMs host transport and optical effects, associated with spin-polarized currents and strongly spin-split bands otherwise only observed in ferromagnets. Chromium Antimonide (CrSb) is due to its crystal symmetry and its compensated order classified as an altermagnet. CrSb exhibits a sizable spin splitting of 1.2 eV which is enabled by the non-relativistic crystal field origin. In my work I investigated the magnetotransport properties of the material in bulk and thin films. The bulk samples were also measured in a high field laboratory in search for a spin-flop transition or the anomalous Hall effect.

MA 9.10 Mon 17:30 H20

Altermagnetic spin wave dispersion in atomistic spin models — •Tobias Dannegger[1], Levente Rózsa[2,3], László Szunyogh[3], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Theoretical Solid State Physics, Institute for Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Budapest, Hungary

Altermagnets have a broken symmetry reflected in the shape of the spin density around the magnetic atoms. Using an ab initio parametrised atomistic spin model of hematite (α-Fe_2O_3), we show that this altermagnetic symmetry breaking induces a remarkably high splitting of 2.8 meV in the isotropic exchange couplings between the Fe spins for equidistant neighbours within the thirteenth coordination shell. We further study the resulting spin-wave dispersion relation and find that, in addition to the relativistic band splitting on the order of 10 GHz present almost throughout the entire Brillouin zone, the altermagnetic asymmetry of the isotropic interactions causes a much larger band splitting of the order of 1 THz, but only along low-symmetry directions in the Brillouin zone.

MA 9.11 Mon 17:45 H20

First-principles calculations of Luttinger ferrimagnets — •Jan Priessnitz[1], Igor Mazin[2], and Libor Šmejkal[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, and Quantum Science and Engineering Center, George Mason University, Fairfax, VA, USA

The discovery of altermagnets demonstrated that it is possible to have a material with zero net magnetization, but broken Kramers' spin degeneracy and large spin-splitting, even without considering relativistic effects (spin-orbit coupling) [1]. The altermagnetic spin polarization promises applications in the field of spintronics.

Apart from altermagnets, there are several other classes of magnets showing such properties, such as the Luttinger compensated ferrimagnets. These are materials containing two or more magnetic sublattices which are not connected by symmetry, but which perfectly compensate each other by the virtue of Luttinger's theorem [2].

In this talk, we will give a brief introduction into Luttinger compensated ferrimagnets and present first-principle calculations of several candidate materials and unconventional properties not seen in conventional magnetic materials.

[1] Šmejkal, L., Sinova, J., & Jungwirth, T. (2022). Physical Review X, 12(3).

[2] Mazin, I. (2022). Editorial, Physical Review X, 12(4).

MA 9.12 Mon 18:00 H20

Magnetic domain features in the altermagnetic Mn_5Si_3 — •Gregor Skobjin[1], Javier Rial[2], Sebastian Beckert[3], Helena Reichlová[3,4], Andy Thomas[3,5], Vincent Baltz[2], Lisa Michez[6], Richard Schlitz[1], Michaela Lammel[1], and Sebastian T.B. Goennenwein[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Université Grenoble Alpes, CNRS, CEA, IRIG-Spintec, France — [3]IFMP, TU Dresden, Germany — [4]Institute of Physics ASCR, Czech Republic — [5]Aix-Marseille Université, CNRS, CINaM, France — [6]IFW Dresden, Germany

Altermagnets are an intriguing novel class of magnetic materials. We exploit the anomalous Hall effect response of micropatterned Mn_5Si_3 thin films to investigate their magnetization relaxation behavior. In experiments at T < 200 K i.e., in the altermagnetic phase, and for magnetic fields for which the samples exhibit large magnetic susceptibility, we observe a strong magnetic aftereffect as well as Barkhausen-like steps in the time-dependent Hall voltage evolution. More specifically, we recorded the evolution of the Hall voltage in micropatterned Hall bars with widths of 10 microns down to 0.1 microns at a series of different magnetic field magnitudes to gain insights into potential domain effects in the altermagnetic phase of Mn_5Si_3. We critically analyze our experimental results and discuss implications for the micromagnetic structure of altermagnetic thin films.

MA 9.13 Mon 18:15 H20

Altermagnetism in twisted magnetic bilayers — •Venkata Krishna Bharadwaj[1], Libor Šmejkal[1,2], and Jairo Sinova[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A recent development in the field of magnetism has introduced a new category of magnetic materials known as altermagnets [1]. These materials form a distinct class of magnetic compounds, characterized by magnetic compensation and the breaking of time-reversal symmetry, leading to a spin-split band structure. This unique band structure exhibits alternating spin polarization in both real and reciprocal spaces. The spin splitting originates from variations in local crystal field anisotropies across different magnetic sublattices. In this study, we introduce a novel approach to achieve altermagnetism in two-dimensional van der Waals materials by twisting bilayers. Furthermore, we explore the physical properties of altermagnets arising in these twisted bilayer structures. Our results lay the groundwork for exploring new possibilities in altermagnetic materials.

[1] L. Šmejkal, et al., Phys. Rev. X 12, 031042 (2022).

MA 10: Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II (joint session MA/TT)

The magnetic moment of the electron lies at the heart of magnetism and spintronics. However, recent research has unveiled the angular momentum and magnetic moment of chiral phonons as fundamental quantities in their own right. These chiral phonons give rise to a plethora of novel lattice phenomena analogous to electronic effects, such as the phonon Hall and phonon Zeeman effects. Moreover, they play a critical role in angular momentum transfer on ultrafast timescales, as seen in the Einstein-de Haas effect. Chiral phonons can also generate effective magnetic fields reaching the tesla scale, inducing magnetization in antiferromagnetic, paramagnetic, and even nonmagnetic materials - a phenomenon reminiscent of the Barnett effect. These advancements showcase phonon chirality and angular momentum as powerful emerging tools for generating and controlling magnetism. This focus session aims to highlight the latest breakthroughs in chiral-phonon magnetism and foster connections between the rapidly evolving field of chiral phononics and the broader magnetism research community.

Coordinators: Dominik M.Juraschek, Eindhoven University of Technology, d.m.juraschek@tue.nl; Martina Basini, ETH Zürich, m.basini@ethz.ch

Time: Tuesday 9:30–12:45 Location: H16

MA 10.1 Tue 9:30 H16

Continuous-wave terahertz spectroscopy on chiral phonons — •Ji Eun Lee, Luca Eisele, Artem Pronin, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

We apply continuous-wave frequency-domain terahertz spectroscopy to study chiral phonons at low frequencies. As samples, we use thin films of materials with soft phonon modes, such as SrTiO3 and (doped) PbTe. Our experimental method utilizes both, measurements of transmission with circular-polarized light and Faraday-rotation experiments. In the talk, our approach to the measurements and preliminary results will be summarized.

MA 10.2 Tue 9:45 H16

Spin-lattice coupling in multiscale modeling: from angular momentum transfer to chiral phonons — •Markus Weissenhofer[1,2], Philipp Rieger[1], Sergiy Mankovsky[3], Akashdeep Kamra[5], MS Mrudul[1], Hubert Ebert[3], Ulrich Nowak[4], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]Freie Universität Berlin, Berlin, Germany — [3]Ludwig Maximilian Universität, München, Germany — [4]Universität Konstanz, Konstanz, Germany — [5]Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Kaiserslautern, Germany

Transfer and manipulation of angular momentum is a key aspect in spintronics. Recently, it has been shown that angular momentum transfer between spins and lattice is possible on ultrashort timescales [1]. To contribute to the understanding of this transfer, we have developed a theoretical multiscale framework for spin-lattice coupling, which is linked to ab-initio calculations on the one hand

and magnetoelastic continuum theory on the other [2], allowing for the study of a wide range of magnetomechanical phenomena. Here I will discuss how this framework can be used to calculate magnon-phonon coupling parameters, emphasizing the importance of a Dzyaloshinskii-Moriya type interaction for angular momentum transfer [2] and revealing the existence of chiral phonons in iron arising from a chirality-selective coupling [3]. [1] Tauchert al., Nature 602, 73 (2022); Luo et al., Science 382, 698 (2023). [2] Mankovsky et al., PRL 129, 067202 (2022); Weißenhofer et al., PRB 108, L060404 (2023). [3] Weißenhofer et al., arXiv:2411.03879.

MA 10.3 Tue 10:00 H16

Chiral phonon-induced magnetization reversal in 2D ferromagnets — •Daniel Bustamante Lopez[1] and Dominik Juraschek[2] — [1]Department of Physics, Boston University, Boston, Massachusetts 02215, USA — [2]Department of Applied Physics and Science Education, Eindhoven University of Technology, Eindhoven, Netherlands

In our previous work, we explored magnonic rectification, where a coherently excited chiral phonon generates an effective magnetic field capable of inducing quasistatic magnetization in antiferromagnetic materials. In this study, we extend this concept to ferromagnetic materials, demonstrating that phononic magnetic fields can achieve permanent magnetization reversal. We focus on two-dimensional chromium-based ferromagnetic crystals, including CrI3, CrGeTe3, and CrCl3, and investigate reversal mechanisms such as damping switching and precessional switching. Our findings reveal that phononic magnetic fields enable robust and permanent magnetization reversal within nanoseconds, highlighting their potential for ultrafast magnetic control.

MA 10.4 Tue 10:15 H16

Chiral phonons in coupled magnon-phonon band structure — •Yelyzaveta Borysenko, Daniel Schick, and Ulrich Nowak — University of Konstanz, Konstanz, Germany

Coupling of spin and lattice degrees of freedom in magnetic materials is a key aspect for angular momentum based information processing. During ultrafast demagnetization, spin angular momentum can be transferred into the lattice creating chiral phonons even in simple centrosymmetric materials [1]. Spin-lattice coupling mechanisms involved in such processes can be approached using first principles calculations, which allow to determine leading energy terms for angular momentum exchange for different materials [2, 3]. Coupled spin-lattice dynamics is then described constructing angular momentum-conserving Hamiltonian linked to ab initio calculated model parameters [4].

Here, we linearize the equations of motion and calculate coupled magnon-phonon dispersions. We discuss how different coupling terms, e.g., of anisotropy or Dzyaloshiskii-Moriya type, can modify magnon and phonon dispersions, open up energy gaps, lift the degeneracy of modes, and lead to avoided crossings in the band structure.

[1] S. R. Tauchert et al., Nature 602, 73 (2022); [2] S. Mankovsky et. al., Phys. Rev. Lett. 129, 067202 (2022); [3] J. Hellsvik et al., Phys. Rev. B 99, 104302 (2019); [4] M. Weißenhofer et al., Phys. Rev. B 108, L060404 (2023)

MA 10.5 Tue 10:30 H16

Phonon Inverse Faraday effect from electron-phonon coupling — •Natalia Shabala and Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

The phonon inverse Faraday effect describes the emergence of a DC magnetization due to circularly polarized phonons. From time-dependent second order perturbation theory and electron-phonon coupling we develop a microscopic formalism for phonon inverse Faraday effect. We arrive at a general and material-independent equation [1]. Using this equation for ferroelectric soft mode in $SrTiO_3$ gives an estimate of effective magnetic field which is consistent with recent experiments [2]. Hence, our approach is promising for shedding light into the microscopic mechanism of angular momentum transfer between ionic and electronic angular momentum, which is expected to play a central role in the phononic manipulation of magnetism.

[1] N. Shabala and R. M. Geilhufe, Accepted to PRL, arXiv:2405.09538, 2024
[2] M. Basini et al., Nature 628, 534 (2024)

MA 10.6 Tue 10:45 H16

Temperature dependent magnon-phonon coupling in YIG/GGG heterostructures — •J. Weber[1,2], M. Cherkasskii[3], F. Engelhardt[3,4,5], S.T.B. Goennenwein[6], S.Viola Kusminskiy[3,5], S. Geprägs[1], R. Gross[1,2,7], M. Althammer[1,2], and H. Huebl[1,2,7] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Munich, Germany — [3]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [4]Department of Physics, University Erlangen-Nuremberg, Erlangen, Germany — [5]Max Planck Institute for the Science of Light, Erlangen, Germany — [6]Department of Physics, University of Konstanz, Konstanz, Germany — [7]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Magnon-phonon coupling in heterostructures has recently gained interest in the context of angular momentum conversion and angular momentum transport via phonons. A typical experimental setting is a bilayer system, where the magnetization dynamics of a magnetic thin film interacts with the elastic standing wave excitations of a non-magnetic bulk crystal. So far, bulk acoustic wave resonators consisting of a ferrimagnetic yttrium iron garnet (YIG) film deposited on a crystalline gadolinium gallium garnet (GGG) substrate have been studied at room temperature due to the favorable magnetic damping properties of YIG [1]. We present a temperature dependent analysis of the magnon-phonon coupling of a YIG/GGG bulk acoustic wave resonator.

[1] K. An et al., Phys. Rev. B **101**, 060407, (2020).

15 min. break

MA 10.7 Tue 11:15 H16

Modeling of the preparation and conservation of coherent phonon (pseudo) angular momentum — •Olga Minakova[1], Maximilian Frenzel[1], Carolina Paiva[2], Joanna M. Urban[1], Michael S. Spencer[1], Martin Wolf[1], Dominik M. Juraschek[2,3], and Sebastian F. Maehrlein[1,4,5] — [1]FHI Berlin — [2]Tel Aviv University — [3]Eindhoven University of Technology — [4]HZDR — [5]TU Dresden

The angular momentum of lattice vibrations - phonon angular momentum - is an underexplored degree of freedom in solid-state systems. Recent experiments have shown that circularly-polarized THz pulses can coherently excite degenerate phonon modes, enabling the preparation of phonon angular momentum states. THz-Kerr effect spectroscopy provides a means to monitor these states by directly measuring vectorial phonon trajectories. To interpret such experiments, it is essential to understand the symmetry properties of the phonon modes that influence the driving and probing processes, as well as the conservation of angular momentum in the crystal lattice. Here, we model the generation and detection of coherent phonon angular momentum, revealing how crystal symmetry dictates the selection rules in the lattice. We show that the form of the Raman tensors associated with the phonon explains the phonon helicity observed in experiments, linking the discrete rotational symmetry of the material to the conservation of pseudo angular momentum in lattice vibrations.

MA 10.8 Tue 11:30 H16

Spin-spin interaction via chiral phonons — •Daniel Schick[1], Markus Weissenhofer[2,3], Akashdeep Kamra[4], and Ulrich Nowak[1] — [1]University of Konstanz, Konstanz, Germany — [2]Uppsala University, Uppsala, Sweden — [3]Free University of Berlin, Berlin, Germany — [4]University of Kaiserslautern-Landau, Kaiserslautern, Germany

Coupling between the magnetic degrees of freedom and phonons has emerged as a topic of great importance for explaining various magnetic phenomena, like ultrafast demagnetization processes [1], and the possibility to affect magnetization dynamics via phonon pumping [2]. We develop a tool to study spin-lattice coupling in atomistic simulations, which conserves total angular momentum. This allows us to precisely retrace the transfer of angular momentum between the spin and lattice systems. We demonstrate the emergence of an effective spin-spin interaction mediated by chiral phonons. This effect can arise from thermal phonons as follows. A spin may precess after coupling to a phonon, with this precession producing chiral phonons, which in turn, affect other spins. A similar effect can be achieved by driving a spin to induce chiral phonons. We discuss the dependence of this interaction on the temperature and strength of the spin-lattice interaction and discuss our findings within the context of phonon-enhanced magnon transport phenomena.

[1] S. R. Tauchert, et. al., Nature **602**, 73 (2022)
[2] R.Schlitz et. al. Phys. Rev. B **106**, 014407 (2022)

MA 10.9 Tue 11:45 H16

Ultrafast generation of multicolor chiral phonons in magnetic and ferroelectric materials — •Omer Yaniv[1] and Dominik M. Juraschek[2] — [1]Tel Aviv University, Tel Aviv, Israel — [2]Eindhoven University of Technology, Eindhoven, Netherlands

Terahertz pulses are powerful tools capable of initiating coherent vibrational motions in solids. Circularly polarized pulses can further excite chiral phonons. Such phonons carry an angular momentum and are able to generate magnetic moments leading to a varying range of phenomena, including the phonon Hall, phonon Zeeman, and phonon inverse Faraday effects. Our study investigates the coherent driving of phonons using multicolor laser pulses, leading to Lissajous trajectories of the atoms. We demonstrate the generation of such multicolor chiral phonons in BaTiO3, a task that presents significant challenges due to the requirement of an exact 1:2 phonon frequency ratio. Achieving this precise ratio is crucial for the generation of closed atomic Lissajous loops. However, we overcome this challenge by creating phonon polaritons with shifted frequencies through the use of optical cavities. This approach allows us to surpass the limitations imposed by the strict phonon frequency ratio. By carefully tuning the cavity parameters, we demonstrate a new pathway for controlling lattice vibrations at ultrafast timescales. We also explore how multicolor phonons tune magnetic properties in monolayer CrI3, a 2D material with strong spin-orbit

coupling and ferromagnetism. By manipulating phonon dynamics, we examine the interaction between lattice vibrations and magnetic order.

MA 10.10 Tue 12:00 H16

Chiral Phonons induced by Magnon-Phonon Coupling — •Hannah Bendin[1], Alexander Mook[2], Ingrid Mertig[1], and Robin R. Neumann[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Johannes Gutenberg University, Mainz, Germany

Chiral phonons, the quasiparticles of circularly polarized lattice vibrations, have recently been investigated due to a range of emerging phenomena. Notably, chiral phonons carry nonzero angular momentum. However, the systems in which they occur still require extensive research. Chiral phonons may, for example, be found in lattices with broken inversion symmetry. Alternatively, they can be induced by the coupling to magnons, the quasiparticles of spin excitations, thereby lifting time-reversal symmetry.

Here, we analyze how magnetoelastic coupling gives rise to magnon-phonon hybridization, which, in turn, generates phonon angular momentum. Conversely, we show how the phonon angular momentum and the spin of the magnons affects their coupling strength. This interplay between magnons and chiral phonons allows for the tunability of the phonon angular momentum.

MA 10.11 Tue 12:15 H16

Ultrafast laser-induced carrier and magnetization dynamics in $SrTiO_3$ from real-time time-dependent DFT — •Andri Darmawan, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Recent experimental studies indicate electric-field-driven ferroelectricity [1] and multiferroicity [2] in the paradigmatic nonmagnetic band insulator $SrTiO_3$ in the terahertz regime. Following a comprehensive study of the optical [3] and x-ray absorption [4] spectra including quasiparticle and excitonic effects, here we explore the response of $SrTiO_3$ to laser excitation. Using real-time time-dependent density functional theory (RT-TDDFT) as implemented in the Elk code, we investigate both linear and circular polarized laser pulses. A complex site- and orbital-dependent temporal dynamics is observed with opposite sign of fluctuations at O and Ti sites and charge transfer from O 2*p* to Ti 3*d* states for linearly polarized light, that breaks dynamically inversion symmetry. Notably, circularly polarized pulses induce a finite transient magnetic moment which is absent for linearly polarized pulses. Funding by DFG within CRC1242 (project C02) and computational time at magnitUDE, amplitUDE and the Leibniz Supercomputer Center (project pr87ro) are gratefully acknowledged.

[1] T.F. Nova et al., Science 364, 1075 (2019)
[2] M. Basini et al., Nature 628, 534 (2024)
[3] V. Begum, M.E. Gruner and R. Pentcheva, Phys. Rev. Mater. 3, 065004 (2019)
[4] V. Begum-Hudde et al., Phys. Rev. Res. 5, 013199 (2023)

MA 10.12 Tue 12:30 H16

Phonon pumping in ferromagnet/nonmagnetic insulator hybrid systems — •Richard Schlitz[1], Luise Holder[1], Johannes Weber[2,3], Mikhail Cherkasskii[4], Fabian Engelhardt[4], Julie Střihavková[5], Matthias Althammer[2,3], Silvia V. Kusminskiy[4,6], Hans Huebl[2,3,7], and Sebastian T. B. Goennenwein[1] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Walther-Meißner-Institut, BAdW, Garching, Germany — [3]School of Natural Sciences, TUM, Garching, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [5]Faculty of Mathematics and Physics, Charles University, Prague — [6]Max Planck Institute for the Science of Light, Erlangen, Germany — [7]Munich Center for Quantum Science and Technology, München, Germany

In ferromagnetic thin films, magnetization dynamics, e.g., driven by ferromagnetic resonance, can coherently couple to phonons. If a ferromagnetic film is deposited on a crystalline substrate with polished parallel faces, the sample stack forms a bulk acoustic resonator, leading to characteristic modifications of the magnetic resonance signal.

In this work, we show that the magnetoelastic coupling can mediate the hybridization of the coherent magnetization dynamics with longitudinal and transverse phonons, with a particular dependence on the orientation of the magnetic field. We extract the magnetoelastic coupling parameters and compare them with theoretical expectations. Our results show that both longitudinal and transverse phonons can be efficiently excited, depending on the magnetic field orientation.

MA 11: Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)

Time: Tuesday 9:30–13:15 Location: H18

MA 11.1 Tue 9:30 H18

Topological orbital Hall effect caused by skyrmions and antiferromagnetic skyrmions — •Lennart Schimpf, Ingrid Mertig, and Börge Göbel — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The topological Hall effect is a hallmark of topologically non-trivial magnetic textures such as magnetic skyrmions. It quantifies the transverse electric current once an electric field is applied and occurs as a consequence of the emergent magnetic field of the skyrmion. Likewise, an orbital magnetization is generated. Here we show that the charge currents are orbital polarized even though the conduction electrons couple to the skyrmion texture via their spin [1]. The topological Hall effect is accompanied by a topological orbital Hall effect even for *s* electrons without spin-orbit coupling. As we show, antiferromagnetic skyrmions and antiferromagnetic bimerons that have a compensated emergent field [2], exhibit a topological orbital Hall conductivity that is not accompanied by charge transport and can be orders of magnitude larger than the topological spin Hall conductivity.

[1] B. Göbel, L. Schimpf, I. Mertig, arXiv pre-print: 2410.00820
[2] B. Göbel, I. Mertig, O. Tretiakov, Physics Reports 895, 1 (2021)

MA 11.2 Tue 9:45 H18

Optimization of orbital torques in ferrimagnets and their relationship with Gilbert damping — •shilei ding, william legrand, hanchen wang, mingu kang, paul noel, and pietro gambardella — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Application of an electric field can induce a non-equilibrium orbital angular momentum in conductive materials whose electronic bands have a k-dependent orbital character. This phenomenon can lead to the current-induced accumulation of orbital momenta in nonmagnetic layers, which can then diffuse into neighboring magnetic layers and interact with the local magnetization through spin-orbit coupling, giving rise to orbital torques. Conversely, the excitation of spin precession in a magnetic layer can give rise to an orbital current, resulting in orbital pumping and dissipation of angular momentum in the nonmagnetic layer. In the first part, I will present the efficacy of converting orbital to spin momenta in ferrimagnetic materials, specifically in the RE-TM ferrimagnet GdyCo100-y. This work underscores the mechanisms that facilitate orbital-to-spin conversion within a magnetic layer at the atomic level. In the second part, I will discuss how the Gilbert damping parameter correlates to spin and orbital torques in magnetic layers adjacent to Pt and CuOx layers, respectively. I will show that CoFe/CuOx bilayers exhibit a favorable combination of efficient orbital torque and minimal increase in Gilbert damping, which is promising for the implementation of orbital torque oscillators with reduced damping compared to spin torque oscillators.

MA 11.3 Tue 10:00 H18

Orbital magnetoresistance in insulating antiferromagnets — •Christin Schmitt[1], Sachin Krishnia[1], Edgar Galíndez Ruales[1], Takashi Kikkawa[2], Duc Tran[1], Timo Kuschel[1], Eiji Saitoh[2], Yuriy Mokrousov[1,3], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, 55128 Mainz, Germany — [2]Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Insulating antiferromagnetic and ferrimagnetic materials are promising candidates for spintronic devices due to their intrinsic properties such as low damping [1]. Recently, orbital angular momentum (OAM) has emerged as a crucial concept in condensed-matter physics. Theoretical and experimental studies have highlighted that the orbital Hall effect (OHE) can enable orbital currents with efficiency orders of magnitude higher than that of spin Hall effects [2]. Here, we investigate magneto-resistance effects in magnetic systems [2,3]. We find that in TmIG the transverse magnetoresistance signal is increased significantly upon replacing Pt, a spin-current generator, by Cu*, a pure orbital-current generator. Further, we explore antiferromagnets with orbital magnetoresistance effects as pure orbital current is crucial for next generation pure orbitronics devices using abundant, cheap and environmentally friendly materials.

[1] R. Lebrun, et al., Nature, 561, 222-225 (2018).
[2] S. Ding, et al., Phys. Rev. Lett. 125, 177201 (2020).
[3] S. Ding et al., Phys. Rev. Lett. 128, 067201 (2022).

MA 11.4 Tue 10:15 H18

Non-reciprocity in magnon mediated charge-spin-orbital current interconversion — •Sachin Krishnia[1], Omar Ledesma-Martin[1], Edgar Galindez-Ruales[1], Felix Fuhrmann[1], Duc Tran[1], Rahul Gupta[1], Marcel Gasser[1,2], Dongwook Go[1,2], Gerhard Jakob[1], Yuriy Mokrousov[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099

Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In magnetic systems, angular momentum is carried by the spin and orbital degrees of freedom. Non-local devices can be used to study angular momentum transport. They consist of parallel heavy-metal nanowires placed on top of magnetic insulators like yttrium iron garnet (YIG), facilitating the transmission of information by magnons, generated by the accumulation of spin at the interface, created via the spin Hall effect (SHE) and detected via the inverse SHE (iSHE). It has been demonstrated that these processes have comparable efficiencies when the role of the detector and injector is reversed, which points to reciprocity of the processes. However, we show that by adding Ru as a source of direct and inverse orbital Hall effect (OHE), the system no longer exhibits this reciprocity. Specifically, the generation of magnons via the combination of SHE and OHE and detection via the iSHE is found to be about 35% more efficient than the inverse process for our system [1]. [1] O. Ledesma et al., arXiv:2411.07044 (2024).

MA 11.5 Tue 10:30 H18

Detection of dynamic x-ray magnetic linear dichroism in NiO — •Timo Kuschel[1], Johannes Demir[1], Olga Kuschel[2], Joachim Wollschläger[2], and Christoph Klewe[3] — [1]Bielefeld University, Germany — [2]Osnabrück University, Germany — [3]Advanced Light Source (ALS), Berkeley, USA

Spin transport through thin antiferromagnetic layers such as NiO has been studied by ferromagnetic resonance (FMR) spin pumping [1], spin Seebeck effect [2], non-local magnon spin transport [3] and x-ray detected FMR (XFMR) [4]. In all these experiments, the spin current has been identified in an adjacent Pt layer [1-3] or FeCo film [4] via inverse spin Hall effect or dynamic x-ray magnetic *circular* dichroism, respectively, after having the NiO layer already passed.

In this contribution, we study Fe_3O_4/NiO/Pt [5] by XFMR and present the identification of dynamic x-ray magnetic *linear* dichroism (XMLD) [6] at the Ni L edges directly in the NiO layer for FMR spin pumping in the adjacent Fe_3O_4 layer. We will analyze the XFMR response depending on the NiO thickness. Further, we will discuss coupling phenomena at the NiO-Fe_3O_4 interface vs. spin transport through the NiO layer as the origin of the dynamic XMLD response.

[1] H. L. Wang et al., Phys. Rev. Lett. 113, 097202 (2014)
[2] W. Lin et al., Phys. Rev. Lett. 116, 186601 (2016)
[3] G. R. Hoogeboom et al., Phys. Rev. B 103, 144406 (2021)
[4] M. Dabrowski et al., Phys. Rev. Lett. 124, 217201 (2020)
[5] L. Baldrati et al., Phys. Rev. B 98, 014409 (2018)
[6] C. Klewe et al., New J. Phys. 24, 013030 (2022)

MA 11.6 Tue 10:45 H18

Manipulating the sign of the interlayer exchange coupling — •Nathan Walker — The Open University, Milton Keynes, UK

We demonstrate, using computer simulations and a non-equilibrium Greens function approach, that the sign of the out-of-equilibrium interlayer exchange coupling (ooeIEC) changes in the presence of an external bias. The system consists of a double barrier connected to an exchange coupled ferromagnetic trilayer. We find a strongly non-linear dependence of the spin current on voltage which results in the exchange coupled tri-layer switching between parallel and antiparallel configurations. Our results are in excellent agreement with earlier theoretical calculations, which predict an approximately 2π topological phase change of the (equilibrium) IEC. We believe that this could act as an energy efficient mechanism for magnetic switching which does not rely on spin-transfer torque (STT). There are potential applications to magnetoresistive random-access memory (MRAM), one of the principal contenders for a universal memory.

MA 11.7 Tue 11:00 H18

Harnessing Orbital Hall Effect in Spin-Orbit Torque MRAM — •J. Omar Ledesma Martin[1,2], Rahul Gupta[1], Chloé Bouard[2], Fabian Kammerbauer[1], Iryna Kononenko[1], Sylvain Martin[2], Gerhard Jakob[1,3], Marc Drouard[2], and Mathias Kläui[1,3] — [1]1 Institute of Physics, Johannes Gutenberg University Mainz, 55099, Mainz, Germany — [2]Staudingerweg 7 — [3]Department of Physics, Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491, Trondheim, Norway

There is considerable potential in the Orbital Hall Effect (OHE) and the Spin Hall Effect (SHE) as electrical means for controlling the magnetization of spintronic devices. Here Ru stands out exhibiting an orbital Hall conductivity four times greater than the spin Hall conductivity of Pt. [1] This work assesses the efficiency of four distinct stacks in devices with perpendicular Magnetic Tunnel Junctions (MTJ). Following the formula Ta/OHE/Pt/[Co/Ni]x3/Co/MgO/CoFeB/Ta/Ru, where the OHE materials are Ru, Nb, and Cr. Additionally, a sample with Pt instead of OHE serves as a reference. The results demonstrate an improvement for the Ru samples, exhibiting higher damping-like torque and significantly lower switching current density compared to both the other samples and the Pt reference. These findings, including first-principle calculations, underscore the potential of Ru as an OHE material for enhancing the performance and power consumption of spintronic devices.

[1] R. Gupta et al., arXiv:2404.02821 (2024). Nature Comm. In press (2024)

15 min. break

MA 11.8 Tue 11:30 H18

Spin and orbital Hall effect in metal systems: extrinsic vs. intrinsic contributions — •Sergiy Mankovsky and Hubert Ebert — LMU of Munich, 81377 Munich, Germany

Kubo's linear response formalism has been used to study the orbital Hall effect (OHE) for non-magnetic undoped and doped metallic systems, focusing on the impact of different types of disorder. Corresponding first-principles calculations of the orbital Hall conductivity (OHC) were performed making use of the KKR Green function method that allows in particular to monitor the impact of the vertex corrections on the OHC. The doping- and temperature-dependence of the OHC have been investigated and compared with corresponding results for the spin Hall conductivity (SHC). The temperature dependent properties of the OHC and SHC determined by thermally induced lattice vibrations (in non-magnetic materials) and spin fluctuations (in magnetic systems) have been accounted for making use of the alloy analogy model. For elemental systems at finite temperature a dominating role of the intrinsic contribution to the temperature-dependent OH and SH conductivities is found. In contrast, the OH and SH conductivities of doped systems at low temperatures are dominated by the SOC-driven extrinsic contributions strongly decreasing at higher temperatures due to the increasing impact of the electron-phonon scattering.

MA 11.9 Tue 11:45 H18

Simulations of spin transport in YIG — •Ben Schwanewedel, Moumita Kundu, and Ulrich Konstanz — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Being synthesized first in 1957, YIG has the lowest Gilbert damping among all known materials. This makes it interesting for spintronic applications and long-range spin transport. In YIG's complex unit cell Fe atoms occupy 20 sublattices leading to 20 magnon bands between 0 and 25 THz. We develop an atomistic spin model for YIG based on exchange interactions from Ref. [1], which were determined through neutron scattering. Further parameters were adapted from Ref. [2]. We varify our study through investigation of the magnon dispersion and comparing it to the results of Ref. [1].

We use atomistic spin dynamics simulations for the model above based on the stochastic Landau-Lifshitz-Gilbert equation to unravel its spin dynamics and spin transport properties. The spin transport is triggered by thermal gradients and and local magnetic fields and it is analyzed using an observable which is proportional to the magnon population. Also, magnon dispersions far from equilibrium are evaluated and discussed.

[1] Princep, Andrew J., et al. "The full magnon spectrum of yttrium iron garnet." npj Quantum Materials 2.1 (2017): 63.

[2] Barker, Joseph, and Gerrit EW Bauer. "Thermal spin dynamics of yttrium iron garnet." Physical review letters 117.21 (2016): 217201.

MA 11.10 Tue 12:00 H18

Orbital Hall effect accompanying quantum Hall effect — •Börge Göbel and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The quantum Hall effect emerges when two-dimensional samples are subjected to strong magnetic fields at low temperatures: Topologically protected edge states cause a quantized Hall conductivity in multiples of e^2/h. Here we show that the quantum Hall effect is accompanied by an orbital Hall effect [1]. Our quantum mechanical calculations fit well the semiclassical interpretation in terms of "skipping orbits". The chiral edge states of a quantum Hall system are orbital polarized akin to an orbital version of the quantum anomalous Hall effect in magnetic systems. The orbital Hall resistivity scales quadratically with the magnetic field making it the dominant effect at high fields.

The discussion can be generalized to systems with effective magnetic fields: The topological Hall effect caused by the emergent field of topological spin textures, such as magnetic skyrmions, is accompanied by an orbital Hall effect, as well [2].

[1] B. Göbel, I. Mertig, Phys. Rev. Lett. 133, 146301 (2024)
[2] B. Göbel, L. Schimpf, I. Mertig, arXiv pre-print: 2410.00820

MA 11.11 Tue 12:15 H18

Large Spin Hall Angle in Mn-based Antiferromagnetic Alloys — •Nabil Menai[1], Martin Gradhand[2], and Derek Stewart[3] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, BS8-1TL, UK — [2]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [3]Western Digital Research Center, San Jose, California 95119, USA

Antiferromagnets (AFMs) have emerged as crucial materials for spintronic technologies for their ability to host spin-dependent transport phenomena, despite their zero net magnetization. Their robustness against external magnetic fields and ultrafast spin dynamics make them ideal for efficient spin-charge interconversion. In this theoretical study, we use density functional theory and Greens function methods to investigate the transport properties of Mn-based binary alloyed AFMs. Our focus is on the total spin Hall conductivity (SHC), account-

ing for both the intrinsic contributions from Berry curvature and the extrinsic effects from skew scattering and side-jump mechanisms. The objective is to identify AFM materials that exhibits a high spin Hall angle (SHA); with an efficient charge-to-spin Hall current conversion ratio. Our results reveal that doping MnPt with Ir significantly enhances the SHA, achieving a value of 8% at room temperature. In contrast, doping with Pd offers temperature stability with lower SHA values. Additionally, we examine the effects of substituting Mn atoms with magnetic transition metals such as Fe and Ni. These findings underscore the potential of antiferromagnetic alloys for efficient spin current generation.

MA 11.12 Tue 12:30 H18

Competing ordinary and Hanle magnetoresistance in Pt and Ti thin films — •Sebastian Sailler[1], Giacomo Sala[2], Denise Reustlen[1], Richard Schlitz[1], Min-Gu Kang[2], Pietro Gambardella[2], Sebastian T.B. Goennenwein[1], and Michaela Lammel[1] — [1]Department of Physics, University of Konstanz — [2]Department of Materials, ETH Zurich

One of the key elements in spintronics research is the spin Hall effect, allowing to generate spin currents from charge currents. A large spin Hall effect is observed in materials with strong spin orbit coupling, e.g. Pt. Recent research suggests the existence of an orbital Hall effect, the orbital analogue to the spin Hall effect, which also arises in weakly spin orbit coupled materials like Ti, Mn or Cr. In any of these materials, a magnetic field perpendicular to the spin or orbital accumulation leads to additional Hanle dephasing and thereby the Hanle magnetoresistance. Here, we studied the magnetoresistance (MR) of Pt thin films over a wide range of thicknesses. Careful evaluation shows that the MR of our textured samples is dominated by the so-called ordinary MR, while the Hanle effect does not play a significant role. Analyzing the intrinsic properties of Pt films deposited by different groups, we find that next to the resistivity, also the structural properties of the film influence which MR dominates. We further show that this correlation can also be found in orbital Hall active materials like Ti. We conclude that in all materials exhibiting a spin or orbital Hall effect, the Hanle MR and the ordinary MR coexist, and that the sample's purity and crystallinity determines which MR dominates.

MA 11.13 Tue 12:45 H18

Orbital Hanle magnetoresistance in Mn thin films — •Min-Gu Kang, Federica Nasr, Giacomo Sala, and Pietro Gambardella — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Momentum-space orbital texture, or orbital character of electrons, enables the orbital Hall effect (OHE), a current-induced flow of nonequilibrium orbital angular momentum in centrosymmetric systems with negligible spin-orbit coupling. This orbital current, which can be orders of magnitude larger than its spin counterpart, offers transformative potential for spin-orbitronics, yet the mechanisms of orbital relaxation remain unclear. In this work, we present temperature-dependent orbital Hanle magnetoresistance and associated orbital relaxation mechanisms in Mn thin films. The results clearly show that the orbital Hanle magnetoresistance depends on the structure of the Mn thin films and can be associated with competing Dyakonov-Perel and Elliott-Yafet orbital relaxation effects. Our study highlights the critical role of orbital relaxation in determining the magnitude of current-induced orbital effects in 3d transition metal films.

MA 11.14 Tue 13:00 H18

Tuning of spin transport properties in 2D ferromagnet VSe_2 by structural polytypes of TaS_2 electrodes — •Biplab Sanyal and Masoumeh Davoudiniya — Department of Physics & Astronomy, Ångströmlaboratoriet, Uppsala University, Box-516, 75120 Uppsala, Sweden

2D magnets and their heterostructures are promising materials for future spintronic applications. Here, we present a study of spin transport through a ferromagnetic monolayer of 1T-VSe_2 with two structural polytypes of TaS_2 electrodes stacked in van der Waals heterostructures. Using density functional theory coupled with the nonequilibrium Green function framework, we explore the impact of TaS_2 electrode polytypes on the device's quantum transport properties. We observe that devices with 1T-TaS_2 electrodes exhibit higher spin-dependent transmission compared to 2H-TaS_2 electrodes. Incorporating MoS_2 as a tunnel barrier, anisotropic tunnel magnetoresistance enhances significantly, reaching 168% for the 1T-device and 1419% for the 2H-device. Spin-transfer torque (STT) analysis shows that its magnitude is highest at 90° (−702 μeV/V for 1T and −1561 μeV/V for 2H devices) and decreases towards 180°. The 1T-device shows superior performance with lower Gilbert damping, reduced critical current density and voltage for magnetization switching, compared to the 2H-device, which requires significantly higher current and voltage. Our predictions reveal the potential of 1T-VSe_2-based heterostructures for advanced spintronic applications.

MA 12: Magnetization Dynamics and Damping

Time: Tuesday 9:30–11:30 Location: H19

MA 12.1 Tue 9:30 H19

Oscillatory dynamics of strongly coupled magnetic domain walls in three-dimensional chiral nanostructures — •Pamela Morales Fernández[1,2], I. Konstantinos Douveas[3], S. Ruiz Gómez[4], E. Zhakina[1], L. Turnbull[1], M. König[1], A. Hierro Rodríguez[5], N. Leo[6], S. Finizio[7], S. Wintz[8], C. Abert[3], D. Suess[3], A. Fernández Pacheco[2], and C. Donnelly[1,9] — [1]MPI CPFS, Germany — [2]TU Viena, Austria — [3]University of Vienna, Austria — [4]ALBA Synchrotron, Spain — [5]Universidad de Oviedo, Spain — [6]Loughborough University, UK — [7]PSI, Switzerland — [8]BESSY II, Germany — [9]Hiroshima University, Japan.

The expansion of nanomagnetism into three dimensions opens opportunities for new topological textures, curvilinear effects, and exotic magnetization dynamics. Here, we investigate the magnetization dynamics in 3D double-helix nanostructures, which host strongly coupled domain wall pairs formed through the interplay of shape anisotropy, chirality, and inter-helix magnetostatic interactions. Using direct 3D nanofabrication techniques, cobalt nano double helices are grown on top of microwave antennas and exposed to GHz magnetic fields. Time-resolved scanning transmission X-ray microscopy reveals enhanced dynamics in the area of the coupled domain walls within the helical conduits. Observed dynamics depend on the geometrical parameters of the system and excitation frequency, matching with micromagnetic simulations that reveal additional higher-frequency modes beyond the reach of the experimental technique. This work provides insights into the physics of 3D nanomagnetism, advancing control for future technologies.

MA 12.2 Tue 9:45 H19

Anisotropic energy dissipation in model Kagome systems — Rajgowrav Cheenikundil[1], Zhiwei Lu[2], Ivan Miranda[3], Manuel Pereiro[4], and •Danny Thonig[1,4] — [1]Örebro University, Sweden — [2]KTH Royal Institute of Technology, Sweden — [3]Linnaeus University, Sweden — [4]University Uppsala, Sweden

Recent efforts have been directed towards understanding spin-orbit mediated phenomena such as the spin Hall effect [1], and energy dissipation phenomena [2], which are enhanced by non-collinear magnetism. Notably, the latter results in anisotropies in energy dissipation that have not been methodically investigated.

We employ the Kubo-Bastin formalism [3] of linear perturbation theory to calculate the non-local Gilbert damping tensor in a model Kagome system with Rashba spin-orbit coupling. This approach is implemented in the Cahmd code [4]. We vary the magnetic state according to different chiralities and phase differences.

Remarkably, the Bastin formalism connects the occurrence of anisotropic damping to a Fermi-sea contribution and, consequently, to spin-spin Berry curvature. Our systematic study examines the dependency of isotropic and anisotropic effective damping, as well as the full non-local damping, on electron lifetimes, Rashba parameters, and other factors. The results of this study pave the way for controlled dissipation in innovative spintronics applications.

[1] Scientific Reports 6, 28076 (2016); [2] Phys. Rev. Lett. 113, 266603 (2014); [3] Phys. Rev. B 102, 085113 (2020); [4] available at https://cahmd.gitlab.io/cahmdweb/

MA 12.3 Tue 10:00 H19

propelling ferrimagnetic domain walls by dynamical frustration — •reza doostani — university of cologne, cologne, germany

In this work, we realize the concept of active matter in a solid state system. By sending a ferrimagnet out of equilibrium by an oscillating magnetic field, we activate rotational goldstone mode where spins start to rotate clockwise or anticlockwise depending on the ferromagnetic component. We see that in this setup, a domain wall moves actively to the left or right due to dynamical frustration. We further discuss the dynamics of these domain walls and the relation between domain wall motion and the external field amplitude, as well as their interaction and consequence of these on the whole system. Furthermore, we continue to study the effect of defects on the movement of domain walls.

MA 12.4 Tue 10:15 H19

Tunable magnetic easy axis orientation with ion irradiation — •Gabriel Gray[1], Kilian Lenz[1], Alexandra Lindner[1], Jürgen Lindner[1], Jürgen Fassbender[1], Fabian Ganss[1], Rodolfo Gallardo[2], and Pedro Landeros[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Material Research, Dresden, Germany — [2]Universidad Técnica Federico Santa María, Department of Physics, Valparaíso, Chile

Our research focuses on the ion-irradiation-induced changes in magneto-crystalline anisotropy and exchange coupling in epitaxially grown Fe thin films in the (110) orientation under ultra-high vacuum conditions on GaAs (110) single crystals. A Cr capping layer was deposited to prevent oxidation. The samples were irradiated with Cr ions at varying kinetic energies and fluences. Subsequent magnetic characterizations were performed using Ferromagnetic Resonance and Vibrating Sample Magnetometry techniques, while structural characterizations where perform using X-ray Diffractometry and Transmission Electron Microscopy.

Our results reveal a clear correlation between ion fluence and modifications in uniaxial magneto-crystalline anisotropy, while cubic anisotropy and the effective magnetization remain largely unaffected. Notably, the observed changes are sufficient to induce a reorientation of the easy axis of magnetization in the system.

MA 12.5 Tue 10:30 H19

Evidence of relativistic field-derivative torque in nonlinear THz response of magnetization dynamics — •Arpita Dutta[1], Christian Tzschaschel[2,3], Debankit Priyadarshi[3], Kouki Mikuni[4], Takuya Satoh[4,5], Ritwik Mondal[6], and Shovon Pal[1] — [1]NISER Bhubaneswar, HBNI, Jatni, India — [2]Max-Born Institute, Berlin, Germany — [3]ETH Zurich, Switzerland — [4]Institute of Science Tokyo, Japan — [5]Quantum Research Center for Chirality, Okazaki, Japan — [6]IIT (ISM) Dhanbad, India

The selective addressing of spins by terahertz (THz) electromagnetic fields via Zeeman torque is, by far, one of the most successful means of controlling magnetic excitations. Here, we show that the conventional Zeeman torque on the spin is not sufficient, rather an additional relativistic field derivative torque (FDT) is essential to realize the observed magnetization dynamics. We accomplish this by exploring the ultrafast nonlinear magnetization dynamics of a ferrimagnetic garnet when excited by two co-propagating THz pulses. Having identified the Kaplan-Kittel mode at 0.48 THz, resulting from the exchange interaction between the rare-earth and transition metal sublattices, we drive this mode to a nonlinear regime. We find that the observed nonlinear trace of the magnetic response cannot be mapped to the magnetization precession induced by the Zeeman torque, while the Zeeman torque supplemented by an additional FDT follows the experimental evidences.

[1] A. Dutta, *et al.*, Phys. Rev. Materials **8**, 114404 (2024).
[2] A. Dutta, *et al.*, arXiv:2408.05510 (2024).

MA 12.6 Tue 10:45 H19

Ferromagnetic resonance linewidth as a probe for investigating magnon-phonon interaction — •Gauravkumar Patel[1], Rodolfo Gallardo[2], Ruslan Salikhov[1], Sven Stienen[1], Kilian Lenz[1], Olav Hellwig[1,3], and Jürgen Lindner[1] — [1]Helmholtz-Zentrum Dresden–Rossendorf, Dresden, Germany — [2]Universidad Técnica Federico Santa María, Valpariso, Chille — [3]Chemnitz University of Technology, 09107 Chemnitz

The Ferromagnetic resonance (FMR) linewidth measurements provide information about dynamic energy losses present in magnetic materials. For materials with high magnetoelastic coupling strength, like Co, the uniform precession can excite the elastic vibrations in the underlying lattice. Using the FMR linewidth as a probe, we investigate this magnon-phonon interaction in Co thin films on Pt seed layers. This interaction results in a non-monotonic behavior of the linewidth as a function of frequency, showing multiple peaks at specific frequencies, in contrast to the typical Gilbert-like linear dependence. The magnon-phonon coupling is more pronounced in Co thin films with higher perpendicular anisotropy. Variation of the Co or Pt layer thickness shifts the linewidth peak position, indicating control over the frequency of the generated phonon.

MA 12.7 Tue 11:00 H19

Landau-Lifshitz damping from Lindbladian dissipation in quantum magnets — •Götz Uhrig — TU Dortmund University

As of now, the phenomenological classical Landau-Lifshitz (LL) damping of magnetic order is not linked to the established quantum theory of dissipation based on the Lindbladian master equation. This is an unsatisfactory conceptual caveat for the booming research on magnetic dynamics. Here, it is shown that LL dynamics can be systematically derived from Lindbladian dynamics using a local mean-field theory. Thereby, the successful LL approach is set on a firm quantum basis in the regime where the Lindblad approach is applicable. Furthermore, we extend the LL dynamics in a systematically controlled way to include not only changes of the orientation of the magnetization $\vec{m}$, but also of its length $|\vec{m}|$. The key aspect is that the Lindbladian relaxation must be adapted to the Hamiltonian $H(t)$ at each instant of time in time-dependent non-equilibrium systems. It is conjectured that this idea holds true well beyond the damping of magnetic dynamics given the appropriate hierarchy of time scales.

MA 12.8 Tue 11:15 H19

Dynamics of electronic phase separation at the laser-induced insulator/metal transition in LPCMO — •Maximilian Staabs, Tim Titze, Karen Stroh, Stefan Mathias, Vasily Moshnyaga, and Daniel Steil — I. Physikalisches Institut, Universität Göttingen, Göttingen, Deutschland

The closely related colossal magnetoresistive manganites LCMO and LPCMO exhibit surprising differences in their transient reflectivity dynamics after nanosecond pulsed laser excitation close to their metal-to-insulator transition (MIT). Transient resistance measurements reveal that both systems show transient metallization effects upon laser excitation in the vicinity of the static MIT. These are, however, weak and on the timescale of the laser pulse for LCMO, but much stronger and long-lived for LPCMO. We attribute the differences between these compounds to the presence of mesoscopic electronic phase separation in LPCMO in the MIT region, stabilized by Jahn-Teller polarons [1]. Laser excitation leads to the annihilation of Jahn-Teller distortions [2,3], thus enabling charge transfer between the formerly separated electronic phases. This process is observed as a collapse of the global electrical resistivity on the nanosecond timescale, whereas the recovery of the insulating phase separated state takes nearly 20 nanoseconds [4].

[1] V. Moshnyaga *et al.*, Phys. Rev. B **89**, 024420 (2014)
[2] M. Fiebig *et al.*, Appl. Phys. B **71**, 211 (2000)
[3] H. Matsuzaki *et al.*, Phys. Rev. B **79**, 235131 (2009)
[4] T. Titze *et al.*, Phys. Rev. Research **6**, 043168 (2024)

MA 13: Altermagnets II

Time: Tuesday 9:30–13:00 Location: H20

MA 13.1 Tue 9:30 H20

Dynamics of the altermagnetic candidate compound UCr_2Si_2C — Nikolaos Biniskos[1], •Manuel dos Santos Dias[2], Karin Schmalzl[3], Andrea Piovano[4], Ursula Bengaard Hansen[4], Michal Vališka[1], and Petr Čermák[1] — [1]Department of Condensed Matter Physics, Charles University, Praha, Czech Republic — [2]Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom — [3]Jülich Centre for Neutron Science at ILL, Forschungszentrum Jülich, Grenoble, France — [4]Institut Laue-Langevin, Grenoble, France

Altermagnets are collinear antiferromagnets where spin degeneracy of the electronic bands or degeneracy of the magnon bands is not enforced by symmetry, potentially enabling diverse physical phenomena. However, it remains challenging to find materials that experimentally exhibit the hallmarks of altermagnetism. UCr_2Si_2C has been recently reported as a high-temperature antiferromagnet with a rare crystal structure that is compatible with altermagnetism [1]. This talk will report on our combined experimental and theoretical investigation of this compound. A large single crystal was successfully grown and experimentally investigated with bulk specific heat and magnetic susceptibility measurements, and through unpolarized and polarized inelastic neutron scattering. These experimental results have been interpreted with density functional theory calculations, providing a unified picture of UCr_2Si_2C and of its prospects as an altermagnet.

[1] Lemoine et al., Inorg. Chem. **57**, 2546-2557 (2018)

MA 13.2 Tue 9:45 H20

Theory of circular dichroism in resonant photoelectron diffraction of altermagnets — •Peter Krüger — Materials Science Dpt, Chiba University, Chiba 263-8522 Japan

Recently we have developed a computational method for resonant photoelectron diffraction (RPED) and its circular dichroism (CD) of magnetic surfaces, by combining ligand field multiplet and multiple scattering theory. The method was successfully tested for ferromagnetic Ni(111) [Phys. Rev. B 107, 075407 (2023)]. Here I apply the new method to the altermagnet MnTe. For a photon energy at the Mn L3-edge resonance and light incidence parallel to the magnetization axis, I show that there is a large, purely magnetic CD signal at the forward focusing peaks of the RPED pattern. This CD signal provides a direct probe of the staggered magnetization in altermagnets, which is closely related to the X-ray magnetic circular dichroism observed in ferromagnets.

MA 13.3 Tue 10:00 H20

New altermagnetic material candidates showing 4*f*-magnetism — •Franziska Walther[1], Johannes Fey[1], Michelle Ocker[1], Libor Šmejkal[2,3], Cornelius Krellner[1], and Kristin Kliemt[1] — [1]Physikalisches Institut, Goethe-Universität 60438 Frankfurt/Main — [2]Max Planck Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [3]Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz

Altermagnets are a novel class of collinear magnetic materials, which are characterised by a vanishing net magnetization while breaking the time-reversal symmetry in the electronic band structure with a unique alternating spin-momentum locking [1]. So far, altermagnetism has been proven for magnetic 3*d*-systems such as CrSb [2], MnTe [3] and Mn_5Si_3 [4] by the time-reversal breaking signature in the band structure or the observation of the anomalous Hall effect. In order to study the altermagnetism arising from local 4*f* moments, we have grown single crystals of lanthanoid-based intermetallic compounds and characterised their physical and chemical properties. We report on the crystal growth and measurements of magnetism, heat capacity and resistivity of the altermagnetic candidates.

[1] L. Šmejkal et al., Phys. Rev. X 12, 031042 (2022)
[2] S. Reimers et al., Nat. Commun. 15, 2116 (2024)
[3] J. Krempaský et al., Nature 626, 517 (2024)
[4] H. Reichlova et al., Nat. Commun. 15, 4961 (2024)

MA 13.4 Tue 10:15 H20

Altermagnetic properties of hematite. — •Edgar Galindez-Ruales[1], Rafael Gonzales-Hernandez[1,2], Gerhard Jakob[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany. — [2]Grupo de Investigacíon en Física Aplicada, Departamento de Física,Universidad del Norte, Barranquilla, Colombia.

Hematite, a prototypical antiferromagnet, has emerged as a promising altermagnet due to its unique magnetic and electronic properties[1]. Unlike conventional antiferromagnets, altermagnets exhibit a nonzero anomalous Hall effect (AHE) due to symmetry-breaking electronic structures despite having no net magnetization. In hematite, we observe anisotropic magnetotransport with a strong crystal orientation dependence, including a striking sign inversion in the Hall effect[2]. Using advanced XMCD and XMLD imaging, we directly visualize and distinguish 180° domains, confirming the interplay between collinear antiferromagnetism and non-centrosymmetric atomic arrangements that drive the altermagnetic behavior. These findings provide robust experimental evidence of hematite*s altermagnetic nature, offering new mechanisms for identifying altermagnetic candidates and establishing hematite as a model system for exploring altermagnetic phenomena. This work paves the way for utilizing altermagnetic materials in spintronic applications, revolutionizing our understanding of magnetic material classification and transport phenomena.

[1] L. Šmejkal et al., PRX 12, 040501 (2022).
[2] E. Galindez-Ruales et al., ArXiv:2310.16907 (2023).

MA 13.5 Tue 10:30 H20

Ferro-spinetic altermagnetic insulators from electronic correlations — •Toshihiro Sato[1,2], Ion Cosma Fulga[1,2], Fakher F. Assaad[3,2], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

While altermagnets are a class of fully compensated antiferromagnets lacking combined time-reversal and translational symmetry, their symmetry allows for unique polarization phenomena when inversion symmetry is broken. In this talk, we introduce an interacting fermion model with emergent ferro-spinetic polarizations in altermagnetic insulators - a spin analog to ferroelectricity. This model is grounded in a two-dimensional Hubbard framework incorporating inversion symmetry-breaking elements. Quantum Monte Carlo simulations demonstrate an altermagnetically ordered state with broken inversion symmetry driven by electron correlations, where spin-up and spin-down polarizations accumulate on opposite edges, with their directions reversibly controlled by the inversion symmetry-breaking factor. While the system retains electron-hole symmetry, resulting in zero ferroelectric charge polarization, breaking this symmetry induces the charge polarization orthogonal to the spin polarization.

MA 13.6 Tue 10:45 H20

Interplay of composition and magnetic properties in VxNbS2: An Altermagnetic candidate — •Sunil Wilfred Dsouza and Jan Minár — New Technologies Research Centre, University of West Bohemia, Univerzitní 8, CZ-306 14 Pilsen, Czech Republic

We investigate the interplay of chemical composition and electronic structure with respect to V atoms in an altermagnetic candidate VxNbS2 in the magnetically ordered state. The results from the first-principles calculations employing coherent potential approximation demonstrate that the electronic band structure exhibits valley-spin splitting induced by bulk magnetic order, which is only slightly affected by disorder and deficiency of V atoms, but an impact on the magnetic exchange coupling can be inferred. The results are interesting for the research on 3d-metal inserted transition-metal dichalcogenides and in a broader context for the understanding and design of Altermagnet- based spintronic materials.

MA 13.7 Tue 11:00 H20

Spin-transfer and topological Hall physics in d-wave altermagnets — •Ricardo Zarzuela — Johannes Gutenberg Universität Mainz, Mainz, Germany

Altermagnets, a novel magnetic phase of matter exhibiting zero net magnetization, anisotropic spin-split isoenergy surfaces and time reversal-symmetry-broken momentum-dependent spin splittings in the electronic band structure, have gained enormous momentum in the recent years due to their potential usage as active elements in Terahertz spintronic-based technologies [1]. In this talk, I will introduce an effective long-wavelength theory for charge carriers flowing within a d-wave altermagnet, from which the spin-splitter effect can be inferred as well as an unconventional spin-transfer response of the electron fluid. Reciprocally, the presence of altermagnetic textures induces the deflection of the electron trajectories. In this regard, I will also discuss how the d-wave nature of the altermagnet yields unconventional features to the topological Hall conductivity, which can be observed experimentally.

[1] L. Šmejkal, J. Sinova and T. Jungwirth, Phys. Rev. X 12, 031042 (2022); ibid. 040501 (2022).

15 min. break

MA 13.8 Tue 11:30 H20

Crystal structure and absence of magnetic order in single crystalline RuO_2 — •Lara Kiefer[1], Felix Wirth[1], Alexandre Bertin[1], Petra Becker[2], Ladislav Bohatý[2], Karin Schmalzl[3], Anne Stunault[4], José Alberto Rodríguez-Velemazan[4], Oscar Fabelo[4], and Markus Braden[1] — [1]II. Physic. Inst., Univ. Cologne, Germany — [2]Inst. Geology a. Mineralogie, Univ. Cologne, Germany — [3]Fz Jülich, Grenoble, France — [4]ILL, Grenoble, France

The recent report of antiferromagnetic order above room temperature in RuO_2 and its identification as an altermagnetic state boosted research on the material [1,2]. However, muon and neutron experiments, along with DFT calculations, recently questioned the existence of magnetic order in RuO_2 and suggested that it only occurs in the presence of vacancies [3-4]. We conducted polarized and unpolarized neutron diffraction experiments on RuO_2 crystals, which were characterized by magnetization, EDX, electrical conductance, and XRD measurements [5]. We did not confirm the proposed structural distortion in our crystals down to 2K. Ruthenium vacancies were below a few percent in our crystals. Polarized neutron experiments did not show magnetic Bragg reflections for the proposed $\vec{k}$=(0,0,0) [2]. Even a smaller ordered moment would have yielded significant intensities. Thus, this antiferromagnetic order is ruled out in our stoichiometric crystals [5].

[1] L. Šmejkal *et al*., 2022, Phys. Rev. X **12(3)**, 031042.
[2] T. Berjilin *et al*., 2017, Phys. Rev. Lett. **118**, 077201.
[3] A. Smolyanyuk *et al*., 2024, Phys. Rev. B. **109**, 134424.
[4] P. Keßler *et al*., 2024, npj Spintronics **2**, 50.
[5] L. Kiefer *et al*., 2024, arXiv, 2410.05850.

MA 13.9 Tue 11:45 H20

Ferroelectric Switchable Altermagnetism — Mingqiang Gu[1], Yuntian Liu[1], Haiyuan Zhu[1], Kunihiro Yananose[2], Xiaobing Chen[1], Yongkang Hu[1], •Alessandro Stroppa[3], and Qihang Liu[1] — [1]Department of Physics and Guangdong Basic Research Center of Excellence for Quantum Science, Southern University of Science and Technology, Shenzhen 518055, China — [2]Korea Institute for Advanced Study, Seoul 02455, Republic of Korea — [3]CNR-SPIN - Via Vetoio - 67100 - Coppito (AQ), Italy.

We propose a novel ferroelectric switchable altermagnetism effect, by synergistically correlating the switching of ferroelectric polarization and the altermagnetic spin splitting. We demonstrate the design principles for the ferroelectric altermagnets and the further symmetry constraints for switching the altermagnetic spin splitting through flipping the electric polarization based on the state-of-the-art spin-group symmetry techniques. 22 ferroelectric altermagnets are found by screening through the 2001 experimental reported magnetic structures in the MAGNDATA database and 2 of them are identified as ferroelectric switchable altermagnets. Using the hybrid improper ferroelectric material [C(NH2)3]Cr(HCOO)3 as an example, we show how the altermagnetic spin splitting is tightly coupled to the ferroelectric polarization, providing an ideal platform for designing electric-field-controllable multiferroic devices. Finally, we find that such manipulation of altermagnetism can be detected by monitoring the physical quantities that are related to the non-vanishing Berry curvature dipole, such as the linearly polarized photogalvanic spin current.

MA 13.10 Tue 12:00 H20

Growth and properties of sputter-deposited altermagnetic RuO_2 thin films — •Maik Gaerner, Martin Wortmann, Judith Bünte, Inga Ennen, Andreas Hütten, Jan Schmalhorst, Timo Kuschel, and Günter Reiss — Bielefeld University, Germany

Altermagnetic materials exhibit time-reversal symmetry breaking and non-relativistic, anisotropic spin splitting in their bandstructure. RuO_2 is widely regarded as such an altermagnetic material, since e.g. spin-torque generation in RuO_2 has been observed [1]. However, muon spin rotation experiments [2] and density functional theory calculations [3] hint at the fragility of the magnetic order in RuO_2.

Here, we report on the growth and characterisation of RuO_2 thin films, deposited on MgF_2-, TiO_2- and MgO-substrates using reactive magnetron sputtering. In contrast to MgF_2-substrates, the lattice mismatch between the commonly used TiO_2-substrates and RuO_2 induces a significant strain on the RuO_2 which can enhance the density of states near the Fermi level [4]. We compare the crystallographic and electronic transport properties of the RuO_2 films, deposited at varying growth conditions and on the different substrates, with regard to the detection of the altermagnetic phase.

[1] Bose et al., Nat. Electron. 5, 267 (2022)
[2] Keßler et al., npj Spintronics 2, 50 (2024)
[3] Smolyanyuk et al., Phys. Rev. B 109, 134424 (2024)
[4] Ruf et al., Nat Commun 12, 59 (2021)

MA 13.11 Tue 12:15 H20

Thermo-electric magnetotransport studies on altermagnetic CrSb — •Sajal Naduvile Thadathil[1,2], T. Kotte[1], C. Müller[3], D. Kriegner[4], J. Pospíšil[4], R. Firouzmandi[5], M. Uhlarz[1], M. C. Rahn[2], T. Speliotis[6], V. Kocsis[5], J. Wosnitza[1,2], H. Reichlova[3], and T. Helm[1] — [1]High Magnetic Field Laboratory Dresden, (HLD-EMFL), HZDR, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany — [3]Institute of Physics, Academy of Science of the Czech Republic — [4]Charles University, Czech Republic — [5]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [6]Institute of Nanoscience and Nanotechnology, NCSR Demokritos

Recent observations of materials exhibiting properties of both ferromagnets and antiferromagnets, characterized by antiparallel magnetic ordering, have led to the classification of a third distinct magnetic phase known as "altermagnetism". In this study, we investigate the thermo-electric and magnetotransport properties of the altermagnetic candidate material CrSb, using bulk and micron-sized structures fabricated from single crystals. We performed measurements of thermal-transport, magnetoresistance (MR) and the Hall effect between 1.8 and 300 K under magnetic fields up to 14 T. Our results reveal a significant nonlinear field dependence of the Hall resistance, confirmed by similar nonlinear behavior in the thermal Hall effect, providing evidence for multiband physics in CrSb. Additionally, we observe a non-saturating MR up to 14 T. These findings provide new insights into the multiband electronic structure of CrSb.

MA 13.12 Tue 12:30 H20

SU(N) altermagnetism: Lattice models, magnon modes, and flavor-split bands — •Pedro Monteiro Cônsoli and Matthias Vojta — Institut für Theoretische Physik, TU Dresden

Altermagnets are magnetically ordered states which, much like antiferromagnets, have zero net magnetization, and yet resemble ferromagnets in that their band structure shows signs of broken time-reversal symmetry. They have stirred great interest lately not only due to their potential for spintronics applications, but also as gateways to unconventional phases of matter. In this talk, we will demonstrate that a generalized form of altermagnetism can occur in SU(N) magnets with $N > 2$. Guided by symmetry principles, we will present a recipe to construct simple Heisenberg models for such generalized altermagnets and apply it explicitly to two-dimensional examples with $N = 2$ and 3. We will then report a comparative analysis based on spin- and flavor-wave calculations which proves that both systems share the same characteristic behavior of insulating altermagnets, namely that their magnon bands are nondegenerate and carry different sets of magnetic quantum numbers. Finally, we will show that the analogy between the models persists when they are supplemented with charge carriers to become metallic.

MA 13.13 Tue 12:45 H20

Quasi-symmetry Constrained Spin Ferromagnetism in Altermagnets — Mercè Roig[1,2], Yue Yu[2], Rune C. Ekman[1], •Andreas Kreisel[1], Brian M. Andersen[1], and Daniel F. Agterberg[2] — [1]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [2]Department of Physics, University of Wisconsin Milwaukee, Milwaukee, Wisconsin 53201, USA

Altermagnets break time-reversal symmetry and their spin-orbit coupling (SOC) allow for an anomalous Hall effect (AHE) that depends on the direction of the Néel ordering vector. AHE and ferromagnetic spin moment share the same symmetry and hence are usually proportional. However, density functional theory (DFT) calculations find that the AHE exists with negligible ferromagnetic spin moment for some compounds, whereas it reaches sizable values for other altermagnets. By examining realistic minimal models for altermagnetism in which the DFT phenomenology is captured, we uncover a general SOC-enabled quasi-symmetry that provides a natural explanation for the amplitude of the ferromagnetic spin moment across the vast range of different altermagnetic materials. Additionally, we derive analytic expressions for the magnetic anisotropy energy, providing a simple means to identify the preferred altermagnetic Néel vector orientation for altermagnets.

MA 14: Focus Session: Strongly Correlated Quantum States in Moire Heterostructures (joint session TT/HL/MA)

In recent years, significant progress has been made in realizing and exploring correlated quantum states in multilayer moiré heterostructures of graphene or transition metal dichalcogenides. These achievements have been made possible by the high level of control and tunability of these systems. Striking phenomena have been demonstrated experimentally, including unconventional superconductivity, fractional quantum anomalous Hall states, Mott-Wigner states and density waves, as well as kinetic ferromagnetism. Moreover, recently novel spectroscopic experimental techniques have been developed which allow for new ways to explore the dynamical response of these exotic states. This focus session will discuss recent experimental advancements as well as theoretical developments in the field of strongly correlated moiré heterostructures.

Organizers: Dmitri K. Efetov (LMU München), Michael Knap (TU München)

Time: Tuesday 9:30–13:15 Location: H36

See TT 18 for details of this session.

MA 15: Poster I

Time: Tuesday 10:00–12:30 Location: P1

MA 15.1 Tue 10:00 P1

Truly Chiral Phonons Arising From Chirality-Selective Magnon-Phonon Coupling — •Philipp Rieger[1], Markus Weissenhofer[1,2], Luca Mikadze[1], M. S. Mrudul[1], Ulrich Nowak[3], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]Freie Universität Berlin, Berlin, Germany — [3]Universität Konstanz, Konstanz, Germany

Growing attention has focused on the angular momentum of phonons, particularly in ultrafast magnetization dynamics. This arises from the circular or elliptical motion of atoms around equilibrium positions, forming collective modes known as chiral phonons.

Structural inversion symmetry (P) breaking is well known to give rise to chiral phonons. Here, we present an alternative mechanism for the generation of chi-

ral phonons, stemming from magnon-phonon coupling in P-symmetric crystal lattices with time-reversal symmetry breaking.

We investigate magnon-phonon coupling in bcc Fe using a first-principles framework. Our calculations reveal the hybridization of magnon and phonon modes, giving rise to magnon-polarons and an avoided crossing (energy gap) in the dispersion relations. Along specific high-symmetry lines in reciprocal space, we observe that magnon coupling transforms degenerate transverse phonon modes into chiral phonons, characterized by an energy splitting between left- and right-handed modes. Our findings challenge conventional magneto-elastic interpretations and reveal zero-point phonon angular momentum and anomalous Hall effects linked to finite (spin) Berry curvatures.

MA 15.2 Tue 10:00 P1

Polymer-free stacking and μ-ARPES of multiferroic $CuCrP_2S_6$ — •Niklas Leuth[1], Tim Jacobs[1], Jeff Strasdas[1], Wendong Wang[2], Roman Gorbachev[2], Elena Voloshina[3], Yuriy Dedkov[3], Marcus Liebmann[1], Vitaly Feyer[4], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH-Aachen University, Germany — [2]National Graphene Institute, University of Manchester, UK — [3]Department of Physics, Shanghai University, China — [4]PGI 6, Forschungszentrum Jülich, Germany

Transition-metal (Tm) phosphorus trisulfides are antiferromagnetic van-der-Waals materials with various magnetic orders, providing a platform for detailed studying and tuning of 2D magnetism [1,2]. The binary Tm compound $CuCrP_2S_6$ exhibits additional ferro-/ antiferroelectricity and magnetoelectric coupling enabling gate induced magnetic orders [2]. We present results on stacking of this material by a fully inorganic transfer process in a glovebox developed by the University of Manchester, leading to polymer-free inter- and surfaces [3]. These stacks are analysed by atomic force microscopy and x-ray photoelectron spectroscopy. After transfer in ultra-high vacuum, they are suitable for surface-sensitive angular-resolved photoelectron spectroscopy (ARPES) with micrometre focus. We tracked the band structure from 300 K to 40 K covering several known phase transitions and discuss changes of the band structure in comparison with density functional theory calculations and analyse the relevant photoelectron matrix elements. [1] J. Mater. Chem. A, 2021, 9, 2560-2591. [2] Nat. Comm., 2024, 15, 3029. [3] Nat. Electron., 2023, 6, 981-990.

MA 15.3 Tue 10:00 P1

Towards time-resolved cubic Magneto-optic Kerr effect measurements — •Farell Keiser, Wentao Zhang, Yuhao Meng, Maik Gaerner, Nicolas Beermann, Hassan Hafez, Savio Fabretti, Timo Kuschel, and Dmitry Turchinovich — Bielefeld University, Germany

The magneto-optic Kerr effect (MOKE) represents an alteration in the polarization of light when it is reflected from a magnetized surface. MOKE-based techniques are widely employed to characterize the magnetic properties of thin films. While many experiments focus on first- or second-order MOKE [1,2], a systematic investigation of the third order "cubic MOKE" (CMOKE) was only reported recently [3]. In this study, we present time-resolved MOKE measurements in Ni(111) thin films to investigate the dynamics of CMOKE. Specifically, we measure MOKE-curves for different sample orientations under strong optical pumping to observe the influence of demagnetization on the CMOKE. Time-resolved MOKE measurements were performed for different sample orientations and pump fluences.

[1] R. Silber et al., Appl. Phys. Lett. 116, 262401 (2020)
[2] R. Silber et al., Phys. Rev. B 100, 064403 (2019)
[3] M. Gaerner et al., Phys. Rev. Applied 22, 024066 (2024)

MA 15.4 Tue 10:00 P1

Cubic magneto-optic Kerr effect in Ni(111) and Co(111) thin films depending on the angle of incidence — •Malte Schaeffer[1], Maik Gaerner[1], Robin Silber[2], Jaroslav Hamrle[3], Martin Wortmann[4], Andrea Ehrmann[4], and Timo Kuschel[1] — [1]Bielefeld University, Germany — [2]VSB-Technical University of Ostrava, Czechia — [3]Charles University Prague, Czechia — [4]Bielefeld University of Applied Science and Arts, Germany

The magneto-optic Kerr effect (MOKE) describes the change in polarization of linear polarized light when reflected from a magnetized sample. It can be utilized to investigate magnetic properties of thin films and microstructures. In most cases, only the linear dependence on the magnetization M and sometimes the quadratic contribution depending on M^2 (QMOKE) are studied [1,2]. The third-order MOKE, so-called cubic MOKE (CMOKE), has only been studied recently [3,4]. In order to separate the individual MOKE contributions, the eight-directional method is used by applying an external magnetic field in eight different in-plane directions. In this contribution, we measured QMOKE and CMOKE in ferromagnetic Ni(111) and Co(111) thin films for different angles of incidence ranging from 45° to normal. We compared the findings with theoretical predictions based on Yeh's matrix formalism.

[1] R. Silber et al., Phys. Rev. B 100, 064403 (2019)
[2] R. Silber et al., Appl. Phys. Lett. 116, 262401 (2020)
[3] M. Gaerner et al., Phys. Rev. Applied 22, 024066 (2024)
[4] See Focus Session 'Magneto-transport and magneto-optics of higher orders in magnetization' at DPG Meeting 2025 in Regensburg

MA 15.5 Tue 10:00 P1

Dynamical Mean Field Theory for Spin Systems at Finite Temperature — •Przemysław Bieniek, Timo Grässer, and Götz Uhrig — Technische Universität Dortmund, Fakultät Physik

In the recent years, a dynamical mean field theory approach for spin systems at infinite temperature (spinDMFT) was developed. It is an approximate technique in the limit of an infinite coordination number, reducing the full dynamics of a spin system to a problem of a single spin interacting with a dynamical environment field. This allows for very efficient computation of spin correlations, which shows good agreement with other computational techniques and excellently describes nuclear magnetic resonance (NMR) experiments.

However, the current version of spinDMFT applies only to systems at infinite temperature and two-site couplings. We aim at extending the technique. One goal is to address finite temperatures, but still above any ordering temperature. To this end, we modify the approach to dynamical Green's functions instead of spin correlations. The second goal is to deal with three-site couplings as they arise in experiments with magic angle spinning. We benchmark the developed techniques for various spin models by comparing the results with other numerical approaches and discuss possible applications.

MA 15.6 Tue 10:00 P1

Spin Textures and Surface State Sequences of a Prototypical Topological Insulator Revealed by Momentum Microscopy — •Wei-Sheng Chiu[1,2], Ina Marie Verzola[3], Ying-Jiun Chen[1,4], Rovi Angelo Beloya Villaos[3], Claus Michael Schneider[1,2], Feng-Chuan Chuang[3], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut PGI-6, 52425 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [3]National Sun Yat-sen University, Department of Physics, 80424 Kaohsiung, Taiwan — [4]Forschungszentrum Jülich,Ernst Ruska-Centre ER-C-1, 52425 Jülich, Germany

As a hallmark of the prototypical topological insulator of Bi_2Se_3, its intriguing topological surface state (TSS) has been extensively studied. By using spin-resolving momentum microscopy (SPEMM) with an Au passivated Ir(100) imaging spin filter, we directly recorded the spin-resolved momentum maps (k_x, k_y) over entire surface Brillouin zone (SBZ) of Bi_2Se_3. In addition to the well-known Dirac cone at the Fermi level, our measurements reveal a sequence of several Dirac-like spin textures and crossings. Our first-principles calculations indicate that those overlooked bands are attributed to Bi_2Se_3 surface states spanning a wide binding energy up to 4 eV below the Fermi level.

MA 15.7 Tue 10:00 P1

A single crystal study of the kagome magnets *R*Mn6Sn6 — •Ana Kurtanidze[1,2], Shingo Yamamoto[1], Klara Uhlirova[3], Yurii Skourski[1], Sergei Zherlitsyn[1], Jeremy Sourd[1], and Joachim Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden,Germany — [3]Materials Growth and Measurement Laboratory (MGML), Charles University, Prague, Czech Republic

The kagome magnets *R*Mn6Sn6 (*R* = Sc, Y, Gd-Lu) with hexagonal structure (P6/mmm) attract attention due to a possible correlation between the observed topological electronic properties and various magnetic phases. We synthesized high-quality single crystals of *R*Mn6Sn6 (*R* = Er and Tm) by a tin-flux method. We performed scanning electron microscopy, energy-dispersive x-ray spectroscopy, and wavelength dispersive x-ray fluorescence measurements to characterize the phase purity of the samples, which showed a composition close to the nominal stoichiometric ratio. We observed approximately 0.25 at.% aluminum impurity, which originated from the alumina crucibles used. In addition to the chemical characterization, we will discuss the magnetic properties from our preliminary magnetization results under magnetic fields applied along the principal crystallographic axes.

MA 15.8 Tue 10:00 P1

Static and dynamic magnetic properties in the Li-rich antiperovskite $(Li_2Fe)ChO$ (Ch = S, Se) — •F.L. Carstens[1], F. Seewald[2], T. Schulze[2,3], N. Grässler[3], M.A.A. Mohamed[3], S. Hampel[3], L. Singer[1], H.-H. Klauss[2], H.-J. Grafe[3], and R. Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany

The recently discovered class of lithium-rich antiperovskites crystallize in cubic antiperovskite crystal structure such that Li^+ and transition metal ions TM^{2+} are randomly distributed at the same atomic position. They octahedrally coordinate central O^{2-} ions while the chalcogens (S^{2-}/Se^{2-}) are at corners of the cubic crystallographic cell. Despite their compelling properties as high-capacity cathode materials, very little is known about their electronic and magnetic properties. Here, we report static magnetisation, Mössbauer, and NMR studies on Li-rich antiperovskite $(Li_2Fe)ChO$ (Ch = S, Se). Our data show a Pauli paramagnetic-like behaviour, a long-range antiferromagnetically ordered ground state and a regime of short-range magnetic order at least up to 100 K. Our results are con-

sistent with predominantly random Li-Fe distribution on the shared lattice position. In addition, the effect of Li-hopping is observed and discussed. Overall, our data elucidate magnetism in a disordered presumably semimetallic system with thermally induced ionic dynamics.

MA 15.9 Tue 10:00 P1

Manipulation of Surface Domains in an Ultrasoft van-der-Waals Ferromagnet — •Stephan Schmutzler[1], Yichen Jin[1], Guangyao Miao[2,3], Florian Kronast[4], Sergio Valencia[4], Zefang Li[5], Martin Weinelt[1], and Cornelius Gahl[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [3]Department of Physics and CSMB, Humboldt-Universität zu Berlin, Berlin 12489, Germany — [4]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [5]School of Physics, Nankai University, Tianjin, China

The layered van-der-Waals material $Cr_2Ge_2Te_6$ (CGT) is a very soft ferromagnet at temperatures below 61 K. We show by X-ray magnetic circular dichroism in photoelectron emission microscopy (XMCD-PEEM) that the surface domain structure of a bulk CGT crystal can be reproducibly switched between topologically different phases by ultrashort laser pulse trains in combination with applying small magnetic fields. The effect is attributed to the transient temperature profile normal to the surface established by the interplay of absorption of light and the low interlayer heat conductivity of the material. The laser parameters accordingly allow for tayloring the sample depth of domain manipulation.

MA 15.10 Tue 10:00 P1

Sensing the Spin States of Individual Lanthanide Atoms on a surface — •Kyungju Noh[1,2,3], Gregory Czap[3], Jairo Velasco Jr.[3,4], Roger M. Macfarlane[3], Harald Brune[3,5], and Christopher P. Lutz[3] — [1]Center for Quantum 467 Nanoscience (QNS), Institute of Basic Science (IBS), Seoul 468 03760, Republic of Korea — [2]Department of Physics, Ewha 469 Womans University, Seoul 03760, Republic of Korea — [3]IBM Almaden Research Center, San Jose, 466 California 95120, United States — [4]Department of Physics, 472 University of California, Santa Cruz, California 95064, 473 United States — [5]Institute of Physics, Ecole 458 Polytechnique Fédérale de Lausanne (EPFL), Lausanne CH-459 1015, Switzerland

Research on single atoms and molecules of lanthanide elements has become a focal point in materials science due to their exceptional magnetic and electronic properties arising from the 4f shell electrons.

Here, we introduce the magnetic property of individual Samarium (Sm) and Europium (Eu) atoms, which has nearly half-filled and half-filled 4f shell each, adsorbed on various binding sites of a MgO thin film. Using electron spin resonance scanning tunneling microscopy (ESR-STM), we analyze the spin structures of Sm and Eu on different binding sites. Titanium (Ti), a well-established atom, serves as a spin sensor to detect interactions with the lanthanide atoms. Our comparison across binding sites reveals distinct spin characteristics of the lanthanides on a surface, which further opens a way to implement lanthanide atoms to quantum devices.

MA 15.11 Tue 10:00 P1

Applications of 3D Nano-Lithography in Magnetism — •Jana Kredl[1], Christian Denker[1], Cornelius Fendler[2], Julia Bethune[1], Nina Meyer[1], Theresa Brinker[1], Finn-F. Stiewe[1], Hauke Heyen[1], Chris Badenhorst[1], Alena Rong[1], Jakob Walowski[1], Robin Silber[3], Mark Doerr[1], Raghvendra Palankar[1], Uwe T. Bornscheuer[1], Marcel Kohlmann[1], Toni Hache[6], Michaela Lammel[4], Alexander Paarmann[5], Andy Thomas[4], Robert Blick[2], Mihaela Delcea[1], and Markus Münzenberg[1] — [1]University of Greifswald, Germany — [2]University of Hamburg, Germany — [3]VSB-Technical University of Ostrava, Czech Republic — [4]IFW Dresden, Germany — [5]Fritz Haber Institute of Max Planck Society, Berlin, Germany — [6]Helmholtz-Zentrum Dresden-Rossendorf, Germany

3D 2-Photon-Lithography, originally developed for 3D photonic crystals, opens a wide range of new possible applications in many fields, e.g. life sciences, micro-optics and mechanics. We will present our recent applications of 3D 2-Photon-lithography and show 3D evaporation masks for in-situ device fabrication using different deposition angles, infra-red laser light focusing lenses directly fabricated on optical fibers, tunnel structures for guiding growth of neurons [1], pillars for investigation of cell mechanics and master-mold fabrication for Polydimethylsiloxane (PDMS) micro-fluidic channels. Based on our experience we will discuss possible applications in magnetism. [1] C. Fendler et al., Adv. Biosys. 5 (2019) doi: 10.1002/adbi.201970054

MA 15.12 Tue 10:00 P1

Straining three-dimensional magnetic nanostructures — •José Claudio Corsaletti Filho, Mohammad Sedghi, Elina Zhakina, Markus König, Elena Gati, and Claire Donnelly — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The study of nanoscale magnetic objects has led to fascinating discoveries over the past few decades. Three-dimensional magnetism offers new opportunities to develop compact energy storage devices and explore spin textures and novel domain walls, which could be crucial for energy-efficient computation. To improve our fundamental understanding and enable the development of new devices, it is important to be able to tune the magnetic properties of materials. One way to achieve the controlled manipulation of magnetic properties is through the application of strain. While the straining of materials is well established for both bulk, and thin film samples, applying strain to 3D magnetic nanostructures remains an open challenge. In this project we develop a protocol to strain three-dimensional cobalt nanostructures grown with focused electron beam induced deposition. By performing in-situ measurements as a function of applied strain, we explore first the mechanical properties of the 3D nanostructures under an electron microscope, and secondly, the evolution of the magnetic properties of the nanostructure with strain. The straining of magnetic nanostructures opens the door to control of magnetic textures in complex geometries, of key importance both to our fundamental understanding, and the development of new devices.

MA 15.13 Tue 10:00 P1

Micromagnetic Simulations of Domain Wall Dynamics in Chiral Nanostructures — •Iason-Konstantinos Douveas[1], Pamela Morales Fernandez[1,8], Sandra Ruiz- Gómez[3], Elina Zhakina[2], Sebastian Wintz[4], Markus König[2], Aurelio Hierro Rodríguez[5], Simone Finizio[6], Luke Turnbull[2], Naëmi Leo[7], Dieter Suess[1], Amalio Fernández-Pacheco[8], Claire Donnelly[2,9], and Claas Abert[1] — [1]Faculty of Physics, University of Vienna, Austria — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]ALBALBA Synchrotron Light Source, CELLS, Spain — [4]Helmholtz Zentrum Berlin BESSY II, Germany — [5]CINN CSIC, University of Oviedo, Spain — [6]Paul Scherrer Institut, Swiss Light Source, Switzerland — [7]Loughborough University, United Kingdom — [8]Institute of Applied Physics, University of Vienna, Austria — [9]International Institute for Sustainability with Knotted Matter, Japan

We investigate domain wall (DW) eigenmodes in three-dimensional chiral magnetic nanostructures through micromagnetic simulations using the finite-element method. Our study focuses on double helices under external magnetic fields, examining the relationship between DW behavior and structural parameters. We employ two computational approaches: a small-scale model for extensive parameter space exploration and a larger structure matching experimental specimens. By implementing X-ray magnetic circular dichroism simulations, we provide direct comparison with experimental data, offering insights into DW mechanics in curved geometries.

MA 15.14 Tue 10:00 P1

Developing a two sublattice model for spin inertia and nutation — •Tarek Moussa[1], Ritwik Mondal[2], and Akashdeep Kamra[1] — [1]Department of Physics, RPTU Kaiserlautern-Landau, Kaiserslautern, Germany — [2]Department of Physics, Indian Institute of Technology (ISM) Dhanbad, India

Recent theoretical and experimental works on ultrafast magnetization dynamics suggest the existence of a finite spin inertia resulting in a nutation mode. Using the Landau-Lifshitz-Gilbert equation, we develop a two sublattice model for the description of spin inertia on the basis of an effective spin-orbit-coupling description and results for two sublattice ferrimagnets. We examine the conditions under which the two-sublattice model leads us to the magnetization dynamics description including spin inertia.

MA 15.15 Tue 10:00 P1

Flip-flop transport of magnetic cuboidal particles in dynamic potential energy landscapes for Lab-on-Chip applications — •Jonas Bugase, Christian Janzen, Arne Vereijken, Yahya Shubbak, Nikolai Weidt, Rico Huhnstock, and Arno Ehresmann — Institute of Physics , University of Kassel, 34132 Kassel

The unique possibility to transport magnetic particles using controlled magnetic forces have resulted in their increased use in bio-applications. We, therefore, present the remotely controlled transport mechanism for cubiodal particles, fabricated using two-photon polymerization (2PP) lithography above a magnetically patterned flat substrate. By sputtering a magnetic exchange bias thin film system on the surface of the polymeric particles, we fix the magnetic moment of the particles along the elongated axis. We characterized the magnetic properties of the custom-made particles and studied their exotic transport within a periodic magnetic stray field landscape, artificially created by parallel stripe domains fabricated via ion bombardment induced magnetic patterning [1]. The shape anisotropy contributions and the rotation dynamics of the particles in a quiescent liquid environment leading to the lateral walking and flipping modes of the particle transport are characterized using optical microscopy. This transport mechanism is promising for the detection of biomolecules in Lab-on-Chip devices [2] and for probing the effective field direction of dynamically transformed magnetic stray field landscapes.

[1] Ehresmann *et al.* (2015), Sensors, (15): 28854.
[2] Lowensohn *et al.* (2020), Langmuir, (36): 7100.

MA 15.16 Tue 10:00 P1

Current status and outlooks in time-resolved scanning transmission X-ray microscopy imaging — Simone Finizio[1], Bart Olsthoorn[2], Joe Bailey[1], Claire Donnelly[3], Sina Mayr[1,4], Ales Hrabec[1,4], and •Jörg Raabe[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]Nordita (KTH), Stockholm, Sweden — [3]MPI-CPFS, Dresden, Germany — [4]DMATL, ETH Zurich, Zurich, Switzerland

Time-resolved X-ray microscopy is a powerful imaging technique that has been extensively employed for the study of dynamical processes in condensed matter systems. In particular, time-resolved scanning transmission X-ray microscopy (TR-STXM) has been the workhorse in the experimental study of magneto-dynamical processes such as magnonics, switching, domain wall motion, and the dynamics of topological magnetic objects.

In this contribution, we will present the current status and outlooks of TR-STXM imaging at soft X-ray energies. The TR-STXM setup of the Swiss Light Source (SLS) will be presented, together with examples of 3D TR-STXM imaging, of periodogram-based imaging, and of how to overcome the limitations given by the X-ray pulse width.

In addition, we will present the planned future developments of the technique in view of the significant increase of coherent photon flux that will be offered by the upgrade of the SLS to a diffraction limited storage ring.

MA 15.17 Tue 10:00 P1

Micro-Hall magnetometry on magnetic grains and nanostructures — •Bereket Ghebretinsae and Jens Müller — Institute of Physics, Goethe University Frankfurt, 60438 Frankfurt (M), Germany

Micro-Hall magnetometry is a highly versatile and extremely sensitive magnetic measurement technique which allows for stray field measurements on micro- to nanosized samples with nanotesla sensitivity. The magnetometer is a Hall sensor based upon an AlGaAs/GaAs heterostructure which hosts a 2DEG whose unparalleled electron mobility in measurements directly translates into an ultrahigh stray-field resolution. Micro-Hall sensors have previously been used for diverse purposes such as resolving the discrete lattice potential inside a YIG thin film [1], pinpointing the onset of the formation of magnetic polarons inside ferromagnetic EuB_6 [2] as well as investigating the magnetostatics and the magnetization dynamics of two- and three-dimensional artificial spin ice systems [3]. Here we outline a (PhD) thesis project which intends to exploit the capabilities and the versatility of micro-Hall magnetometry to investigate a variety of magnetic systems of current scientific interest. We explain how micro-Hall measurements on specially prepared micron-sized YIG flakes, exchange-biased ferromagnetic bricks, and most of all, three-dimensional Co_3Fe nanotetrapod lattices serve to elucidate their characteristic properties and add upon our current understanding of the magnetism in these systems.

[1] K. Novoselov *et al.* Nature **426**, 812–816 (2003)
[2] M. Pohlit *et al.* Phys. Rev. Lett. **120**, 257201 (2018)
[3] L. Keller *et al.* Sci Rep. **8**, 6160 (2018)

MA 15.18 Tue 10:00 P1

Impact of sample dimensions on the anomalous Hall effect response — •Dominik Vogel, Denise Reustlen, Sebastian Sailler, Gregor Skobjin, Michaela Lammel, Richard Schlitz, and Sebastian T. B. Goennenwein — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

The anomalous Hall effect (AHE) enables an electrical detection of the magnetization in ferromagnetic conductors. In typical AHE measurements, the voltage transverse to both the applied charge current and magnetic field is detected. Recording this voltage as a function of magnetic field strength and polarity allows one to infer the magnetic hysteresis loop of a given magnetic microstructure. However, the absolute magnitude of the AHE voltage characteristically scales with the sample dimensions. In particular, the smaller the width w of the respective studied Hall bar microstructure, the smaller the Hall voltage signal for constant current density. In order to establish the minimal sample dimensions required for a detectable AHE signal, we have systematically varied the dimensions of Hall bar microstructures patterned into thin Co/Pt multilayers with perpendicular magnetic anisotropy and measured their Hall response as a function of field magnitude and current density. We critically discuss the scaling of the Hall voltage with sample dimensions observed and its implications for Hall effect-based experiments in magnetic nanostructures.

MA 15.19 Tue 10:00 P1

Bright days ahead - Soft X-ray scanning microscopy at 4th generation light-sources — •Simone Finizio[1], Tim Butcher[1,2], Lars Heller[1], Benjamin Watts[1], Blagoj Sarafimov[1], Mirko Holler[1], and Jörg Raabe[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]Max-Born-Institut, Berlin, Germany

Diffraction limited synchrotron (DLSR), or 4th generation, light sources are now delivering an increase in the coherent photon flux of several orders of magnitude compared to the current 3rd generation storage ring design, revolutionizing synchtrotron-based experiments.

For scanning transmission X-ray microscopy (STXM), the increase in coherent photon flux will allow us to routinely perform high-resolution imaging, as it will tackle all the issues occurring for high-resolution X-ray optics. In addition, the combined increase in coherent photon flux, in the available (GPU) computational power, and in the performances of 2D soft X-ray detectors will also enable for the routine performing of high-resolution soft X-ray ptychographic imaging.

In this presentation, we will show the current status of the commissioning of a new combined STXM and soft X-ray ptychography endstation at the SoftiMAX beamline of the MaxIV DLSR, and the first results in the ptychographic imaging of the magneto-electric coupling between ferroelectric domains and spin cycloid in freestanding BiFeO3 thin films, which fully exploit the sub-5nm spatial resolutions achievable with the technique.

MA 15.20 Tue 10:00 P1

Theory of Magnetization Dynamics Control by Phonons — •Meritxell Valls Boix and Alexander Mook — Johannes Gutenberg University, Mainz

Spin-lattice coupling plays a crucial role in facilitating angular momentum exchange between the lattice and magnetic subsystems. In this work, we explore how this coupling can be harnessed to enhance the lifetime of magnons in ferromagnetic materials. Specifically, we focus on the interaction between propagating surface acoustic waves and a proximate magnetic system, where these waves generate a torque on the spins. Using perturbation theory, we derive the effective field arising from magneto-rotational coupling and subsequently define the resulting torque. In particular, we investigate whether a damping-like component of the torque can emerge, which could act as an anti-damping mechanism to counteract the intrinsic magnon damping.

MA 15.21 Tue 10:00 P1

Prospects of spin dynamic mean-field theory for nuclear magnetic resonance — •Timo Gräßer and Götz S. Uhrig — Condensed Matter Physics, TU Dortmund University, Germany

The recently developed dynamic mean-field theory for spins at infinite temperature (spinDMFT) [1] is perfectly tailored to simulate NMR experiments. The underlying idea of spinDMFT is to couple a spin to a dynamic Gaussian mean-field with second moments that are self-consistently linked to the spin's autocorrelations. The approach can be straight-forwardly improved by considering clusters of spins quantum-mechanically in a mean-field background [2,3]. As such, the extension to a non-local spinDMFT (nl-spinDMFT) has been successfully benchmarked for calcium fluoride (CaF_2) and adamantane ($C_{10}H_{16}$) [3]. Due to the low computational requirements and the high flexibility of the method, it can be applied to various scenarios in NMR such as magic angle spinning (MAS) or spin diffusion.

[1] T. Gräßer et al., Phys. Rev. Research 3, 043168 (2021).
[2] T. Gräßer et al., Phys. Rev. Research 5, 043191 (2023).
[3] T. Gräßer et al., Solid State NMR 132, 101936 (2024).

MA 15.22 Tue 10:00 P1

Micromagnetic simulation of an X-shaped crossing controlled by the orientation of an external bias magnetic field — •Sven Niehues, Robert Schmidt, Jannis Bensmann, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster, Germany

Magnonics is a well-known research field in solid-state physics, which studies magnetic phenomena and the propagation of spin waves and their respective quanta, called magnons. The possibility of steering the propagation direction of spin waves in magnetic insulators such as yttrium iron garnet (YIG) is of crucial importance for the realization of magnonic logic devices. By changing the orientation of the external bias magnetic field relative to the propagation direction, the propagation of spin waves can be manipulated. In this work, numeric simulations of an X-shaped YIG crossing are presented, which allows the steering of spin waves from one input arm into all three output arms at selected frequencies by rotation of the magnetic bias field.

MA 15.23 Tue 10:00 P1

Coupled dynamic modes of a skyrmion chain in a synthetic antiferromagnet (SAF) — •Kauser Zulfiqar[1,2,3], Samuel Holt[1,3], Martin Lang[1,3], Swapneel Amit Pathak[1,3], and Hans Fangohr[1,3,4] — [1]Max Planck Institute for the Structure and Dynamics of the Matter, Hamburg, Germany. — [2]University of Hamburg, Hamburg, Germany. — [3]Center for Free Electron Laser, Hamburg, Hamburg, Germany. — [4]University of Southampton, Southampton, United Kingdom.

Synthetic antiferromagnets (SAFs) are multilayer structures with ferromagnetic layers coupled via RKKY interaction [1]. Skyrmions in SAFs are smaller than in ferromagnetic systems, and studying their modes provides insights into their dynamics and stability, enhancing their potential for spintronic devices [2].

In this work, we expand on previous studies of skyrmion dynamics in circular geometries [3] by exploring a chain of Néel-type skyrmions in a rectangular strip using finite-difference micromagnetic simulations [4]. We use the ringdown method to excite the system with a sinc pulse. Through Fourier analysis, we identify individual modes and observe hybrid and coupled breathing modes among layers.

This work is funded by Marie Skłodowska-Curie (grant 101152613), MaMMoS (Horizon Europe, grant 101135546), and HEC-DAAD (ID 57630247).

[1]. Physical Review B 94, 064406 (2016) [2]. Applied Physics Letters 118, 082403 (2021) [3]. Physical Review B 102, 104403 (2020) [4]. IEEE Transactions on Magnetics 58, 1-5 (2022)

MA 15.24 Tue 10:00 P1

Spin dynamics in ferrimagnetic heterostructures — •Felix Fuhrmann[1], Akashdeep Akashdeep[1], Sven Becker[1], Mathias Weiler[3], Gerhard Jakob[1,2], and Mathias Kläui[1,2,4] — [1]Institute of Physics, University of Mainz, Germany — [2]Graduate School of Excellence "Materials Science in Mainz" (MAINZ), Germany — [3]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische UniversitätKaiserslautern-Landau, 67663 Kaiserslautern, Germany — [4]Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway

Magnons emerge as promising information carriers for energy-efficient technology. To advance magnon-based devices, crucial materials requirements must be addressed. Yttrium Iron Garnet (YIG, $Y_3Fe_5O_{12}$) and related garnets, like Gadolinium Iron Garnet (GdIG, $Gd_3Fe_5O_{12}$), stand out due to low damping and large magnon propagation lengths. Using pulsed laser deposition, we fabricated YIG/GIG heterostructures and simulated their magnetic properties. Our findings reveal ferromagnetic coupling between Fe sublattices, leading to complex magnetic response and nontrivial temperature dependence [1]. Experiments on spin current generation via spin Seebeck effect and spin pumping at ferromagnetic resonance align with our micromagnetic simulations [2]. These results provide insights for magnon-based devices and highlight YIG/GIG heterostructures' potential in spintronics applications. [1] S. Becker et al., Phys. Rev. Appl., 16, 014047 (2021). [2] F. Fuhrmann et al., ArXiv:2303.15085 (2023).

MA 15.25 Tue 10:00 P1

Magnetization fluctuations probed via the anomalous Hall effect — •Nadine Nabben[1], Giacomo Sala[2], Ulrich Nowak[1], Matthias Krüger[3], and Sebastian T. B. Goennenwein[1] — [1]Universität Konstanz — [2]ETH Zürich — [3]Universität Göttingen

Fluctuation phenomena inherently limit the precision of physical measurements, making it essential to understand the underlying mechanisms for improving measurement accuracy. In particular, analyzing magnetic fluctuations provides valuable insights into magnetization behavior and domain wall dynamics. We employ the anomalous Hall effect to electrically investigate low-frequency magnetization fluctuations in thin ferromagnetic layer stacks with perpendicular magnetic anisotropy. By examining the anomalous Hall effect noise at different points in the hysteresis loop, we probe the distinct types of magnetic noise associated with different magnetization states. Our results show that Barkhausen noise, exhibiting a characteristic $1/f^2$ frequency dependence, dominates as long as magnetic relaxation processes occur. In contrast, quasi-stationary magnetization fluctuations generate noise that obeys a $1/f$ frequency dependence. We discuss how these findings offer new perspectives on magnetic fluctuation mechanisms and their implications for both fundamental understanding and technical applications.

MA 15.26 Tue 10:00 P1

Micromagnetic Mumax3 simulations of spin-waves under the influence of stray field landscapes — •Fabian Samad[1,2], Attila Kákay[2], and Olav Hellwig[1,2] — [1]University of Technology Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

In most spin-wave application concepts the capability of manipulating and confining the spin-waves is pivotal. One promising way is the usage of hybrid systems [1,2], where the spin-wave transport layer is not directly manipulated, e.g. by patterning, but instead is influenced by a "programming" layer. In our study, we choose for the programming layer a synthetic antiferromagnet (SAF) with perpendicular magnetic anisotropy (PMA) [3], which acts on a spin-wave transport layer via its stray field. The SAF can exhibit a variety of magnetic states depending on the energy parameters and the applied magnetic field, making it – and thus the hybrid system – field-reconfigurable. By performing Mumax3 simulations, we investigate the influence of the stray field of various magnetic patterns in the SAF on the spin-wave dispersion in a layer with YIG-type properties. Particularly, we focus on regular and periodic magnetic domains in the SAF, which can be stabilised e.g. by means of focussed ion beam irradiation and manipulated with external magnetic fields [4].

References: [1] Qin et al., Nano Letters 22, 5294 (2022) [2] Szulc et al., ACS Nano 16, 14168 (2022) [3] Hellwig et al., JMMM 319, 13 (2007) [4] Samad et al., APL 119, 022409 (2021)

MA 15.27 Tue 10:00 P1

Quantum spin liquid mimicry in correlated proton disorder double hydroxide perovskite $CuSn(OD)_6$ — •Anton Kulbakov[1], Ellen Haeussler[2], Aswathi Mannathanath Chakkingal[1], Nikolai Pavlovskii[1], Kaushick Parui[1], Sergey Granovsky[1], Sebastian Gass[3], Laura Teresa Corredor Bohorquez[3], Anja Wolter[3,4], Vladimir Pomjakushin[5], Darren Peets[1], Thomas Doert[2], and Dmytro Inosov[1,4] — [1]IFMP, TUD, Dresden, Germany — [2]Faekultaet fuer Chemie und Lebensmittelchemie, TUD, Dresden,Germany — [3]IFW, Dresden, Germany — [4]Wuerzburg-Dresden ct.qmat, TUD, Dresden, Germany — [5]PSI, Villigen, Switzerland

In a magnetic double perovskite hydroxide $CuSn(OD)_6$, the frustration of the proton network coexists with magnetic frustration on the distorted fcc sublattice. Structural distortions, which are most pronounced in the Cu^{2+} compounds due to the Jahn-Teller effect, partially alleviate both frustrations. On the other hand, the quantum spin $S = \frac{1}{2}$ promotes quantum fluctuations that lower the ordering temperature. Proton disorder is also expected to suppress long-range order tendencies from most general considerations, as it should lead to variations in the exchange constants, which can effectively be described as bond disorder in the spin model. In certain scenarios, these can destroy long-range order in favor of spin-liquid-mimicry.

MA 15.28 Tue 10:00 P1

Observation of the spiral spin liquid in a triangular-lattice material — •Nikita Andriushin[1], Stanislav Nikitin[2], Oystein Fjellvag[2,3], John White[2], Andrey Podlesnyak[4], Dmytro Inosov[1], Marein Rahn[6,1], Marcus Schmidt[5], Michael Baenitz[5], and Aleksandr Sukhanov[6,1] — [1]TU Dresden, Germany — [2]PSI, Switzerland — [3]IFE, Norway — [4]ORNL, USA — [5]MPI CPfS, Dresden, Germany — [6]Augsburg University, Germany

The spiral spin liquid (SSL) is a highly degenerate state characterized by a continuous contour or surface in reciprocal space spanned by a spiral propagation vector. Although the SSL state has been predicted in a number of various theoretical models, very few materials are so far experimentally identified to host such a state. Via combined single-crystal wide-angle and small-angle neutron scattering, we report observation of the SSL in the quasi-two-dimensional delafossite-like $AgCrSe_2$ [1]. We show that it is a very close realization of the ideal Heisenberg J_1–J_2–J_3 frustrated model on the triangular lattice. By supplementing our experimental results with microscopic spin-dynamics simulations, we demonstrate how such exotic magnetic states are driven by thermal fluctuations and exchange frustration.

[1] N. D. Andriushin, *et al*., arXiv:2410.04954 (2024).

MA 15.29 Tue 10:00 P1

Magnetism in i-Tb-Cd quasicrystals — •Andreas Kreyssig — Institute for Experimental Physics 4, Ruhr-Universität Bochum, 44801 Bochum, Germany

i-Tb-Cd orders as icoshedral quasicrystal with the magnetic Tb3+ ions arranged in Tsai-type clusters. We studied the magnetic correlations and excitations by elastic and inelastic neutron scattering on single-grain isotopically enriched samples. The measurements of the crystalline electric field excitations demonstrated that the Tb3+ moments are directed along the local fivefold axes of the Tsai-type clusters. By using a simple Ising-type model for the moment configurations on a single Tb3+ icosahedron, we calculated the magnetic diffuse scattering for the low-energy configurations and identified the most likely moment configuration in a single cluster by comparison with our diffuse neutron scattering signals. We further studied the role of intercluster interactions for magnetic frustration and the magnetic scattering.

This work was supported by the U. S. DOE, BES, DMSE, under Contract DE-AC02-07CH11358. This research used resources at HFIR and SNS, U. S. DOE Office of Science User Facilities operated by the Oak Ridge National Laboratory.

MA 15.30 Tue 10:00 P1

Magnetism in i-Tb-Cd quasicrystals — •Andreas Kreyssig[1,2], P. Das[2], G. S. Tucker[2], A. Podlesnyak[3], Feng Ye[3], Masaaki Matsuda[3], T. Kong[2], S. L. Bud'ko[2], P. C. Canfield[2], R Flint[2], P. P. Orth[2,4], T. Yamada[5], and A. I. Goldman[2] — [1]Experimental Physics IV, Ruhr University Bochum, Bochum, Germany — [2]Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, USA — [3]Neutron Scattering Division, Oak Ridge National Laboratory, USA — [4]Department of Physics, Harvard University, Cambridge, USA — [5]Department of Applied Physics, Tokyo University of Science, Tokyo, Japan

i-Tb-Cd orders as icoshedral quasicrystal with the magnetic Tb^{3+} ions arranged in Tsai-type clusters. We studied the magnetic correlations and excitations by elastic and inelastic neutron scattering on single-grain isotopically enriched samples. The measurements of the crystalline electric field excitations demonstrated that the Tb^{3+} moments are directed along the local fivefold axes of the Tsai-type clusters. We calculated the magnetic diffuse scattering for the low-energy configurations using an Ising-type model for the moment arrangements on a single Tb^{3+} icosahedron. By comparison with our diffuse neutron scattering signals, we identified the most likely moment configuration in a single cluster. We further studied the role of intercluster interactions for magnetic frustration and the magnetic scattering.

This work was supported by the U. S. DOE, BES, DMSE, Contract DE-AC02-07CH11358, and resources at HFIR and SNS, U. S. DOE.

P. Das, A. Kreyssig, et. al., Phys. Rev. **B** 108, 134421 (2023).

MA 15.31 Tue 10:00 P1

Frustrated magnetism in hydrogenated hexagonal Boron Nitride — •Maksim Ulybyshev, Manish Verma, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We study monolayer hexagonal boron nitride (h-BN) with hydrogen adatoms arranged in a regular triangular lattice. Extensive density functional theory (DFT) calculations reveal a flat band formed by electronic states localized near the adatoms, situated within the band gap of h-BN. Based on these results, we construct a tight-binding model that captures the essential features of this band structure and derive an effective Hamiltonian for electrons in the flat band. This effective Hamiltonian incorporates the effects of long-range Coulomb interactions projected onto the flat band using a technique previously validated by Quantum Monte Carlo simulations of similar systems. We demonstrate that the lack of particle-hole symmetry in this system causes the projected long-range Coulomb interactions to induce frustrated spin couplings between electrons localized near neighboring adatoms. Depending on the spatial configuration of the adatoms, this frustration can give rise to various nontrivial magnetic states.

MA 15.32 Tue 10:00 P1

Geometrical frustration mediated unconventional magnetism in a Kondo lattice Ce3ZrBi5 — •Saswata Halder, Arumugam Thamizhavel, and Kalobaran Maiti — Tata Institute of Fundamental Physics, Mumbai, India

Kondo lattice materials with geometric frustration offer fertile ground for exploring exotic new physics with a field-induced fractional magnetization platform. In this work, we investigate hexagonal Ce3ZrBi5 with 1D Bi chains and a frustrated Ce-kagome network to understand its magnetic properties. Density functional theory (DFT) calculations reveal the presence of a non-trivial electronic structure, that changes significantly in the presence of SOC. The temperature dependent magnetization for Ce3ZrBi5 show the presence of two antiferromagnetic (AFM) transitions below TN = 4.9 K; highlighting a complex and highly anisotropic magnetic landscape. The magnetization shows a peculiar nature where the moments align along the CEF hard axis; contrary to conventional antiferromagnets. The unconventional magnetization can be attributed to multiple observables: geometric frustration, presence of competing Kondo and RKKY nergy scales and strong spin- orbit coupling (SOC). Field-induced metamagnetic transitions are observed in the isothermal magnetization data which follows the one-third magnetization rule observed in frustrated Kagome lattices. Specific heat and transport measurements highlight inherent Kondo-lattice characteristics in Ce3ZrBi5. Our work establishes Ce3ZrBi5 and related materials as a unique platform for exploring low-dimensional quantum fluctuations in frustrated antiferromagnets.

MA 15.33 Tue 10:00 P1

Flat bands and megnetoelectric effect in XX sawtooth chain with three-spin interactions — •Karen Baghdasaryan[1], Vadim Ohanyan[2,3], Ostap Baran[4], and Oleg Derzhko[4] — [1]Ludwig-Maximilians-Universität, München, Germany — [2]Yerevan State University, Yerevan, Armenia — [3]CANDLE Synchrotron Research Institute, Yerevan, Armenia — [4]Institute for Condensed Matter Physics, Lviv, Ukraine

We present an exact analysis of the XX sawtooth chain with three-spin interactions and the Katsura-Nagaosa-Balatsky (KNB) mechanism. Using Jordan-Wigner fermionization, we identify all zero-temperature phases of the model and observe the emergence of a flat band in the free-fermion spectrum. These flat bands result in jumps in observables such as magnetization and dielectric polarization as functions of both magnetic and electric fields.

MA 15.34 Tue 10:00 P1

Two-dimensional coherent spectroscopy as a probe for spin-1 single ion bound states — •Sagar Ramchandani[1], Yoshito Watanabe[1], Simon Trebst[1], and Ciarán Hickey[2,3] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [3]Centre for Quantum Engineering, Science, and Technology, University College Dublin, Dublin 4, Ireland

Nonlinear spectroscopy has emerged as a powerful prospect to probe quantum magnets by extracting information from higher-order responses. In this work, we report on the implementation of 2-dimensional coherent spectroscopy (2DCS) in the context of the Su(n)ny Julia package for modelling atomic-scale magnetism. We employ this code (and its semi-classical approach) to study the properties of spin-1 single ion bound states (SIBS), motivated in part by recent experiments on FeI_2.

MA 15.35 Tue 10:00 P1

Theoretical study on in-plane, out-of-plane, and transverse anisotropic magnetoresistance effects for ferromagnetic films — •Satoshi Kokado[1] and Masakiyo Tsunoda[2] — [1]Shizuoka University, Hamamatsu, Japan — [2]Tohoku University, Sendai, Japan

We theoretically study the in-plane [1], out-of-plane [2], and transverse anisotropic magnetoresistance (AMR) effects [3] for a strong ferromagnet, Fe_4N. We here use the electron scattering theory with an extrinsic mechanism, in which the conduction electron is scattered into the conduction state and the localized d states by impurities and so on [4]. The in-plane and out-of-plane AMR effects exhibit the negative AMR ratio with the twofold symmetry, while the transverse AMR effect shows the positive AMR ratio with the fourfold symmetry. The calculation results agree qualitatively well with the respective experimental results [1,2,3] for Fe_4N. In addition, the peak structures of the AMR ratios reflect the probability densities of the current direction of the single atomic d states.

[1] M. Tsunoda et al., APEX **3**, 113003 (2010).
[2] M. Tsunoda et al., unpublished.
[3] K. Kabara et al., AIP advances **6**, 055818 (2016).
[4] S. Kokado et al., J. Phys. Soc. Jpn. **91**, 044701 (2022), J. Phys. Soc. Jpn. **81**, 024705 (2012), Adv. Mater. Res. **750-752**, 978 (2013), Jpn. J. Appl. Phys. **55**, 108004 (2016), J. Phys. Soc. Jpn. **88**, 034706 (2019).

MA 15.36 Tue 10:00 P1

Preparation and characterization of $Co_{20}Fe_{80}Si_x$ thin films — •Florian Knossalla, Maik Gaerner, Luca Kempe, Karsten Rott, Jan Schmalhorst, and Günter Reiss — Bielefeld University, Germany

In spintronics, materials with favorable magnetic properties, such as large magnetic polarization and a high Curie temperature are essential. By means of machine learning, different Fe-Co-Si compounds were identified as promising [1]. This study focuses on the investigation of alloys with the composition $Co_{20}Fe_{80}Si_x$.

The samples were fabricated using DC and RF magnetron co-sputtering. Subsequently, temperature-dependent resistance measurements, investigations of the ordinary and the anomalous Hall effect were performed alongside with measurements of the anisotropic magneto-resistance.

The magnetic polarization decreased with increasing silicon content, from approximately 2 T for $Co_{20}Fe_{80}$ to about 0.5 T for $Co_{20}Fe_{80}Si_{100}$. In the latter, a phase transition at 60K was observed, which coincides with the appearance of a linear nonsaturating magnetoresistance. Interestingly, $Co_{20}Fe_{80}Si_{50}$ exhibited a higher magnetic polarization than $Co_{20}Fe_{80}Si_{25}$, as well as twice the charge carrier density compared to $Co_{20}Fe_{80}$.

[1] Timothy Liao u. a. Phys. Rev. Materials 7, 034410(2023)

MA 15.37 Tue 10:00 P1

Real-time in-situ giant magnetoresistance measurements in Co/Cu multilayers during sputter deposition — Michael Mattern, •Luca Kempe, Jan Schmalhorst, and Günter Reiss — Bielefeld University, Faculty of Physics, Germany

Magnetoresistive sensors generate important input information that is further processed in complex microelectronic systems in a wide range of applications. For optimization purposes or the investigation of new material combinations, a permanent analysis of the influence of deposition conditions on the magnetoresistive performance is necessary. Today, research and development in the field of magnetic sensor technology is slowed down due to slow feedback from results of ex-situ characterization of samples into modelling and production. This study presents an experimental technique for real-time in-situ measurements of magnetoresistive effects, such as giant magnetoresistance (GMR), during the sputtering process. As an example, an oscillating in-plane magnetic field with an amplitude of 420 Oe and a frequency of 10 Hz was applied to samples of cobalt/copper multilayers during film growth. By employing advanced instrumentation with a sampling rate of 20 kS/s and the implementation of real-time GMR amplitude calculation, we were able to obtain and analyze complete R versus H curves within 100 milliseconds. Correlations between the magnetic response of these samples and structural changes at different stages of film deposition are shown.

MA 15.38 Tue 10:00 P1

Quantitative study of the spin Hall magnetoresistance in a yttrium iron garnet/Pt heterostructure — •Denise Reustlen, Sebastian Sailler, Davina Schmidt, Richard Schlitz, Michaela Lammel, and Sebastian T. B. Goennenwein — Department of Physics, University of Konstanz, 78457 Konstanz

The spin Hall magnetoresistance (SMR) is a well-known and extensively studied phenomenon in the field of spintronics. The SMR is most commonly observed in heterostructures consisting of a ferromagnetic insulator and a normal metal with a large spin orbit interaction. In this study, we use yttrium iron garnet as the ferrimagnetic insulator and platinum as the normal metal due to its relatively large spin Hall angle. While the SMR is usually measured locally, on a single Hallbar structure, the data obtained often are used to gauge the magnetic quality of the underlying magnetic insulator or of the magnet/metal interface. Interestingly, however, up to now little is known about the SMR statistics in one Hallbar and the scatter of the SMR magnitude across several Hallbars on a single sample. Given that the SMR is a local effect, it is relevant to ascertain the significance of a single measurement as a representative measure for the entire sample. We thus have patterned more than 200 nominally identical SMR microstructures into a single YIG/Pt bilayer and studied the statistical distribution of the SMR as a function of position across the entire sample. Our results demonstrate that the SMR amplitude is robust and provide the basis for a consistent comparison of the SMR.

MA 15.39 Tue 10:00 P1

Spin Textures Stability in Exfoliated Fe3GaTe2 Two-Dimensional Magnets — •Kai Litzius[1], Yara Mahboub[2], Krishnanjana Puzhekadavil Joy[2], Steffen Wittrock[1], Lilian Prodan[1], István Kézsmárki[1], and Felix Büttner[1,2] — [1]University of Augsburg, Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Two-dimensional (2D) van der Waals magnets have emerged as an exciting area of research, providing unique opportunities to study magnetism in reduced dimensions. Among these materials, Fe3GaTe2 is particularly notable for its exceptionally high Curie temperature [1], which enables investigations and device applications at room temperature. Moreover, its structural and compositional similarity to Fe3GeTe2, one of the most extensively studied 2D magnets, suggests significant potential for tuning its magnetic properties [2,3], making it a promising candidate for both fundamental research and spintronic device applications. In this study, we explore the spin texture stability of Fe3GaTe2 thin flakes, prepared through mechanical exfoliation, using magnetic force microscopy (MFM). We also assess their resistance to oxidation [4] and degradation under ambient conditions, confirming their robust performance. These results highlight Fe3GaTe2 as a high-TC, stable 2D magnet, well-suited to advancing research in 2D magnetism and enabling next-generation spintronic technologies. References: [1] H. Shi et al., Nano Lett. 24, 11246 (2024). [2] Y. Wu et al. Nat. Commun. 11, 3860 (2020). [3] M. T. Birch et al. 2D Mater. 11, 025008 (2024). [4] D. S. Kim et al. Curr. Appl. Phys. 30, 40 (2021).

MA 15.40 Tue 10:00 P1

Electrical detection of spin currents in magnetic insulators — •Ankita Nayak[1], Matthias Kronseder[2], Nynke Vlietstra[3], Hans Huebl[3,4,5], Jeroen A. Heuver[6], Beatriz Noheda[6], Maxim Mostovoy[6], Christian Back[3,4], and Aisha Aqeel[1,3,4] — [1]University of Augsburg, 86135, Augsburg, Germany — [2]Department of Physics, Regensburg University, 93053, Regensburg, Germany — [3]Department of Physics, Technical University Munich, 85748 Garching b. München, Germany. — [4]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, D-80799, München, Germany. — [5]Walther -Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748, Garching, Germany, — [6]Zernika Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, Groningen, The Netherlands.

We investigate the spin current-induced phenomena, such as spin Hall magnetoresistance and the spin Seebeck effect within Pt films deposited on a non-collinear magnet [1], CoCr2O4 (CCO). CCO is a spinel with a collinear ferrimagnetic state below Tc = 94 K and non-collinear magnetic phases at lower temperatures [2]. We investigated the SMR and the SSE at different temperatures (5K-300K) [2]. The temperature-dependent behavior of both SMR and SSE signals exhibits a noticeable variation correlated with different magnetic phases of CCO. This study offers insights into spin-current-driven phenomena, paving the way for potential spintronic applications. [1]. A. Aqeel, et al., Phys. Rev. B 103 (10), L100410 (2021). [2]. A. Aqeel, Phys. Rev. B 92 (22), 224410 (2015).

MA 15.41 Tue 10:00 P1

First principle study of Spin and charge transport properties in CrO2/CrI3/Td-WTe2/CrO2 based device heterostructures — •Nivedita Pandey and Oscar Granas — Department of Physics and Astronomy, Uppsala University, SE-751 20 Uppsala, Sweden

Van der Waals heterostructures are attractive for spintronic applications due to tunability of electronic, and magnetic properties. Herein, we show that precise control over spin injection and filtering can be achieved by interfacing magnetic and non-magnetic 2D layers, and these properties are robust to electrode attachment. We study a bilayer of CrI3/WTe2, using electrode CrO2 to design a promising spintronic device. We use density functional theory, capturing charge transport and thermal properties through the use of the non-equilibrium Green function. Integration of ferromagnetic CrI3 with either metallic or semiconducting phase of WTe2 results in substantially different properties of the interface. Further, the coupling between magnetism, and charge/spin transport has been studied in detail for both parallel magnetization and anti-parallel magnetization case. The spin polarized current with variation in the electrode temperature has been calculated for the designed CrO2/CrI3/WTe2/CrO2 device, further the spin filtration efficiency is extracted to understand the effect of temperature on spin filtration. The proposed device shows a spin filtration efficiency of around 100% at the studied temperatures. In addition, a high thermal magnetoresistance has been obtained for the designed device.

MA 15.42 Tue 10:00 P1

Workflow for Robust Code and Data Management exemplified for the numerical calculation of the Hopf index — •Jonas Nothhelfer, Ross Knapman, and Karin Everschor-Sitte — Universität Duisburg-Essen

Structured workflows for code and data management are essential in scientific projects to ensure reproducibility and quality. We will discuss these workflows from a system administrator's perspective, emphasizing the infrastructure and tools needed to support scientific computing. Using a recent scientific project as a case study, we present an example workflow that makes the projects numerical methods for calculating the three-dimensional topological Hopf index accessible [1]. Not only do we offer Python scripts, but we also develop extensions for the standard micromagnetic software tool, Mumax3 [2]. Code management is handled through GitLab, ensuring access to the most current versions of code [3], while Zenodo is used to provide persistent identifiers for released versions [4].

[1] R. Knapman, et al. arxiv:2410.22058 (2024).
[2] A. Vansteenkiste, et al. AIP Adv. 4, 107133 (2014).
[3] https://git.uni-due.de/twist-external/numericalhopfindexcalculation.
[4] https://zenodo.org/records/14007386, https://zenodo.org/records/14006428.

MA 15.43 Tue 10:00 P1

Angle-resolved calculation of magnetocrystalline anisotropy using symmetry-adapted Wannier functions — •Hiroto Saito and Takashi Koretsune — Tohoku University, Sendai, Japan

Magnetocrystalline anisotropy is one of the most fundamental physical quantities that determine the properties of magnetic materials. However, since its value is often very small, dense k-mesh is needed to accurately calculate it using first-principles calculations. We have previously developed a method to calculate magnetocrystalline anisotropy with high precision and low computational cost by constructing a Wannier tight-binding model that incorporates both crystal and spin symmetries, and by using the time-reversal-symmetry operation to separate the magnetization and spin-orbit interaction [1, 2].

Recently, a systematic approach for generating a complete set of symmetry-adapted multipole bases has been developed to describe the electronic degrees of freedom in crystals [3]. In this study, we apply this method to demonstrate that symmetry-adapted Wannier Hamiltonians for magnetic materials can be expanded using multipole bases. This finding highlights the feasibility of constructing symmetry-based effective models directly from first-principles calculations. As a practical application, we report the calculation results of the magnetic anisotropy of anomalous Hall conductivity.

[1] T. Koretsune, Comput. Phys. Commun. **285**, 108645 (2023).
[2] H. Saito *et al*., Comput. Phys. Commun. **305**, 109325 (2024).
[3] H. Kusunose *et al*., Phys. Rev. B **107**, 195118 (2023).

MA 15.44 Tue 10:00 P1

Discretization Anisotropy In Micromagnetics — Samuel Holt[1,2], •Andrea Petrocchi[1,2], Martin Lang[1,2], Swapneel Pathak[1,2], and Hans Fangohr[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Faculty of Engineering and Physical Sciences, University of Southampton, Southampton SO17 1BJ, United Kingdom

Micromagnetics models the physics of magnetic systems using partial differential equations to express quantities such as the magnetization, energy density, and effective field. The discretization of these equation onto a regular lattice produces anisotropy. Its impact is extensive and includes phenomena such as the energy-minimizing rotation of magnetic structures, preferred directions, and creating artificial magnetization structures.

Despite this, the consequences of discretization anisotropy and how to mitigate against it are rarely discussed in the context of micromagnetics. A thorough understanding of these effects is important for the accurate interpretation of simulation results and for enhancing the overall fidelity of micromagnetic modeling. In this work we focus on these errors introduced by using finite difference approximations in micromagnetic simulations.

Funded by EU Horizon 2020, grants 101152613 and 101135546.

MA 15.45 Tue 10:00 P1

Magnetization Reconstruction from Magnetic Field Measurements Using Physics-Informed Inverse Problems — •Alexander Setescak, Florian Bruckner, and Claas Abert — University of Vienna, Austria

Understanding the magnetization of topological spin textures is crucial for advancing spintronic applications. This work covers a physics-informed framework for reconstructing magnetization from high-resolution magnetic field measurements, such as those obtained via nitrogen-vacancy (NV) magnetometry. The approach leverages the micromagnetic equilibrium condition as a critical constraint in the inverse problem, ensuring the reconstructed magnetization satisfies the fundamental energy minimization principles.

The reconstruction process is formulated as an optimization problem, where a loss functional is designed to minimize discrepancies between measured and computed magnetic fields while imposing physical and regularization constraints. Efficient gradient computation is achieved through a combination of backpropagation algorithms and the adjoint method, enabling accurate and robust parameter optimization.

Preliminary results reveal detailed magnetization structures consistent with theoretical predictions and experimental observations. This demonstrates the potential of the proposed framework to investigate tailored magnetic configurations on the nanoscale, thereby laying the groundwork for future advancements in spintronic device engineering.

MA 15.46 Tue 10:00 P1

Synthetic Data Training Strategies for Magnetic Phase Classification — •Marcelo Arlego[1,2], Agustín Medina[1], and Carlos Lamas[1] — [1]Instituto de Física La Plata, La Plata, Argentina. — [2]Institute for Theoretical Physics TU-BS

In this work, we explore the potential of artificial neural networks trained with a synthetic catalogue of spin patterns, examining their ability to generalize and classify phases in complex models beyond the simplified training context.

Specifically, we investigate the transition from order to disorder in a diluted Ising model, a problem for which no exact solution exists, and where most current analytical and numerical techniques face significant difficulties.

Despite these obstacles, we used direct methods to achieve consistency in determining percolation densities and transition temperatures.

Our results suggest that a simple yet strategic training approach for neural networks can help in understanding complex physical phenomena, with potential applications beyond condensed matter physics.

MA 15.47 Tue 10:00 P1

Simulation of magnetoelastic mode filters for surface acoustic waves — •Bernhard Emhofer[1], Michael Karl Steinbauer[1], Peter Flauger[1], Matthias Volz[3], Matthias Küss[2], Stephan Glamsch[2], Manfred Albrecht[2], Hubert Krenner[3], and Claas Abert[1] — [1]University of Vienna — [2]University of Augsburg — [3]University of Münster

Surface acoustic wave (SAW) propagation critically depends on the waveguide geometry, with a key challenge being the independent excitation of specific mode types such as Rayleigh and shear modes.

In this study, we employ micromagnetic simulations, specifically the python library magnum.np [1], to explore a novel approach for selectively absorbing specific acoustic modes via magnetoelastic coupling. This coupling occurs through the excitation of spin waves in a thin magnetic film, layered on top of the waveguide. To achieve controlled mode filtering, the equilibrium magnetization is manipulated by varying the angle and strength of an external magnetic field. The distinct resonance configurations for Rayleigh and shear modes observed experimentally [2], enable their selective attenuation.

Simulations performed for a $LiNbO_3$ substrate with a 108 nm thick Ni film show that SAWs experience significant attenuation, with the maximum displacement at the surface reduced by around 70% after 13 wavelengths. These results demonstrate the potential of magnetoelastic interactions for precise mode filtering.

[1] F. Bruckner et al., Sci. Rep. 13, 12054 (2023).
[2] M. Küß et al., Phys. Rev. Appl. 15, 034046 (2021).

MA 15.48 Tue 10:00 P1

Revealing rich magnetic phases and novel spin-wave spectra in Orthorhombic perovskite TbCrO3: a frsfprinciples study — •Fengyi Zhou — Faculty of Applied Sciences, Macao Polytechnic University, Macao SAR, 999078, China

The experimental measurements have revealed the orthohombic perovskite $TbCrO_3$ crystal exhibits rich magnetic structures with temperature variation. Specifically, a long-range canted AFM state of Cr^{3+} ions is formed below T_N^{Cr} = 157.9 K. At a lower temperature (below T_N^{Tb} ~ 7.7 K), the Tb^{3+} ions exists a long-range antiferromagnetic (AFM) order. Furthermore, a weak competition between the FM and AFM interactions within the Cr^{3+} ions is observed at 15 K. Importantly, a strong coupling between the spin orders of the Cr^{3+} and Tb^{3+} ions is observed at 1.8 K. As the temperature decreases, the magnetic moment of Tb disappears first. Currently, in-depth theoretic research is appealing and urgently needed to explore these complex magnetic interactions, magnetic phase transition and spin wave spectra of $TbCrO_3$.

Based on the first-principles study, this study presents the entire magnetic landscape of $TbCrO_3$ including the magnetic ground state, equilibrium state, and excited state. Meanwhile, we clarified the detailed magnetic exchange mechanisms including the isotropic Heisenberg exchange and the antisymmetric Dzyaloshinskii-Moriya interaction, as well as single ion anisotropy. Finally, the spin wave spectrum considered adiabatic and temperature-dependent relationships is also evaluated.

MA 16: Topological Insulators (joint session MA/HL)

Time: Tuesday 14:00–15:15 Location: H16

MA 16.1 Tue 14:00 H16

Topological Hall effects on two-dimensional Archimedean lattices — •L.V. Duc Pham[1,2], Nicki F. Hinsche[2], and Ingrid Mertig[2] — [1]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, Bergstraße 66c, 01062 Dresden, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany

Archimedean lattices are a family of tilings in which the two-dimensional plane is filled with different regular polygons while maintaining the vertices configuration. Kagome, the most famous member of the Archimedean lattices familiy, was studied extensively in a wide variety of theoretical works. Another lattice of this type, the snub square lattice, was also used as an approximant for quasi crystals [1]. The rich geometry of these systems gives rise to various unconventional nano ribbon edge configurations and therewith various possible topological edge states. In this work, we calculate the band structures of all 8 pure Archimedean lattices using a tight-binding method including s and p orbitals and study topological properties of these lattices, such as topological edge states, the $\mathbb{Z}_2$ invariance and the quantum spin Hall conductivity within the Kubo formalism [2].

[1] Roy, Sumalay, et al. "The Kepler tiling as the oldest complex surface structure in history: X-ray structure analysis of a two-dimensional oxide quasicrystal approximant." Zeitschrift für Kristallographie-Crystalline Materials 231.12 (2016): 749-755

[2] Sinova, Jairo, et al. "Spin hall effects." Reviews of modern physics 87.4 (2015): 1213-1260

MA 16.2 Tue 14:15 H16

Spin topology, spin-orbit coupling and entanglement — •Gunnar Felix Lange[1], Wojciech Jankowski[2] und Robert-Jan Slager[2,3] — [1]Department of Physics, University of Oslo, Norway — [2]TCM Group, Cavendish Laboratory, University of Cambridge, UK — [3]Theoretical Physics Group, University of Manchester, UK

Topological systems with time-reversal symmetry are of great theoretical and practical interest. Theoretically, such phases often rely on studying the topology in each spin sector separately, as in the spin Hall effect.

This requires identifying the spin degree of freedom in the band structure, which is not always straightforward in the presence of spin-orbit coupling. This field has received renewed interest in recent years, leading to the concept of spin topology.

In this talk, we will discuss some recent results on spin topological phases, with a particular focus on spin-orbit coupling and its interplay with entanglement.

MA 16.3 Tue 14:30 H16

Fractionally Charged Vortices at Quantum Hall/Superconductor Interfaces — •Enderalp Yakaboylu and Thomas Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg

We investigate interface states between a type-II *s*-wave superconductor (SC) and a Chern insulator describing an integer quantum Hall (QH) system. We find that an effective pairing interaction at this boundary gives rise to two emergent Abelian Higgs fields, representing the two paired electrons at the SC/QH interface, coupled to a gauge field that incorporates both Chern-Simons and Maxwell terms. We use this model to investigate the effect of magnetic flux vortices in the SC on the QH system. In particular, we find vortex solutions in which the Cooper pairs give rise to topological fractionally-charged vortices localized at the interface.

MA 16.4 Tue 14:45 H16

Local and Global Topological Characteristics of Local Magnetic Moments Coupled to Chern Insulators — •Devesh Vaish and Michael Potthoff — I. Institute of Theoretical Physics, Department of Physics, University of Hamburg

A magnetic impurity, modelled as a classical spin and locally exchange coupled to a Chern insulator may cause in-gap bound states. Their nature can be very different depending on the (k-space) topological phase of the Chern insulator. Here we study several impurity spins coupled to a QWZ model and analyze, for different k-space topological phases, the additional "local" topological properties on the manifold of impurity-spin configurations (S-space). In case of $R > 1$ spins, the R-th spin-Chern number serves as a topological invariant on S-space. Varying the local exchange-coupling strength, we find local topological phase transitions and relate them to Fermi-energy crossings of in-gap states. In addition, we compute the first spin-Chern number for various physically motivated closed two-dimensional sub-manifolds of the full configuration space and relate those to the R-th spin-Chern number.

MA 16.5 Tue 15:00 H16

Non-relativistic linear Edelstein effect in noncollinear EuIn2As2 — •Adriana Nayra Alvarez Pari[1], Rodrigo Jaeschke Ubiergo[1], Atasi Chakraborty[1], Jairo Sinova[1,5], and Libor Smejkal[1,2,3,4] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany — [2]Max Plank Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic — [5]Department of Physics, Texas A & M University, Texas, USA

Motivated by the ongoing interest in understanding the actual magnetic ground state of the promising axion insulator candidate EuIn2As2, we present here a spin symmetry analysis and *ab-initio* calculations, aiming to identify specific exchange-dominated physics that could offer insights into the current debate. We investigate two non-collinear coplanar magnetic orders reported in this compound: the *helical* and *broken-helical* phases [1]. Our symmetry analysis shows that magnetic-exchange alone results in the formation of an out-of-plane odd-wave order in momentum space in both phases. Additionally, we identify an in-plane g-wave order that emerges exclusively in the *broken-helical* phase, providing a distinguishing feature for this phase. Furthermore, we report a non-relativistic Edelstein effect with a distinct out-of-plane polarized spin density that dominates over spin-orbit coupling effects.

[1] Pari, Nayra A. Álvarez, et al. "Non-relativistic linear Edelstein effect in non-collinear EuIn2As2." *arXiv:2412.10984* (2024)

MA 17: Micro- and Nanostructured Magnetic Materials

Time: Tuesday 14:00–15:00 Location: H18

MA 17.1 Tue 14:00 H18

Thin films of a dinuclear Fe^{2+} complex on HOPG: Spin-crossover studies using X-ray absorption spectroscopy — •Marcel Walter[1], Sebastien Elie Hadjadj[1], Clara Trommer[2], Jorge Torres[1], Jendrik Gördes[1], David Swerev[1], Christian Lotze[1], Chen Luo[3], Florin Radu[3], Felix Tuczek[2], Sangeeta Thakur[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Institut für Anorganische Chemie, Christian-Albrechts Universität zu Kiel — [3]Helmholtz Zentrum Berlin for Materialien und Energie

The spin-crossover (SCO) properties of the dinuclear complex $[\{Fe(H_2B(pz)_2)_2\}_2\mu - (ac(bipy)_2)]$ deposited as (sub)-monolayer and thin film by an ultra-high-vacuum liquid-jet deposition technique on highly oriented pyrolytic graphite (HOPG) were studied by X-ray absorption spectroscopy. A comparison of the SCO properties of thin films and a dropcast sample indicates that the spin-switching capability of the thin films is lower due to substrate*molecule interactions. The similar switching properties of the dropcast sample as of a bulk powder sample confirm that the SCO properties are not affected by the presence of solvent necessary for deposition. The soft-X-ray-induced excited spin-state trapping (SOXIESST) effect is pronounced in all samples, although the light-induced high-spin (HS) fractions of the dropcast and the thin-film samples on HOPG are higher as compared to the HS fraction attained by SOXIESST, which confirms the sensitivity of the complex to light.

MA 17.2 Tue 14:15 H18

Magnetic Characterization of Antidot Arrays in NiFe Thin Films: Insights from Ferromagnetic Resonance and Micromagnetic Simulations — •Zeynep Reyhan Ozturk[1] and Fikret Yildiz[2] — [1]SESAME, Amman, Jordan — [2]Gebze Technical University, Kocaeli, Türkiye

Antidot arrays, patterned magnetic films with regular nonmagnetic holes, are gaining attention for their unique behaviors and applications in data storage and sensors [1]. These arrays modify magnetic properties by introducing stray field energy, enabling control over magnetic anisotropy and magnetization reversal [2].

Optimizing antidot size, spacing, and lattice symmetry allows precise control of switching fields, magnetoresistance, and spin-wave modes, making them ideal for advanced technologies [3]. Their dynamic behavior, particularly localized spin-wave modes, sets them apart from continuous films.

This study combines ferromagnetic resonance (FMR) and micromagnetic simulations to reveal the influence of antidot geometry on magnetic performance. Insights gained optimize thin-film properties for next-generation devices.

1.Kwon et al., Phys. Rev. B, 2013.
2.Duine et al., Phys. Rev. B, 2007.
3.Park et al., J. Appl. Phys., 2015.

MA 17.3 Tue 14:30 H18

Effect of Ag addition on structure, morphology and magnetism of CoCrFeMnNi micro powders prepared by HEBM — •Emmanouil Kasotakis, Ivan Tarasov, Tatiana Smoliarova, Michael Farle, and Natalia Shkodich — Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany

We fabricated (CoCrFeMnNi)-Agx (x=0; 2; 5; 10 wt.%) high entropy alloy nanocrystalline (~10 nm) microparticles which are paramagnetic at room temperature (Tc = 80 K) by a two-step high energy ball milling (HEBM) [1] process in Argon at 700/1400 rpm. An elemental powder blend of Co, Cr, Fe, Mn, Ni was milled for 60 min to produce single phase FCC Cantor alloy with a homogeneous distribution of the principal elements, followed by 10 min of HEBM with the addition of Ag. By varying the Ag concentration, we modified the morphology. For 2 and 5 wt.% Ag (Cantor + Ag) we find flake-like core shell particles, and for 10 wt.% Ag, we obtain round homogeneous particles, with a lattice expansion of the FCC phase. Annealing cycles up to 700 K in a magnetic field of 1 T magnetic field increased M at 9 T up to 2.5-fold (14 Am^2/kg) for homogeneous particles (x = 10 wt.%) and Hc up to 5-fold (41 kA/m) for core shell particles (x = 2 wt.%) at 310 K. We acknowledge DFG financial support (project ID: FA209/27-1).

[1] N.F. Shkodich, M. Spasova, M. Farle, et al. J. Alloys Compd. 816, 152611 (2020).

MA 17.4 Tue 14:45 H18

Fabrication and characterization of freestanding magnetic nanostructures for microwave to photon transduction — •Matthias Grammer[1,2], Jonny Qiu[3], Sebastian Sailler[4], Sebastian T. B. Goennenwein[4], Matthias Althammer[1,2], Stephan Geprägs[1,2], Michaela Lammel[4], Eva Weig[3], and Hans Huebl[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]School of Computation, Information and Technology, TUM, Garching, Germany — [4]Department of Physics, University of Konstanz, Konstanz, Germany

Efficient transduction between microwave and optical photons is critical for quantum network applications. Engelhard et al. [1] proposed a trasduction scheme based on collective magnetic and elastic excitations as mediators between the microwave and the optical regime. Implementing this concept requires co-localization of microwave, magnetic and elastic excitations within a suspended microstructure resembling an optomechanical crystal (OMC). In this presentation we present our progress towards the fabrication of a OMC based on the ferrimagnetic insulator yttrium iron garnet (YIG). To realize freely suspendend structures we explore two fabrication strategies: (i) the structuring of grown YIG/SiO_x/GGG heterostructures and (ii) the integration of YIG on semiconductor substrates. We will report on fabrication aspects and the characterization of the resulting devices using e.g. scanning electron microscopy and magneto-optical Kerr effect measurements.

[1] F. Engelhardt et al., Phys. Rev. Applied 18, 044059 (2022).

MA 18: Functional Antiferromagnetism

Time: Tuesday 14:00–15:30 Location: H19

MA 18.1 Tue 14:00 H19

Switching of magnetic domains in a noncollinear antiferromagnet at the nanoscale — •Atul Pandey[1,2], Prajwal Rigvedi[1], Edouard Edouard[3], Jitul Deka[1], Jiho Yoon[1], Wolfgang Hoppe[2], James M. Taylor[2], Stuart S. P. Parkin[1], and Georg Woltersdorf[1,2] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Institute of Physics, Martin Luther University Halle Wittenberg, Von Danckelmann Platz 3, 06120 Halle, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Nothnitzer Straße 40, 01187 Dresden, Germany

Antiferromagnets that display very small stray magnetic field are ideal for spintronic applications. Of particular interest are non-collinear, chiral antiferromagnets of the type Mn_3X (X=Sn, Ge), which display a large magnetotransport response that is correlated with their antiferromagnetic ordering. The ability to read out and manipulate this ordering is crucial for their integration into spintronic devices. These materials exhibit a tiny unbalanced magnetic moment such that a large external magnetic field can, in principle, be used to set the material into a single antiferromagnetic domain. However, in thin films of Mn_3Sn, we find that such fields induce only a partial magnetic ordering. By detecting two orthogonal in-plane components of the magnetic order vector, we find that the non-switchable fraction has a unidirectional anisotropy. This also enables us to visualize switching along multiple easy axes in Mn_3Sn. Studying the switching at the nanoscale allows us to correlate the pining behavior to crystal grain boundaries in the Mn3Sn nanowire structures.

MA 18.2 Tue 14:15 H19

Understanding the role of spin non-conserving on magnon excitation — •Hebatalla Elnaggar — Sorbonne University, Paris, France

Conventional wisdom suggests that one photon that carries one unit of angular momentum (1h) can change the spin angular momentum of a magnetic site with one unit (*M* = *1h) at most following the selection rules. This implies that a two-photon process such as 2*3* resonant inelastic X-ray scattering (RIXS) can change the spin angular momentum of a magnetic system with a maximum of two units (*M* = * 2h). Herein we describe a triple-magnon excitation in *-Fe2O3 and various perovskite thin films, which contradicts this conventional wisdom that only 1- and 2-magnon excitations are possible in a resonant inelastic X-ray scattering experiment [1].

We observe an excitation at exactly three times the magnon energy, along with additional excitations at four and five times the magnon energy, suggesting quadruple and quintuple magnons as well. Guided by theoretical calculations, we reveal how a two-photon scattering process can create exotic higher-rank magnons due to spin non-conserving interactions.

References: 1- H. Elnaggar, et. al., Magnetic excitations beyond the single- and double-magnons, Nat. Commun. 14, 2749 (2023).

MA 18.3 Tue 14:30 H19

Domain wall patterns in granular Cr_2O_3 thin films — •Igor Veremchuk[1], Oleksandr V. Pylypovskyi[1], Peter Rickhaus[2], Natascha Hedrich[3], Artem V. Tomilo[1], Tobias Kosub[1], Kai Wagner[3], Brendan Shields[3], Gediminas Seniutinas[2], Vicent Borras[2], Paul Lehmann[3], Liza Žaper[2], Paulina J. Prusik[1], Pavlo Makushko[1], René Hübner[1], Jüren Fassbender[1], Denis D. Sheka[4], Patrick Maletinsky[3], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V.,01328 Dresden, Germany — [2]Qnami AG, CH-4132 Muttenz, Switzerland — [3]University of Basel, Basel CH-4056, Switzerland — [4]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

Cr_2O_3 provides possibility to control its magnetic order parameter by an external electric field rendering it a prospective material for spintronic applications. We developed a material model for granular thin Cr_2O_3 films. The coupling between the grains influences the equilibrium domain pattern due to pinning of antiferromagnetic domain walls at the grain boundaries. By the characterization of the experimentally measured domain patterns via fractal dimension, we determine the inter-grain exchange coupling [1]. In contrast to extended films, finite-size samples can be set into a single-domain state even via a zero-field cooling procedure. Such a sample should be small enough for the propagation of thermally driven domain walls through the energy landscape formed by grain boundaries [2].

[1] O. V. Pylypovskyi et al., Phys. Rev. Appl. 20, 014020 (2023). [2] P. Rickhaus, O. V. Pylypovskyi et al., Nano Lett. 24, 13172 (2024).

MA 18.4 Tue 14:45 H19

Domain walls properties and spin-flop transition in Cr_2O_3 — •Paulina J. Prusik[1,2], Igor Veremchuk[1], Florin Radu[3], Andrey N. Anisimov[1], Pavlo Makushko[1], Georgy V. Astakhov[1], Sophie F. Weber[4], René Hübner[1], Nicola A. Spaldin[4], Kirill D. Belashchenko[5], Jürgen Fassbender[1,2], Denys Makarov[1], and Oleksandr V. Pylypovskyi[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V. — [2]Dresden University of Technology, 01062 Dresden, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany — [4]ETH Zürich, 8093 Zürich, Switzerland — [5]University of Nebraska-Lincoln, Lincoln, NE 68588, USA

A room-temperature magnetoelectric uniaxial antiferromagnet Cr_2O_3 is a prospective material for spintronics and fundamental research [1,2]. We derive a σ-model for Cr_2O_3 and show the presence of a symmetry-breaking term relevant for non-collinear magnetic textures. It couples the magnetic field with a gradient of the Néel vector. Analyzing quantum magnetometry images of antiferromagnetic domain walls, we can properly describe the material parameters of Cr_2O_3. Furthermore, this term results in lowering of the spin-flop field for thin films of Cr_2O_3 by a factor of two comparing with single crystals. This finding is confirmed by X-ray magnetic linear dichroism measurements.

[1] J. Han et al., Nat. Mater. 22 (2023) 684; He et al, Nat. El. (2024) [2] P. Makushko et al., Nat. Comm. 13, 6745 (2022); O.V. Pylypovskyi et al., Phys. Rev. Let. 132, 226702 (2024); S.F. Weber et al., Phys. Rev. Lett. 130, 146701 (2023)

MA 18.5 Tue 15:00 H19

Current pulse driven switching mechanisms in antiferromagnetic Mn_2Au — •Jonathan Bläßer[1], Sonka Reimers[1], Yuran Niu[2], Evangelos Golias[2], Francesco Maccherozzi[3], Miriam Fischer[1], Guzmán Orero Gámez[1], Mathias Kläui[1], and Martin Jourdan[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]MAX IV Laboratory, Lund, Sweden — [3]Diamond Light Source, Chilton, Didcot, Oxfordshire, UK

In antiferromagnetic spintronics, reorientation of the staggered magnetization driven by current pulses can originate from different mechanisms. Investigating Mn_2Au, for longer pulses [Rei23] the thermal contribution is dominant. However, for pulses in the nanosecond range Néel spin-orbit torque switching is demonstrated.

[Rei23] S.Reimers et al., Nat Commun. 14, 1861 (2023)

MA 18.6 Tue 15:15 H19

Amplifying the antiferromagnetic spin Seebeck effect through topological magnons — Feodor Svetlanov Konomaev and •Kjetil Magne Dørheim Hals — Department of Engineering Sciences, University of Agder, 4879 Grimstad, Norway

Topological magnons emerge as topologically protected spin wave states at the edges of magnets. Here, we theoretically explore how these surface states can be harnessed to amplify the spin Seebeck effect (SSE) in antiferromagnets (AFMs) interfaced with normal metals (NMs). Based on a microscopic model of a kagome AFM, we demonstrate that broken mirror symmetry, combined with the Dzyaloshinskii-Moriya interaction (DMI), drives the system into a topological phase hosting spin-polarized magnons at the boundaries. Notably, linear response calculations reveal that in AFM/NM heterostructures, the topological magnons exhibit strong coupling to the metals charge carriers, resulting in a substantial enhancement of the SSE. The relative contribution of the topological magnons is found to be 4-5 times greater than that of the trivial magnon bands. Moreover, our results show that this enhancement is highly sensitive to the strength of the DMI.

MA 19: Magnetic Imaging and Sensors

Time: Tuesday 14:00–15:15 Location: H20

MA 19.1 Tue 14:00 H20

Green synthesis of R-type hexagonal ferrite magnetic nanoparticles and their electrochemical sensor for levofloxacin — •SAJJAD HUSSAIN — Centre of Excellence in Solid State Physics, University of the Punjab, Lahore

The usage of Levofloxacin (LEV) has increased in recent years for the treatment of bacterial infections in both human and veterinary fields. In this context, there has been a significant demand for the development of a highly sensitive and cost-effective approach to LEV quantification. In this study, R-type hexagonal ferrite nanoparticles (SrSn2Fe4O11-NPs) were prepared by an auto-ignition methodology and various analytical techniques were used for the material characterization, including X-ray diffraction (XRD), Field emission scanning electron microscopy (FE-SEM), X-ray photoelectron spectroscopy (XPS), Brunauer Emmett and Teller (BET) analysis, dynamic light scattering (DLS), and vibrating sample magnetometer (VSM) analysis. The characterization confirmed that the prepared material has a crystalline structure single-phase with a crystalline size of 35.02 nm. The R-type hexagonal ferrite nanoparticles were immobilized on a glassy carbon electrode (GCE) by a simple drop-casting approach to developing an efficient electrochemical sensor (SrSn2Fe4O11-NPs) for sensitive and selective LEV detection through an extended concentration range (0.06 * 10*6 to 170 * 10*6 M) and a low detection limit of (41.5nM). The developed sensor was applied successfully to quantitatively determine LEV in clinical samples and pharmaceutical preparations with excellent recoveries from 95.2 to 102.5 %.

MA 19.2 Tue 14:15 H20

Signatures of Berezinskii-Kosterlitz-Thouless transitions in magnetic films in Nitrogen Vacancy Magnetometry — •Mark Potts and Shu Zhang — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Nitrogen vacancy magnetometry provides sensitive measurements of the correlation functions of magnetic degrees of freedom in a material. Recent experiments have applied this technique in the study of two dimensional thin films, candidates for realising the topological Berezinskii-Kosterlitz-Thouless phase transition. We present calculations of frequency dependent relaxation rates for nitrogen vacancy centres coupled to an XY-type magnetic film, and identify features characteristic of the transition to quasi-long ranged order, and show that algebraic spin correlations are inherited by the relaxation rate as a temperature dependent power-law at low frequencies.

MA 19.3 Tue 14:30 H20

Development of an Ultra High Vacuum and Low Temperature Scanning NV Magnetometer — •Sandip Maity[1], Ricardo Javier Peña Román[1], Dinesh Pinto[1,3], Klaus Kern[1,3], and Aparajita Singha[2,1] — [1]Max Planck Institute for Solid State Research, Stuttgart, German — [2]Technische Universität Dresden, Dresden, Germany — [3]Institut de Physique, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The nanoscale spatial resolution and calibration-free quantifiable magnetic field measurement capabilities of nitrogen-vacancy (NV) centers have enabled us to investigate the properties of magnetic spin textures with high magnetic sensitivity through scanning probe microscopy across a wide range of temperatures and pressure. I will be discussing the development of a scanning probe magnetometer capable of imaging magnetic nanostructures under ultra-high vacuum and low temperature. Moreover, we have integrated commercial NV tips with a home-built tip holder equipped with an AFM amplifier and microwave excitation on the tip (not on the sample), allowing us to have a magnetic image of any sample region without restriction. To exploit the quantifying nature of NV magnetometry using Optically Detected Magnetic Resonance, a coherent microwave (MW) delivery to the probe is mandatory. I will also discuss different means of delivering MW to the NV probes through different designs of the tip holders and how effective they are in coherently manipulating the NV spin states.

MA 19.4 Tue 14:45 H20

On-surface Spin Characterization using Shallow NV Centers in Diamond — •Olga Shevtsova[1,2], Atharva Paranjape[2], Lisa Ebo[2,3], Bernhard Putz[4], Ulrich Ziener[4], Marvin Grünhagen[5], Rainer Herges[5], and Aparajita Singha[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Universität Konstanz, Konstanz, Germany — [4]Universität Ulm, Ulm, Germany — [5]Christian-Albrechts-Universität zu Kiel, Kiel, Germany

As interest in quantum systems surges due to their potential applications in quantum computing, information storage, and sensing, molecular spins emerge as promising candidates for these technologies. Unlike conventional systems such as superconducting qubits and trapped ions, molecular spins offer unique advantages in stability, tunability, and scalability. However, key challenges remain in assessing their coherent properties, which are crucial for practical application. Existing techniques face limitations in terms of environmental requirements, complexity, and invasiveness. In this context, Nitrogen-Vacancy (NV) centers in diamonds emerge as a highly suitable solution, as they can operate at a wide range of temperatures and provide non-invasive optical readout. This study aims to leverage on the capabilities of NV-center-based sensors to probe the coherent properties of molecular spins, thus providing insights into their viability as stable and controllable components for future quantum technologies.

MA 19.5 Tue 15:00 H20

Imaging magnetic vortices in a van der Waals magnet at room temperature with scanning NV magnetometry — •Carolin Schrader[1], Elias Sfeir[1], Mário Ribeiro[2], Giulio Gentile[2], Alain Marty[2], Céline Vergnaud[2], Frédéric Bonell[2], Isabelle Robert-Philip[1], Matthieu Jamet[2], Vincent Jacques[1], and Aurore Finco[1] — [1]Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France — [2]Université Grenoble Alpes, CEA, CNRS, IRIG-SPINTEC, Grenoble, France

Two-dimensional van der Waals (vdW) magnets have gained significant attention for their potential application in spintronics, however, this would require room temperature magnetism and large-scale fabrication. Recently, ferromagnetic order at room temperature has been demonstrated in thin Fe_5GeTe_2 grown by Molecular Beam Epitaxy (MBE). Here, we employ scanning NV magnetometry to quantitatively image the magnetic texture in MBE-grown Fe_5GeTe_2 at the nanoscale. We use the single spin of the nitrogen-vacancy (NV) defect in diamond to investigate the effect of patterning on the magnetic order and demonstrate the stabilisation of magnetic vortices in various micron-sized structures at room temperature. Upon application of an external magnetic field of a few mT we obtain a single ferromagnetic domain in these structures, which allows us to extract a saturation magnetisation of about 160 kA/m. Our results show the role of confinement for the stabilisation of complex magnetic structures in 2D magnets and highlight the potential of the room temperature vdW magnet Fe_5GeTe_2 for applications in spintronics.

MA 20: Magnonics II

Time: Wednesday 9:30–13:15 Location: H16

MA 20.1 Wed 9:30 H16

Wavenumber-dependent magnetic losses in YIG-GGG heterostructures at millikelvin temperatures — •David Schmoll[1], Andrey A. Voronov[1], Rostyslav O. Serha[1], Denys Slobodianiuk[2], Khrystyna Levchenko[1], Claas Abert[1], Sebastian Knauer[1], Dieter Suess[1], Roman Verba[2], and Andrii V. Chumak[1] — [1]University of Vienna, Vienna, Austria — [2]V.G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, Kyiv, Ukraine

With its low magnetic damping, the ferrimagnet yttrium iron garnet (YIG), grown on gadolinium gallium garnet (GGG), is the most promising material for magnon based quantum technologies, wich demand long decoherence times. While such samples are already well established at room temperature, further knowledge needs to be acquired at millikelvin temperatures, due to the paramagnetic character of the GGG substrate. We report on propagating spin-wave spectroscopy studies at temperatures between 4 K to 26 mK and the recorded change of the dissipation rate. Additionally, we compute the dispersion and the dissipation rate of the layered YIG-GGG magnetic system quasi- analytically and with micromagnetic simulations, allowing us to investigate the magnon losses with respect to wavenumber. Contrary to room temperature, we observe a significant increase of the magnetic losses with k at cryogenic temperatures, introduced by the dipolar coupling between the ferrimagnetic YIG film and the partially magnetized GGG substrate. Our theoretical calculations predict a steady decrease of the dissipation for short-wavelength exchange magnons.

MA 20.2 Wed 9:45 H16

Exchange enhanced switching in quantum antiferromagnets with dephasing and relaxation — •Asliddin Khudoyberdiev and Götz S. Uhrig — Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

One requirement for ultrafast storage devices is that they can be operated in the terahertz (THz) regime. Suitable candidates are antiferromagnets because of their characteristic frequencies range. The efficient control of their order is the focus of a plethora of current studies. Recently, we established a quantum approach, time-dependent Schwinger boson mean-field theory, to reverse the sublattice magnetization in anisotropic quantum antiferromagnets by means of external static and oscillating magnetic fields [1,2]. We also showed that the exchange enhancement for staggered control fields persists on the quantum level so that significantly lower fields are sufficient to switch the order [3]. Our quantum theory incorporates dephasing, i.e., the destructive interference of the contributions of all spin modes at their respective frequencies, which results in a slow, non-exponential decrease of the oscillations after the switching [2,3]. This must be distinguished from spin-lattice relaxation which induces faster decay of oscillations. Our methodological progress including Lindblad dissipators allows us to address the differences between dephasing and spin-lattice relaxation in the switching processes. [1] K. Bolsmann, A. Khudoyberdiev, and G. S. Uhrig, PRX Quantum 4, 030332 (2023) [2] A. Khudoyberdiev and G. S. Uhrig, Phys. Rev. B 109, 174419 (2024) [3] A. Khudoyberdiev and G. S. Uhrig, arXiv:2407.00472.

MA 20.3 Wed 10:00 H16

Non-linear processes in YIG based spin-wave transducers — •Matthias Wagner, Felix Kohl, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Spin waves are considered as promising candidates for the realization of future signal processing devices. Due to their fundamental equation of motion, spin-wave dynamics are inherently non-linear. For the practical application of spin-wave based devices, this non-linear nature can either be a perspective or a challenge, depending on the desired use case. Therefore, a systematic study on the impact of non-linear dynamics on a potential spin-wave based device is instructive. For this purpose, spin-wave transducers patterned on yttrium iron garnet (YIG) films are investigated. Using micro-focused and time-resolved Brillouin light scattering spectroscopy, the power-limiting non-linear processes as well as their scattering dynamics are analysed. The characterization is complemented by propagating spin-wave spectroscopy measurements to study the corresponding impact of the non-linear processes on the output of the spin-wave transducers. The results of this work provide an important foundation to develop new concepts of signal processing devices using spin waves. This research is funded by the European Union within HORIZON-CL4-2021-DIGITAL-EMERGING-01 (No. 101070536,MandMEMS).

MA 20.4 Wed 10:15 H16

Higher Order Resonances in Periodically Driven Magnon Systems — •Jan Mathis Giesen, Alexandre Abbass Hamadeh, Philipp Pirro, Imke Schneider, and Sebastian Eggert — RPTU, Kaiserslautern, Germany

We analyze resonant excitations of ferromagnetic magnons via microwave pumping below the threshold frequency using Floquet theory. A special feature of parameteric resonance is the possibility to create magnons with higher energy

than the driving frequency, which allows for new tuning possibilities. We develop a theoretical framework that analytically predicts the region of resonances and resonance thresholds in thin films of ferro- and ferri-magnetic materials as a function of damping, amplitude and frequency. The results are compared with micomagnetic simulations.

MA 20.5 Wed 10:30 H16

SAW-Induced Spin Wave Excitation in Ferromagnetic Epitaxial Thin Films — •Alfons Georg Schuck, Sebastian Kölsch, and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Surface acoustic wave (SAW) excitation of spin waves in ferromagnetic thin films has recently gained significance due to the potential for the realization of novel microwave devices and applications in magnonics. So far, SAW excitation has commonly been accomplished by use of piezoelectric substrate materials, such as $LiNbO_3$, on top of which the ferromagnetic thin film is deposited [1]. This approach has severe limitations with regard to studying SAW-spin wave coupling effects in epitaxial magnetic thin films. For epitaxy to occur, selected substrate materials and crystal orientations have to be used; and these substrate materials tend not to be piezoelectric.

Here we show how textured piezoelectric AlN thin film transducer structures can be fabricated on different substrate materials by means of reactive RF sputtering. By proper selection of the material for the interdigital transducer electrode structures and standard UV lithography, the frequency range up to about 3 GHz becomes available for spin wave excitation. Selected examples of SAW-induced spin wave excitation in epitaxial magnetic thin films are presented and compared to results obtained on Nickel thin films as commonly used reference material. Complementary simulations of the SAW attenuation are shown and the influence of the magnetic anisotropy is described.

[1] M. Weiler et. al., Phys. Rev. Lett. **106**, 117601, **2011**

MA 20.6 Wed 10:45 H16

Integrated hybrid magnonic-spintronic system for tunable broadband signal filtering and microwave generation — •Abbas Koujok[1], Abbass Hamadeh[1,2], Leandro Martins[3], Felix Kohl[1], Björn Heinz[1], Ricardo Ferreira[4], Alex Jenkins[4], Ursula Ebels[3], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Université Paris-Saclay, Centre de Nanosciences et de Nanotechnologies, CNRS, 91120, Palaiseau, France — [3]Univ. Grenoble Alpes, CEA, CNRS, Grenoble INP, IRIG, Spintec, Grenoble, France — [4]International Iberian Nanotechnology Laboratory (INL), 4715-31 Braga, Portugal

Non-conventional beyond-the-state-of-the-art signal processing schemes require parallelism, scalability, robustness and energy efficiency to meet the demands of complex data-driven applications. Magnonic and spintronic circuits are potential candidates that can aid in fulfilling these requirements. Hereby, an experimental proof-of-concept for a novel hybrid magnonic-spintronic device is proposed. Using spintronic auto-oscillations, this device can generate a broad, GHz-wide RF signal and filter this signal in a selective and tunable manner using a magnonic circuit. This research is funded by the European Research Council within the Starting Grant No. 101042439 "CoSpiN" and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - TRR 173-268565370 (project B01). U.E. acknowledges financial support from CEA PTC-21ID26 MINOS.

MA 20.7 Wed 11:00 H16

Spatially Resolved Investigation of Spin Wave frequency Multiplication — •Roméo Beignon[1], Chris Körner[2], Rouven Dreyer[2], Georg Woltersdorf[2], Vincent Jacques[1], and Aurore Finco[1] — [1]Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Interactions between spin waves and magnetic textures offer promising tools for designing magnonic devices. Among new developments, a frequency multiplication phenomenon has been observed in permalloy microstructures [1]. This generation of a high harmonic frequency has been observed using magnetic resonance measurements on NV center ensembles.

Here, we use scanning NV-center microscopy to investigate this phenomenon further. Our aim is to obtain maps of the harmonic generation with a spatial resolution of about 50 nm, and to correlate them with the magnetic state of the Py microstructures (edges, domain walls, ...).

Our results show that we can detect the spin wave frequency comb with a single NV center in a scanning probe tip. Furthermore, we are able to spatially map the effect of each harmonic on the NV center separately, revealing a non-trivial behavior. These measurements are a first step towards the understanding of the interplay between the non-linear process that generates the harmonics and the magnetic texture.

[1] Köerner et al., Science 375. 1165-1169 (2022)

15 min. break

MA 20.8 Wed 11:30 H16

Tayloring spin-wave transducers for integrated RF application — •Felix Kohl, Björn Heinz, Matthias Wagner, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Current advances in magnonics are increasingly targeted at improving the functional applicability of integrated magnonic devices. Despite the widespread use of transducers based on dynamic Oersted field excitation, there are still inefficiencies due in part to a discrepancy between the scientific understanding of magnetic responses and the technical requirements for practical implementation. Using propagating spin-wave spectroscopy, we investigated spin-wave transducers patterned on yttrium-iron-garnet (YIG) films, demonstrating the capability to tailor transducer characteristics, such as non-reciprocity towards a desired use case. Supported by a modelling approach, our measurements provide a useful framework for designing efficient, application-specific transducers and pave the way for integrated and standalone RF devices such as isolators and filters. This work is an important step towards scalable, energy-efficient magnonic application and demonstrates the potential of magnonics to become a future technology. This research is funded by the European Union within HORIZON-CL4-2021-DIGITAL-EMERGING-01 (No. 101070536,MandMEMS).

MA 20.9 Wed 11:45 H16

Investigation of parallel parametric signal amplification in YIG nanostructures — •Akira Lentfert, Björn Heinz, David Breitbach, Burkard Hillebrands, and Philipp Pirro — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

In the pursuit of advanced information processing beyond traditional CMOS technologies, various magnonic circuits and devices such as magnon transistors, majority gates, and half adders have been developed. However, for an extended magnonic network, a phase-conserving and sensitive amplification of spin waves is required. One of the candidates is the use of the parallel parametric pumping process. A phase-conserving signal amplification in microscopic metallic waveguides has already been demonstrated in previous works. In this work, we focus on the phase dependence of the parallel parametric amplification processes in Damon-Eschbach (DE) geometry in yttrium iron garnet (YIG) nanowaveguides for propagating spin waves. Due to the low spin-wave damping in YIG, other damping mechanisms such as radiative losses have a significant impact on the pumping processes. Time-resolved micro-focused Brillouin light scattering spectroscopy is used to study the phase-dependent amplification of short spin-wave pulses. This project has been supported by the EU Horizon research and innovation program within the SPIDER project (No. 101070417) and by DFG (TRR 173-268565370: Spin+X).

MA 20.10 Wed 12:00 H16

Nanoscaled Spin-Wave Frequency Selective Limiter (FSL) for 5G Technology — •Kristýna Davídková[1], Khrystyna Levchenko[1], Florian Bruckner[1], Roman Verba[2], Fabian Majcen[1], Qi Wang[3], Carsten Dubs[4], Vincent Vlaminck[5], Jan Klíma[6], Michal Urbánek[6], Dieter Suess[1], and Andrii Chumak[1] — [1]University of Vienna, Austria. — [2]Institute of Magnetism, Ukraine. — [3]School of Physics, China. — [4]INNOVENT e. V. Technologieentwicklung, Germany. — [5]IMT Atlantique, France — [6]CEITEC BUT, Czech Republic

Power limiters are essential devices in radio frequency communications systems to protect the input channels from large incoming signals. Nowadays-used semiconductor limiters suffer from high electronic noise and switching delays when approaching the GHz range, which is crucial for the modern generation of 5G communication technologies aiming to operate at the EU 5G high band (24.25-27.5 GHz). The proposed solution is to use ferrite-based Frequency Selective Limiters (FSLs), which maintain their efficiency at high GHz frequencies, although they have only been studied at the macroscale so far. We demonstrate a proof of concept of nanoscale FSLs based on spin-wave transmission affected by four-magnon scattering phenomena in a 97-nm-thin YIG film. Spin waves were excited and detected using coplanar waveguide transducers of the smallest feature size of 250 nm. The FSLs are tested in the frequency range up to 25 GHz, and the key parameters are extracted (power threshold, power limiting level, insertion losses, bandwidth) for different SW modes and transducer lengths.

MA 20.11 Wed 12:15 H16

Uniaxial strain response of antiferromagnetic magnons — •Manuel Knauft, Arthur von U.-S. Schwark, Yiran Liu, Lichen Wang, Sajna Hameed, Matteo Minola, and Bernhard Keimer — Max Planck Institute for Solid State Research, Stuttgart, Germany

With the suggested paradigm shift away from conventional transistors towards lower loss devices, magnonics has attracted considerable attention in recent years. Generation, manipulation and detection of magnons are prerequisites for successful integration into microstructured chips. We will present ideas and results of using uniaxial strain to control magnon behavior in perovskite antiferromagnets. In particular, recent work on iridates has shown that the magnon energy can be varied by as much as 40 % with small uniaxial strain of about

0.1 % [1]. Building on those findings, we discuss alternative approaches. Furthermore, through spatially inhomogeneous strain environments, we will also demonstrate ideas of guiding magnons as investigated using finite element simulation and confocal Raman scattering.

[1] Kim *et al.*, Nat. Commun. **13**, 6674 (2022)

MA 20.12 Wed 12:30 H16

cavity-enhanced optical manipulation of Antiferromagnetic magnon-pairs — •Tahereh Parvini — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Str.8, 85748 Garching, Germany

The optical manipulation of magnon states in antiferromagnets (AFMs) holds the potential for advancing AFM-based computing devices. In particular, two-magnon Raman scattering processes are known to generate entangled magnon-pairs with opposite momenta. We propose to harness the dynamical backaction of a driven optical cavity coupled to these processes, to obtain steady states of squeezed magnon-pairs, represented by squeezed Perelomov coherent states. The system's dynamics can be controlled by the strength and detuning of the optical drive and by the cavity losses. In the limit of a fast (or lossy) cavity, we obtain an effective equation of motion in the Perelomov representation, in terms of a light-induced frequency shift and a collective induced dissipation which sign can be controlled by the detuning of the drive. In the red-detuned regime, a critical power threshold defines a region where magnon-pair operators exhibit squeezing, a resource for quantum information, marked by distinct attractor points. Beyond this threshold, the system evolves to limit cycles of magnon-pairs. In contrast, for resonant and blue detuning regimes, the magnon-pair dynamics exhibit limit cycles and chaotic phases, respectively, for low and high pump powers. Observing strongly squeezed states, auto-oscillating limit cycles, and chaos in this platform presents opportunities for future quantum technologies.

MA 20.13 Wed 12:45 H16

Predicting the future with magnons — •Zeling Xiong[1,2], Christopher Heins[1,2], Katrin Schultheiss[1], Helmut Schultheiss[1], Thibaut Devolder[3], and Joo-Von Kim[3] — [1]Helmholtz-Zentrum Dresden Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]Centre de Nanosciences et de Nanotechnologies, CIderNRS, Université Paris-Saclay, France

The Mackey-Glass (MG) time series data describes how density of mature circulating cells change over time using time delayed differential equations. This is a standard problem to test the performance of physical reservoirs. Here, we used different magnon reservoir systems to carry out such time series prediction task. By connecting several reservoirs together we increase the reservoir depth which yielded very accurate long-time future prediction.

MA 20.14 Wed 13:00 H16

Dynamic Control of Spin-Wave Propagation for Advanced Computing Applications — •Dmitrii Raskhodchikov[1], Kirill Nikolaev[2], Jannis Bensmann[1], Rudolf Bratschitsch[1], Vladislav Demidov[2], Sergey Demokritov[2], and Wolfram Pernice[1,3] — [1]Institute of Physics and Center for Nanotechnology (CeNTech), Muenster, Germany — [2]Institute of Applied Physics, Muenster, Germany — [3]Kirchhoff-Institute for Physics, Heidelberg, Germany

Spin waves, collective excitations of electron spins in magnetic materials, have attracted significant interest for spin-wave and neuromorphic computing applications. A key challenge in utilizing spin waves for these technologies is achieving precise control over their propagation. This study investigates methods to regulate spin-wave dynamics by manipulating parameters like the external magnetic field, excitation frequency, and the integration of external memory elements, including phase-change materials.

Our results show that varying the external magnetic field influences the dispersion relation of spin waves, allowing for tunable propagation velocities and wavelengths. Adjusting the excitation frequency enables selective excitation of spin-wave modes with desired properties. Furthermore, incorporating phase-change materials allows for dynamic modulation of spin-wave propagation through localized changes in magnetic anisotropy or damping. This approach provides a foundation for adaptive control mechanisms essential for spin-wave-based information processing.

MA 21: Frustrated Magnets I

Time: Wednesday 9:30–12:45 Location: H18

MA 21.1 Wed 9:30 H18

Ab-initio exploration of complex magnetism of frustrated Mn and Cr films on hexagonal metallic surfaces — •Selcuk Sözeri[1,2] and Samir Lounis[2,1] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

We employ ab initio first-principles simulations to explore the complex magnetic behavior in antiferromagnetic (AFM) systems. Specifically, we investigate Mn films on an Ag(111) substrate, where spin-polarized STM experiments established Néel order as the ground state for a single Mn layer [1,2] in contrast to previous predictions. Our focus extends to the interplay of Heisenberg exchange interactions, leading to magnetic frustration, and higher-order magnetic interactions when increasing the thickness of Mn films, which can host complex three-dimensional AFM spin-textures. Additionally, we examine the magnetic properties of multiple AFM Cr layers deposited on a PdFe bilayer supported by an fcc Ir(111) substrate. Instead of being in a Néel state, a single Cr layer prefers a row-wise AFM state, which hosts single and catenated intrinsic AFM skyrmions [3]. For thicker Cr films, we monitor the emergence of new topological magnetic objects.

– Project funded by DFG (SPP 2137: LO 1659/8-1).

– [1] Gao, et al., PRL 101, 267205 (2008); [2] Sözeri et al., submitted (2024); [3] Aldarawsheh et al., Nat. Commun.13, 7369 (2022); Front. Physics. 11, 335 (2023).

MA 21.2 Wed 9:45 H18

Dilatometry studies on the spin supersolid candidate materials $K_2Co(SeO_3)_2$ and $Rb_2Co(SeO_3)_2$ — •Erik Walendy[1], Kwangwoo Shin[2], Jae-Ho Chung[2], Kwang-Yong Choi[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Physics, Korea University, Seoul 02841, Korea

The layered triangular lattice material $K_2Co(SeO_3)_2$ has recently attracted attention due to the presence of a high-field spin supersolid phase between 18 and 21 T, at 2 K [1]. We report high-resolution capacitance dilatometric studies on single crystals of $K_2Co(SeO_3)_2$ and $Rb_2Co(SeO_3)_2$. Pronounced anomalies in thermal expansion and magnetostriction measurements at the phase boundaries imply significant magnetoelastic coupling. We obtain the uniaxial strain dependencies of the field-induced phases and construct the magneto-elastic phase diagrams.

[1] T. Chen et al. arXiv:2402.15869 (2024).

MA 21.3 Wed 10:00 H18

NMR Study of the $S = 1/2$ 1D Heisenberg Antiferromagnetic Chain $Cu(C_6H_8N_2)ClBr$ — •Marlis Schuller[5], Monika Jawale[1], Avinash Mahajan[1], Sanjay Bachhar[1], Saikat Nandi[1], Rahul Kumar[2], Athinarayanan Sundaresan[2], John Wilkinson[3], Rabindranath Bag[4], Sara Haravifard[4], Norbert Büttgen[5], Thomas Gimpel[5], and István Kézsmárki[5] — [1]Department of Physics, IIT Bombay, IN — [2]CPMU, JNCASR, IN — [3]ISIS Facility, STFC Rutherford Appleton Laboratory, GB — [4]Department of Physics, Duke University, US — [5]EPV, Institute of Physics, University of Augsburg, DE

$Cu(C_6H_8N_2)ClBr$ is a possible candidate for realising the frustration-induced quantum spin-liquid phase, as proposed in a recent theoretical study by Uematsu *et al.* (JPSJ **90**, 124703 (2021)) on the random-bond $S = 1/2$ Heisenberg antiferromagnet on the zigzag chain. Based on μSR and bulk susceptibility data, it does not display any long-range order down to 88 mK. Mixing chlorine and bromine may generate randomness in the nearest-neighbour exchange necessary to satisfy the criteria from the aforementioned proposal. We investigated this compound by ^{1}H-NMR, and determined the spin-lattice relaxation rate $1/T_1(T)$ to probe low-energy excitations. Our study revealed a discontinuity in the relaxation rate at a characteristic temperature of approximately 2.5 K, where anomalies were observed in the specific heat and μSR experiments. These experimental results imply the emergence of a dimerised ground state.

MA 21.4 Wed 10:15 H18

Geometric design of frustrated magnetic textures in ferrotoroidal spin chains — •Oleksandr V. Pylypovskyi[1], Enrico Di Benedetto[2], Carmine Ortix[3], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]Università degli Studi di Palermo, 90123 Palermo, Italy — [3]Università di Salerno, IT-84084 Fisciano (SA), Italy

Design of geometric shapes in magnetic nanosystems provides a possibility to tune their magnetic responses [1] and even enable multiferroicity by a finite geometry-driven toroidal moment [2]. Here, we consider the effects of ring-like geometries with a constant torsion on properties of 3D ferro- (FM) and anti-

ferromagnetic (AFM) spin chains. Their magnetic state is primarily determined by the knots in geometry with a high curvature, which corresponds to a localized geometry-driven Dzyaloshinskii–Moriya interaction (DMI). This DMI favors the twist of the order parameter at the knot. For the AFM chains with even and odd number of spins, the number of knots in their geometry allows designing the ground-state magnetic texture characteristic either for the spin system with or without geometric frustration. While the FM chains with the easy tangential axis of magnetization host a large toroidal moment for the whole sample, AFM hard-axis chains split into toroidal domains by geometric knots. To conclude, the localized geometry-driven DMI offers a possibility to design frustrated magnetic textures in spin chains.

[1] D. Makarov et al., Adv. Mater. 34, 2101758 (2022). [2] C. Ortix, J. van den Brink, Phys. Rev. Research, 5, L022063 (2023).

MA 21.5 Wed 10:30 H18

High-temperature expansion of dynamical spin correlator: Dyn-HTE — •Ruben Burkard[1], Benedikt Schneider[2,3], and Björn Sbierski[1] — [1]Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Currently, there is a scarcity of theoretical methods to calculate dynamical correlation functions at finite temperatures in frustrated spin systems. To address this challenge, we extend the well-established method of high-temperature expansion to the dynamical two-point Matsubara Green's function, which we calculate to high order in perturbation theory. We consider Heisenberg models with one coupling constant J, arbitrary spin length, and without external magnetic field. We use resummation techniques to extrapolate our results to temperatures down to about $T \approx 0.2J$. Our method also gives an analytical expression for the frequency dependence, enabling analytical continuation to real frequencies. Using the dynamical information of the Matsubara correlator, we aim to study spin-liquid phases with this approach in the future.

MA 21.6 Wed 10:45 H18

Pseudo-Majorana Functional Renormalization for Frustrated XXZ-Z Spin-1/2 Models — Ruben Burkard[1], Benedikt Schneider[2], and •Björn Sbierski[1] — [1]Universität Tübingen — [2]LMU München

The numerical study of high-dimensional frustrated quantum magnets remains a challenging problem. Here we present an extension of the pseudo-Majorana functional renormalization group to spin-1/2 XXZ type Hamiltonians with field or magnetization along spin-Z direction at finite temperature. We consider a U(1) symmetry-adapted fermionic spin representation and derive the diagrammatic framework and its renormalization group flow equations. We discuss benchmark results and application to two anti-ferromagnetic triangular lattice materials recently studied in experiments with applied magnetic fields: First, we numerically reproduce the magnetization data measured for CeMgAl11O19 confirming model parameters previously estimated from inelastic neutron spectrum in high fields. Second, we showcase the accuracy of our method by studying the thermal phase transition into the spin solid up-up-down phase of Na2BaCo(PO4)2 in good agreement with experiment.

15 min. break

MA 21.7 Wed 11:15 H18

NMR study of the field-induced magnetic states in Cu-based mineral $Cu_2(OH)_3NO_3$ — •Yoshihiko Ihara[1], Issei Niwata[1], Aswathi M. Chakkingal[2], Dmytro Inosov[2], and Darren Peets[2] — [1]Hokkaido University, Sapporo, Japan — [2]TU Dresden, Dresden, Germany

Magnetic ground states are stabilized at low temperature by minimizing the energy costs for magnetic moments interacting with each other. When the interactions compete by geometrical frustration in the case of a non-bipartite lattice or by the bond-dependent sign of interactions, the magnetic ground state cannot be easily selected and the perturbation by external fields can modify the ground state introducing a nontrivial magnetic state with intriguing properties. Here, we focus on the Cu-based mineral rouaite, $Cu_2(OH)_3NO_3$, in which $S = 1/2$ Cu^{2+} spins construct both ferromagnetic (FM) and antiferromagnetic (AFM) chains in a unit cell. Competing FM and AFM interactions result in complicated field-temperature phase diagram with at least three different magnetic states. We study the magnetic structure and the low-energy magnetic excitations by measuring the NMR spectra and the nuclear spin-lattice relaxation rate. The low-field magnetic structure is identified and compared with the results of neutron diffraction measurements. We will also discuss the external magnetic field effect on the magnetic ground state from the results of NMR measurements at higher magnetic fields.

MA 21.8 Wed 11:30 H18

Magnetic Properties of the Frustrated Cu-based Quantum Magnets Posnjakite, Kobyashevite, and Ktenasite — Kaushick K. Parui[1], Anton A. Kulbakov[1], Roman Gumeniuk[2], Sergey Granovsky[1], Dmytro S. Inosov[1], and •Darren C. Peets[1] — [1]IFMP, TU Dresden, Germany — [2]IEP, TU Bergakademie Freiberg, Germany

Posnjakite, kobyashevite, and ktenasite are copper hydroxide sulphates in which the magnetic copper sites are arranged in distorted-triangular planes. Such a magnetic sublattice is expected to lead to strong geometric frustration, which can produce exotic magnetic order. We report the synthesis of all three materials and the results of our investigations into their low temperature magnetic properties by magnetization, specific heat, and diffraction. All three compounds indeed exhibit low magnetic transition temperatures with high frustration factors, confirming that frustration plays a key role in selecting their magnetic ground states.

MA 21.9 Wed 11:45 H18

The role of quantum fluctuations in rare-earth pyrochlore oxides — •Lasse Gresista[1], Daniel Lozano-Gómez[2], Simon Trebst[1], and Yasir Iqbal[3] — [1]Institute for Theoretical Physics, University of Cologne — [2]Institut fur Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universitat Dresden — [3]Department of Physics and Quantum Center for Diamond and Emergent Materials (QuCenDiEM), Indian Institute of Technology Madras, Chennai, India

Rare-earth pyrochlore oxides provide a rich platform for exploring exotic magnetic phenomena, ranging from the highly degenerate spin-ice states governed by emergent gauge theories in $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$, to order-by-disorder effects in $Er_2Ti_2O_7$, multi-phase magnetism in $Yb_2Ti_2O_7$, and the ongoing quest to realize a quantum spin liquid state in experiment. Many of these materials are well described by localized spin-$\frac{1}{2}$ moments on a pyrochlore lattice coupled via anisotropic interactions. While the classical limit of this model has been extensively studied, a full quantum mechanical treatment remains challenging. In this work, we investigate the general spin-$\frac{1}{2}$ Hamiltonian using a pseudo-fermion functional renormalization group approach, which incorporates quantum fluctuations beyond mean-field theory. Our results reveal a significant shift in phase boundaries compared to the classical model, alongside the emergence of disordered regions without conventional magnetic order. This highlights the importance of quantum fluctuations when interpreting experimental observations in pyrochlore magnets.

MA 21.10 Wed 12:00 H18

Dynamical response of the Kitaev quantum spin liquid in the $KJ\Gamma$-model under external magnetic field — •Peng Rao[1], Roderich Moessner[2], and Johannes Knolle[1,3,4] — [1]Physics Department, Technical University of Munich, TUM School of Natural Sciences, 85748 Garching, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

We study the dynamical structure factor of the Kitaev quantum spin liquid (KQSL) generally, i.e. away from the solvable Kitaev limit, in the $KJ\Gamma$-model with external magnetic field. Using Majorana mean field theory, we compute spin susceptibility by including Majorana interactions in the random phase approximation (RPA). At zero field for the pure Kitaev model, RPA reproduces qualitatively spin susceptibility in the adiabatic approximation, which is close to the exact result. Small non -Kitaev couplings J and Γ induce sharp low-energy magnon modes as Majorana bound states. Larger couplings or finite field generally tend to weaken the KQSL and cause the sharp modes to condense, whence the system becomes magnetically ordered. However in specific paramter regimes, magnetic field may destroy the zero-field magnetic order and stabilize KQSL at intermediate field values, thus exemplifying the proposed 'field-induced KQSL'.

MA 21.11 Wed 12:15 H18

Short-range spin correlations in the 3D face-centred frustrated spin-$\frac{5}{2}$ system $MnSn(OH)_6$ — •Kaushick K. Parui[1], Anton A. Kulbakov[1], Ellen Häussler[2], Nikolai S. Pavlovskii[1], Roman Gumeniuk[3], Thomas Doert[2], Maxim Avdeev[4], Dmytro S. Inosov[1], and Darren C. Peets[1] — [1]IFMP, TU Dresden, Germany — [2]AC II, TU Dresden, Germany — [3]IEP, TU Bergakademie Freiberg, Germany — [4]ANSTO, Australia

Manganese tin hydroxide, $MnSn(OH)_6$, is an A-site-vacant double perovskite with magnetic Mn^{2+} ions on a face-centred sublattice, creating frustration that may lead to exotic magnetism. Combined x-ray and neutron diffraction data analysis reveals tetragonal $P4_2/n$ symmetry with precise H/D positions. Despite dominant antiferromagnetic interactions among Mn^{2+} moments, evidenced by a negative Curie-Weiss temperature, the lack of a sharp thermodynamic transition down to 350 mK implies the absence of long-range magnetic order. This suppression of the magnetic order hints towards a large frustration factor >10. Low-temperature neutron diffraction performed at 20 mK shows the absence of sharp magnetic Bragg peaks but reveals broad diffuse peaks, indicating 3D anti-

ferromagnetic short-range interactions with a correlation length of roughly three unit cells.

MA 21.12 Wed 12:30 H18

Understanding the Hamiltonian of α-$RuCl_3$ through Nonlinear Spin-Wave Analysis — •Jonas Habel[1,2], Roderich Moessner[3] und Johannes Knolle[1,2,4] — [1]Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [4]Blackett Laboratory London, UK

The precise values of the magnetic exchange couplings in α-$RuCl_3$ are of significant interest to understand the proposed Kitaev spin-liquid phase. A common method for extracting them involves fully field-polarizing the magnetic moments, performing an inelastic neutron scattering (INS) experiment, and fitting a non-interacting (linear) spin-wave theory to the data. However, due to magnetic frustration, magnon many-body interactions are strong in α-$RuCl_3$ and cannot be neglected, even at high fields. We present a procedure for fitting an interacting (nonlinear) spin-wave theory to INS data, explicitly accounting for these many-body interactions. This reveals a significant renormalization of the exchange couplings compared to linear spin-wave estimates.

MA 22: Caloric Effects in Ferromagnetic Materials

Time: Wednesday 9:30–11:30 Location: H19

MA 22.1 Wed 9:30 H19

Utilizing frustration in Gd- and Yb-based oxides for milli-Kelvin adiabatic demagnetization refrigeration — •Tim Treu[1], Prachi Telang[1], Marvin Klinger[1], Alexander Tsirlin[2], Anton Jesche[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Felix Bloch Institute for Solid-State Physics, University of Leipzig

Gadolinium- and Ytterbium-oxide based frustrated magnets have recently been characterised as excellent millikelvin adiabatic demagnetization refrigerants [1]. They offer several advantages over conventional paramagnetic hydrated salts, such as higher entropy density at similar minimum temperatures, chemical stability and UHV compatibility. We present a comprehensive study of the structural, magnetic and thermodynamic properties as well as the adiabatic demagnetisation refrigeration performance of several different Gd- and Yb-based oxides (including [1-2] and further unpublished results). For the temperature range between 0.03 and 2 K, a systematic comparison of the field-induced entropy density change and the refrigerant capacity is provided, demonstrating the advantages of frustrated magnets for low-temperature ADR.

Work supported by the German Research Foundation through the project 514162746 (GE 1640/11-1).

[1] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025).
[2] P. Telang et al., arXiv:2411.04805

MA 22.2 Wed 9:45 H19

High-throughput design of all-d-metal Heusler alloys for transverse thermoelectric applications — •Fu Li, Hao Wang, Ruiwen Xie, and Hongbin Zhang — Technical University of Darmstadt, 64287 Darmstadt, Germany

Magnetic materials with prominent topological transport properties have been attracting significant attention due to the underlying intriguing physics and great potentials in various applications. Among these, Heusler alloys are particularly interesting because of their compositional flexibility which enables tunability of their physical properties via chemical doping. In this work, we perform high-throughput density functional theory calculations to evaluate the effects of chemical doping on the intrinsic anomalous Hall conductivity (AHC) and anomalous Nernst conductivity (ANC) in all-d-metal Heusler compounds, where chemical alloying with neighboring elements is considered using the virtual crystal approximation. The AHC and ANC are computed using the tight-binding Hamiltonian by automatically constructing the maximally localized Wannier functions. It is observed that rigid band model does not apply in all cases, because not only the Fermi energy has been shifted, but also the band structure has modified significantly. For (Pt0.7Ir0.3)2RhFe, detailed analysis reveals that the significant AHC and ANC are originated from the Weyl points close to the Fermi energy. These findings highlight the critical importance of chemical doping in the development of high-performance materials.

MA 22.3 Wed 10:00 H19

Electronic structure of all-*d*-metal Ni(-Co)-Mn-Ti vs. *p-d* Ni_2MnSn: DFT and XAS insights — •Olga Miroshkina[1], Johanna Lill[1], Benedikt Eggert[1], Benedikt Beckmann[2], David Koch[2], Franziska Scheibel[2], Katharina Ollefs[1], Wolfgang Donner[2], Oliver Gutfleisch[2], Heiko Wende[1], and Markus Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

All-*d*-metal Heusler alloys are a new class of promising caloric materials for energy efficient solid-state refrigeration [1]. We investigate the peculiar differences of the electronic structure between *d-d* Ni(-Co)-Mn-Ti and *p-d* Ni_2MnSn by combining density functional theory and x-ray absorption spectroscopy (XAS). To retrieve the distinctive characteristics of *d-d* orbital hybridization in K- and $L_{2,3}$-edges spectra, we correlate the features in the electronic densities of states (DOS) and XAS. The comparison of *d-d* Ni(-Co)-Mn-Ti with the conventional *p-d* Ni_2MnSn enables us to reveal the impact of the third *d*-element on magnetic and vibrational properties. The correlation of the calculated and measured XAS shows the presence of (partial) disorder not only in all-*d*-metal systems, but also in *p-d* Ni_2MnSn sample. This is consistent with our earlier findings of the traces of atomic disorder in the vibrational DOS [2]. Therefore, the interatomic hybridization in all-*d*-metal Heusler compounds can be utilized as an intrinsic control parameter for designing high-performance caloric materials.

[1] B. Beckmann *et al.*, *Acta Materialia* **246** 118695 (2023).
[2] O. Miroshkina *et al.*, *Phys. Rev. B* **106**, 214302 (2022).

MA 22.4 Wed 10:15 H19

Magnetocrystalline anisotropy of magnetocaloric Fe_2AlB_2 single crystals — •Nicolas Josten[1], Ralf Meckenstock[1], Anna Semisalova[1], Benedikt Beckmann[2], Konstantin Skokov[2], Oliver Gutfleisch[2], Hanna Pazniak[3], Thierry Ouisse[3], Michael Farle[1], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg Essen, Germany — [2]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany — [3]LMGP, Grenoble INP, CNRS, Université Grenoble Alpes, France

Fe_2AlB_2 is a low-cost, low weight and easily synthesized material composed of abundant elements for magnetocaloric applications near room temperature [1]. It is a ferromagnetic MAB phase with an orthorhombic crystal structure and a Curie-temperature T_C = 274 K [2]. The low crystal symmetry of Fe_2AlB_2 leads to a significant magnetocrystalline anisotropy up to around 1 MJ·m^{-3} at 10 K. We determined the temperature-dependent magnetocrystalline anisotropy constants of a bulk Fe_2AlB_2 single crystal using the Sucksmith-Thomson method and broadband ferromagnetic resonance measured along principal crystallographic directions. Both methods show perfect quantitative agreement.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) * Project-ID 405553726 * SFB/TRR 270.

[1] B. Beckmann et al. J. Appl. Phys. 133, 173903 (2023)
[2] T. N. Lamichhane et al. Phys. Rev. Mater. 2, 084408 (2018)

MA 22.5 Wed 10:30 H19

Effect of boron doping on the magnetocaloric properties in $La(Fe, Si)_{13}$ — •M. Strassheim[1,2], C. Salazar-Mejía[1], J. Wosnitza[1,2], and T. Gottschall[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany

Traditional refrigeration methods rely on gases and toxic refrigerants, contributing to environmental degradation and energy inefficiencies. In contrast, magnetocaloric materials offer a promising alternative, with the ability to produce large, reversible thermal changes when exposed to magnetic fields. Among these, $La(Fe,Si)_{13}$-based compounds stand out due to their excellent magnetocaloric effect at near-room temperatures, relatively high transition temperatures, and comparatively low cost of the base elements, making them ideal candidates for practical applications. The influence of elements such as hydrogen and carbon on interstitial sites of the $La(Fe,Si)_{13}$ lattice is already well understood, but boron doping is not. We present a study of the latter in regard of magnetization and transition temperature with a perspective of both room-temperature and cryogenic applications.

MA 22.6 Wed 10:45 H19

Direct measurements of the adiabatic temperature change of a dysprosium single crystal — •E. Bykov[1], T. Gottschall[1], J. Wosnitza[1,2], C. Salazar Mejia[1], M. D. Kuz'min[3], Y. Mudryk[4], and D. L. Schlagel[4] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Aix-Marseille Université, IM2NP, Marseille, France — [4]Ames Laboratory, U.S. Department of Energy, Iowa State University, Ames, USA

Heavy rare-earth elements in the Gd-Tm series have unique magnetic properties due to their electronic structure. The exchange between $4f$ electrons occurs via RKKY interactions and, therefore, is extremely sensitive to the ionic radii of the elements, exhibits anisotropy, and shows pronounced magnetoelastic coupling. This leads to various magnetic phase diagrams with different helicoidal magnetic structures despite similar chemical and physical properties of the $4f$ elements.

The high total angular momentum enables significant magnetocaloric effects, which is relevant for magnetic refrigeration applications. Gadolinium, for instance, exhibits a notable magnetocaloric effect at room temperature, serving as a comparative standard. Prior research at the Dresden High Magnetic Field Laboratory demonstrated record magnetocaloric effects in terbium. Holmium's broad plateau in ΔT_{ad} at 5 T suggests potential in cryogenic applications, such as for hydrogen liquefaction. Continuing our study of the magnetocaloric effect of the $4f$ elements, we present our recent results for a dysprosium single crystal.

MA 22.7 Wed 11:00 H19

Estimation of the inverse giant barocaloric effect in Fe_2P — •Sven Wiesekopsieker[1,2], Tapas Samanta[1], Chris Taake[1], Judith Bünte[1], Andreas Hütten[1], and Luana Caron[1,2] — [1]Faculty of Physics, Bielefeld University, Bielefeld 33501, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin 12489, Germany

The Fe_2P system has so far been explored with respect to the magnetocaloric effect, linked to it's first-order magnetostructural transition between a ferromagnetic high volume phase at low T and a paramagnetic low volume phase at high T. Both phases show a hexagonal structure ($P\bar{6}2m$ space group) [1]. This transition also gives rise to the barocaloric effect (BCE), which we studied by means of an indirect method, consisting of magnetization measurements under pressure and ambient pressure differential scanning calorimetry [2]. Application of pressure shifts the transition by −45.8(1.0) K/GPa. It is accompanied by a transition entropy change of $|\Delta S_{tr}| = 1.06(0.16)$ J/(kg K), similar to that reported by Hudl et al. Under application of 0.74 GPa a moderate adiabatic temperature change of -0.65 K is observed.

[1] A. Koumina et al., Ann. Chim. Sci. Mat. 23, 177 (1998)
[2] X. J. He et al., J. Mater. Sci. 52, 2915 (2017)
[3] M. Hudl et al., Phys. Rev. B 90, 144432 (2014)

MA 22.8 Wed 11:15 H19

Towards the hydrogenation of DyCo2 for cryogenic magnetocaloric liquefaction applications — •Allan Döring, Imants Dirba, Fernando Maccari, Konstantin Skokov, and Oliver Gutfleisch — TU Darmstadt, Darmstadt, Germany

Hydrogen can play an important role in the carbon-neutral society. Liquid H2 stands out for its higher volume-to-energy ratio. However, the current liquefaction method sums up to 34% of the costs to liquefy H. The magnetocaloric cooling could be one alternative to improve the efficiency of this process. Hence, research for materials with intense magnetocaloric effect (MCE) between 20 K and 77 K is needed. Those materials exhibit the peak of the MCE at transition temperatures, such as the Curie temperature (TC). Further, the MCE is stronger in heavy rare-earth (Re) based compounds, such as ReCo2. However, some of the ReCo2 materials exhibit giant MCE in temperatures above 77 K, and one way to shift down TC of such compounds is by introducing H as interstitial atoms. The TC of DyCo2 was shifted down by 120 K through the hydrogenation processK. Further, partially hydrogenated samples showed two distinct TCs. By X-ray diffraction analysis a crystalline state was confirmed with distorted lattices. The magnetic entropy changes were measured in non-hydrogenates, partially and fully hydrogenated samples, revealing a peak of entropy change at 25 K after hydrogenation. The reversibility of hydrogenation and its microstrutuctre was also investigated. We acknowledge the HyLICAL project through grant 101101461.

MA 23: Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization I

Magneto-transport and magneto-optic effects linear in the magnetization M (e.g. anomalous Hall effect (AHE), Faraday effect or magneto-optic Kerr effect (MOKE)) are important magnetic phenomena in spintronics and magneto-optics for the characterization of magnetic samples by vectorial magnetometry, microscopy, spectroscopy and pump probe experiments. However, already some time ago, it has been shown that the angular dependence of the anisotropic magnetoresistance and of magneto-optic effects contains higher-order-in-M terms. In the last decade, these effects beyond the linear dependence on M, e.g. quadratic effects proportional to M^2, have been mainly utilized to investigate antiferromagnetic materials.

Recently, the third-order MOKE proportional to M^3, so-called cubic MOKE, was reported to be sensitive to the structural domain twinning in thin-film samples of (111) orientation. By investigating AHE and MOKE of higher orders in M, the multipolar structure of the Berry curvature in magnetization space can be probed. These additional higher-order contributions in standard Hall or polar MOKE setup geometries are able to trace the in-plane magnetization while the linear effect keeps sensitive to the out-of-plane magnetic moment. This can be utilized, for example, to detect spin-orbit torques magneto-optically.

This Focus Session introduces the main magneto-transport and magneto-optic effects of higher orders in magnetization, draws connections between both research fields, distinguishes between already known and new higher-order effects and presents first applications beyond the study of antiferromagnets by quadratic effects.

Coordinators: Timo Kuschel, Bielefeld University, tkuschel@physik.uni-bielefeld.de;
Jaroslav Hamrle, Charles University, Prague, jaroslav.hamrle@matfyz.cuni.cz

Time: Wednesday 9:30–13:00 Location: H20

Invited Talk MA 23.1 Wed 9:30 H20

Magneto-transport effects in crystalline magnetic films — •Sebastian T. B. Goennenwein — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

The magneto-transport response of magnetically ordered materials – such as the anisotropic magneto-resistance (AMR), or the anomalous Hall effect (AHE) – has been extensively studied in the last decades. While the magneto-transport response of amorphous or polycrystalline samples can often be described by comparatively simple expressions, the implications of crystal symmetry lead to a much richer and more complex response in single-crystalline specimens [1]. In particular, higher-order terms with a seemingly 'unconventional' dependence on the magnetization can be allowed by symmetry, and indeed also be detected in experiment [2].

In the presentation, I will first review the implications imposed onto the magneto-transport response by crystal symmetry, and then discuss typical experimental results, focusing on crystalline (Ga,Mn)As films as a prototypical and well-studied example [3,4]. If time permits, I will furthermore touch upon the impact of crystalline symmetry onto the magneto-thermopower response.

[1] R. R. Birss, *Symmetry and Magnetism* (North-Holland, Amsterdam, 1966)
[2] P. K. Muduli *et al.*, Phys. Rev. B **72**, 104430 (2005)
[3] W. Limmer *et al.*, Phys. Rev. B **74**, 205202 (2006)
[4] W. Limmer *et al.*, Phys. Rev. B **77**, 205210 (2008)

Invited Talk MA 23.2 Wed 10:00 H20

Cubic magneto-optic Kerr effect in thin films depending on structural domain twinning and crystal orientation — •Robin Silber[1], Maik Gaerner[2], Jaroslav Hamrle[3], and Timo Kuschel[2] — [1]VSB - Technical University of Ostrava, Czechia — [2]Bielefeld University, Germany — [3]Charles University, Czechia

Many of the second-order effects in magnetization in magneto-transport and magneto-optics are of practical importance in research and applications today. In the case of magneto-optic Kerr effect (MOKE), the second-order effect (quadratic MOKE) has been utilized to e.g. study antiferromagnetics [1] or to investigate spin-orbit torques in insulating structures [2], while the third-order effect (cubic MOKE, CMOKE) has only been discussed rarely so far [3, 4]. Here we provide a solid theoretical background for the phenomenological description of CMOKE for (111)- and (001)-oriented cubic crystal structures and compare the results with the experimental data collected on Ni(111) and Ni(001) thin film samples. CMOKE manifests as a three-fold angular dependence in Ni(111) thin films while for Ni(001) a four-fold angular dependence of CMOKE is predicted. The dependence on the incidence angle is changing from one to the other crystal orientation. Furthermore, the strength of the CMOKE is also sensitive to the

degree of twinning of the Ni(111) thin film [4].
[1] V. Saidl et al., Nat. Photonics 11, 91 (2017).
[2] M. Montazeri et al., Nat. Commun. 6, 8958 (2015).
[3] A. V. Petukhov et al., J. Appl. Phys. 83, 6742 (1998).
[4] M. Gaerner et al., Phys. Rev. Applied 22, 024066 (2024).

MA 23.3 Wed 10:30 H20

Unconventional Magneto-Optical Effects — •Rudolf Schäfer and Ivan Soldatov — Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

Numerous magneto-optical reflection effects will be discussed that have hardly been considered in the past and that lead to intensity-based domain contrast in the absence of analyser and compensator in a wide-field magneto-optical microscope: (i) The transverse Kerr effect can be applied for in-plane magnetized material. (ii) In- and out-of-plane magnetized material can be imaged by circularly polarized light, leading to domain contrasts with different symmetry as the conventional Kerr contrast. (iii) Plane-polarized light at a specific angle can be employed for both in-plane and perpendicular media (Oppeneer effect). (iv) Perpendicular light incidence leads to a contrast on in-plane materials that is quadratic in the magnetization and to a domain boundary contrast. In case (iii), the contrast is generated by magnetic circular dichroism, while magnetic linear dichroism is responsible for the contrast in case (iv). The latter, being due to the diagonal elements in the quadratic dielectric magneto-optical tensor has a different symmetry as the conventional linear birefringence (Voigt) effect which is due to the off-diagonal elements. The domain*boundary contrast is caused by the magneto-optical gradient effect, which also exists as birefringence and dichroic effect. Reference: R. Schäfer, et al., Appl. Phys. Rev. 8, 031402 (2021)

MA 23.4 Wed 10:45 H20

Multipolar anisotropy in anomalous Hall effect from spin-group symmetry breaking — •Zheng Liu — University of Science and Technology of China, Hefei, China

Traditional view of the anomalous Hall effect (AHE) in ferromagnets is that it arises from the magnetization perpendicular to the measurement plane and that there is a linear dependence on the latter. However, this view is squarely challenged by a number of experiments recently, urging for a thorough theoretical investigation on the fundamental level. We find that for strong magnets, it is more appropriate and fruitful to regard the AHE as a spin-group symmetry breaking phenomenon where the critical parameter is the spin-orbit interaction strength, which involves a much smaller energy scale. Born out of our framework is a rich multi-polar relationship between the anomalous Hall conductivity and the magnetization direction, with each pole being expanded progressively in powers of the spin-orbit coupling strength. For the leading order contribution, i.e., the dipole, its isotropic part corresponds to the traditional view, and its anisotropic part can lead to the in-plane AHE where the magnetization lies within the measurement plane. Beyond the dipolar one, the octupolar structure offers the leading order source of nonlinearity and hence introduces unique anisotropy where the dipolar structure cannot. The dipolar and octupolar structure offers a unified explanation for the in-plane AHE recently observed in various ferromagnets. Our theory lays the ground for decoding the coupling between various transport and optical phenomena and the magnetic orders.

15 min. break

Invited Talk MA 23.5 Wed 11:15 H20

electrical and optical detection of the multipolar structure in the magnetization space — •Dazhi Hou — University of Science and Technology of China, Hefei, China

The anomalous Hall effect (AHE) in ferromagnetic materials has traditionally been understood to originate from a dipolar magnetization, with the effect typically showing sensitivity to out-of-plane magnetization. In contrast, we present compelling evidence that the AHE fundamentally arises from multipolar contributions to the magnetization. This discovery enables the observation of AHE under in-plane magnetization in cubic ferromagnets such as iron and nickel, challenging the conventional view. The magnitudes of these multipoles align with theoretical predictions from our recently proposed multipolar structure of Berry curvature in magnetization space. Notably, the octupole term can dominate the AHE in certain conditions, as observed in a van der Waals ferromagnet. Furthermore, we introduce a novel MOKE geometry that detects both the magnitude and direction of the perpendicular magnetization component, enabled by the multipolar structure of Berry curvature. This orthogonal MOKE geometry reveals unique angle-dependent behaviors, providing a direct probe of the magnetization multipoles at optical frequency. Our findings offer new insights into the quantum geometry of magnetization and open new avenues for probing magnetic orders across both electrical and optical domains, offering a unified framework for the study of multipolar magnetization in the context of Berry curvature.

MA 23.6 Wed 11:45 H20

Polarization variation method for investigation of magnetic and magneto-optical anisotropies — •Tomáš Ostatnický, Zeynab Sadeghi, Jozef Kimák, Peter Kubaščík, Eva Schmoranzerová, Lukáš Nádvorník, František Trojánek, and Petr Němec — Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

We present a newly developed method for all-in-one measurement of both magnetic anisotropy and anisotropy of magneto-optical (MO) coupling in magnetic materials. It fully relies on the quadratic MO response (in magnetization) of a sample. The method works in both the reflection and transmission at near-normal incidence, it is not limited by presence of components with linear MO response in setup and it does not require sample rotation during the experiment; it therefore allows measurements with a sample placed inside a cryostat. Measurement scheme is based on a scanning of the probe beam polarization change upon rotation of external magnetic field for several linear polarization of the probe laser. Numerical analysis of the full set of data allows us to recover magnitude and anisotropy of the MO coupling coefficient and we further determine the magnetic anisotropy of the sample by a fitting procedure. We demonstrate the precision of the method by characterizing several GaMnAs ferromagnetic samples with different Mn contents. Reliability of the method is confirmed by a perfect fit of the MO coupling constants with the predictions based on the G-tensor formalism and by a mutual agreement of magnetic anisotropic constants, determined from data acquired at different wavelengths.

MA 23.7 Wed 12:00 H20

Magnetic polymorphism in 2D layered antiferromagnets — •Shiwei Wu — Department of Physics, Fudan University

Polymorphism, commonly denoting the variety of molecular or crystal structures, is a vital element in many natural science disciplines. In van der Waals layered antiferromagnets, a new type of magnetic polymorphism is allowed by having multiple layer-selective magnetic structures with the same total magnetization. However, resolving and manipulating such magnetic polymorphs remain a great challenge. In this talk, I will report the use of phase-resolved magnetic second-harmonic generation microscopy to elucidate such magnetic polymorphism in the 2D semiconducting layered antiferromagnet CrSBr, and demonstrate how the magnetic polymorphs can be deterministically switched in an unprecedented layer-selective manner. With the nonlinear magneto-optical technique unveiling the magnetic symmetry information through the amplitude and phase of light, we could unambiguously resolve the polymorphic spin-flip transitions in CrSBr bilayers and tetralayers. Remarkably, the deterministic routing of polymorphic transitions originates from the breaking of energy degeneracy via a magnetic layer-sharing effect: the spin-flip transitions in a tetralayer are governed by the laterally extended bilayer, which acts as a *control bit*. We envision such controllable magnetic polymorphism to be ubiquitous for van der Waals layered antiferromagnets, and could lead to conceptually new design and construction of spintronic and opto-spintronic devices for probabilistic computation and neuromorphic engineering.

MA 23.8 Wed 12:15 H20

Anisotropy of the contributions to the orbital magnetization — •Milan Vrána[1,2] and Jaroslav Hamrle[1,2] — [1]Charles University, Prague, Czech Republic — [2]Czech Technical University, Prague, Czech Republic

The general definition of orbital magnetization is the change in the grand canonical potential, Ω, with respect to the external magnetic field: $\mathbf{m}_{\mathrm{orb}} = -\partial\Omega/\partial\mathbf{B}$. The orbital magnetization consists of two distinct contributions [1]. The first term originates from the orbital motion of electrons and is given by $\mathbf{m}_{\mathrm{dip}} = -\frac{e}{2}\langle\psi|\mathbf{r}\times\mathbf{v}|\psi\rangle$. The second term, $\mathbf{m}_{\mathrm{kden}}$, has been reinterpreted as arising from changes in the density of $\mathbf{k}$-points in phase space due to the concurrent presence of both the magnetic field and the Berry curvature, Ω [2]. This violates Liouville's theorem, leading to an expansion or contraction of the phase space volume by a factor of $(1 + \frac{e}{\hbar}\mathbf{B}\cdot\Omega)$. In the model material bcc Fe, we demonstrate that $\mathbf{m}_{\mathrm{kden}}$ is negligible in the [100] magnetization direction, whereas $\mathbf{m}_{\mathrm{dip}}$ is negligible in the [111] direction. It demonstrates different nature of the orbital magnetization for different magnetization directions. However, the magnitude of the total orbital magnetization, $\mathbf{m}_{\mathrm{orb}} = \mathbf{m}_{\mathrm{dip}} + \mathbf{m}_{\mathrm{kden}}$, remains nearly independent of the magnetization direction.

[1] F. Aryasetiawan, K. Karlsson, *Modern theory of orbital magnetic moment in solids*, J. Phys. Chem. Solids **128**, 87 (2019).
[2] Di. Xiao, *Berry Phase Modification to Electron Density of States and Its Applications*, dissertation, Texas University (2007).

Invited Talk MA 23.9 Wed 12:30 H20

Ultrafast Néel order dynamics detected by time-resolved magneto-optical Voigt effect — •Haibin Zhao — Fudan University, Shanghai, China

The time-resolved magneto-optical (MO) Voigt effect can be principally utilized to study the Néel order dynamics in antiferromagnetic (AFM) materials. In this talk, I will present the quench of AFM order by ultrafast laser pulses in both collinear and noncollinear AFM spin configurations in antiferromagnets with

negligible net magnetization probed by the time-resolved MO Voigt effect. For CoO with collinear spin configuration, the quench time of Néel order slows down pronouncedly near the Néel temperature (TN). In contrast, for Mn3Sn with an inverse triangular spin structure, The AFM order quench time shows negligible change with increasing temperature approaching the TN. This atypical behavior can be explained by the influence of weakened Dzyaloshinskii-Moriya interaction rather than the smaller exchange splitting on the diminished AFM order near TN. The temperature-insensitive ultrafast spin manipulation can pave the way for high-speed spintronic devices either working at a wide range of temperature or demanding spin switching near TN. The modulated Voigt angle in Mn3Sn is significantly larger than the polarization rotation due to the crystal-structure related linear dichroism effect and the modulated MO Kerr angle arising from the ferroic ordering of cluster magnetic octupole.

MA 24: Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets (joint session TT/MA)

In recent years, significant progress has been made in understanding strongly correlated quantum magnets, with a particular focus on fractionalized states of matter such as quantum spin liquids. These achievements in understanding have been made possible by remarkable developments in both materials science and experimental techniques. In particular, improvements in both traditional experimental tools (e.g., inelastic neutron scattering, Raman scattering, resonant X-ray scattering, etc.) and the introduction of innovative techniques such as 2D coherent THz spectroscopy and sophisticated noise experiments have advanced studies of quantum matter to qualitatively new levels of insight. This focus session will discuss these recent advancements in nonlinear spectroscopy techniques along with theoretical inroads in describing the nonlinear spectroscopic signatures of complex quantum magnets.

Organizers: Simon Trebst (Universität zu Köln), Johannes Knolle (TU München)

Time: Wednesday 9:30–12:45 Location: H36

See TT 27 for details of this session.

MA 25: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr I (joint session HL/MA)

The session is the first part of the focus session on the physics of the van der Waals magnetic semiconductor CrSBr, with a main session on Friday morning. The focus session is jointly organized by HL and MA.

Time: Wednesday 15:00–15:30 Location: H15

See HL 37 for details of this session.

MA 26: Ultrafast Magnetization Effects I

Time: Wednesday 15:00–18:45 Location: H16

MA 26.1 Wed 15:00 H16

Terahertz field assisted magneto-optical effects in nonmagnetic substrates — •Sergey Kovalev[1], Igor Ilyakov[2], Anneke Reinold[1], Patrick Pilch[1], Ahmed Ghalgaoui[1], Ruslan Salikhov[2], Jürgen Lindner[2], Cong Li[3], Jianbing Zhang[3], Pu Yu[3], and Zhe wang[1] — [1]Fakultät Physik, Technische Universität Dortmund, Dortmund, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Tsinghua University, China

Coherent control of matter on ultrafast timescales is attracting much attention due to numerous applications in advanced technologies. Strong terahertz (THz) fields are highly demanded in many of these studies, which focus on the control of carrier flow, spin dynamics, orbital polarisation and various aspects of nonlinear electron dynamics. For these studies it is very important to understand and disentangle different THz field induced processes occurring in the investigated systems and their substrates. In this contribution, we present two effects that occur in fused silica [1] and in LaAlO3 driven by strong THz field, resulting in rotation of laser pulse polarisation. These observations are due to the magneto-optical effect in amorphous systems or the Kerr electro-optical effect in anisotropic systems. Our results show that in general these effects should be carefully considered in the studies of ultrafast THz magnetisation dynamics by ultrafast pump-probe approaches. [1] S. Kovalev et al., Optics Letters 49, 4749 (2024)

MA 26.2 Wed 15:15 H16

Photoinduced spectral manipulation of coherent magnonics in ultrathin iron garnets — •Volker Wiechert[1], Moritz Cimander[1], Hanchen Wang[2], William Legrand[3], Pietro Gambardella[2], and Davide Bossini[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Materials, ETH Zürich, Hönggerbergring 64, CH-8093 Zürich, Switzerland — [3]Unité Mixte de Physique, CNRS, Université Paris-Saclay, Palaiseau 91767, France

Iron garnets, particularly Bi:YIG thin films, are promising materials for magnonics and magnetotransport due to their low damping and tunable magnetic properties through doping or external magnetic fields [1]. Recent advances demonstrate the ability of ultrashort laser pulses to excite, control, and even switch magnetization with minimal heating [2-4]. In this study, we investigate Bi:YIG single crystals in quasi-2D ultrathin form (~20 nm), using a femtosecond, balanced-detection scheme to capture simultaneous optical and magneto-optical responses. Our findings reveal two pathways for modifying magnetic resonance eigenfrequency: an impulsive femtosecond modification of magneto-crystalline anisotropy and a nanosecond lattice-mediated heating effect. This dual effect is quantitatively identified in time-resolved experiments, with potential applications in other quasi-2D ultrathin magnetic systems exhibiting temperature-dependent phase transitions.

[1] C. Holzmann et al., ACS Appl. Nano Mater. 5(1), 2022
[2] F. Hansteen et al., PRB 73, 2006
[3] L. Soumah et al., PRL 127, 2021
[4] A. Stupakiewicz et al., Nature 542, 2007

MA 26.3 Wed 15:30 H16

Ultrafast Entropy Production in Non-Equilibrium Magnets — •Finja Tietjen and R. Matthias Geilhufe — Chalmers University of Technology, Gothenburg, Sweden

We present an ultrafast thermodynamics framework to model heat generation and entropy production in laser-driven ferromagnetic systems. By establishing a connection between the magnetic field strength of the laser pulse and magnetization dynamics we model time-dependent entropy production rates and deduce the associated heat dissipation in epitaxial and polycrystalline FeNi and CoFeB thin films. Our theoretical predictions are validated by comparison to experimental magnetization dynamics data, shedding light on thermodynamic processes on picosecond timescales.

Crucially, we incorporate recently observed inertial spin dynamics, to describe their impact on heat generation in pump-probe experiments. As such, this formalism provides novel insights into controlling heat production in magnetic systems, and contributes to advancing the understanding of non-equilibrium

thermodynamics in magnetic systems, with implications for future experimental protocols in spintronics and nanotechnology.

[1] F. Tietjen, & R. M. Geilhufe (2024). Ultrafast Entropy Production in Non-Equilibrium Magnets. arXiv preprint arXiv:2410.23205.

MA 26.4 Wed 15:45 H16

Spin-lattice modeling of elastic waves generated by ultrafast demagnetization in fcc Ni — •Ievgeniia Korniienko[1], Pablo Nieves[2], Alberto Fraile[3], Roberto Iglesias[2], and Dominik Legut[1] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — [2]University of Oviedo, Oviedo, Spain — [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain

Picosecond ultrasonics is a fast growing and advanced research field with broad application to the imaging and characterization of nanostructured materials as well as at a fundamental level. Experiments that provide direct, layer-specific, and quantitative information on the picosecond strain response [1], however, face comparably limited theoretical descriptions and modeling. In our work we propose a 3D model on the base of atomistic spin-lattice simulations [2] for laser-induced elastic response. As an example for testing our modeling approach we use ferromagnetic fcc Ni. Such choice allows us not only to calculate the lattice elastic response including ultrafast thermal expansion, but also to characterize the magnetic contribution to stress in this material [3]. The theoretical approach presented in our work [3] can be useful for further interpretations of experiments in the picosecond ultrasonics, as well as for providing other required parameters (like ultrafast thermal expansion coefficient) in micromagnetic models, e.g. within a multiscale approach. References: [1] M. Mattern, et al.: Photoacoustics 31, 100503 (2023); [2] P. Nieves, et al.: Phys. Rev. B 103, 094437 (2021); [3] I. Korniienko, et al.: Phys. Rev. Research 6, 023311 (2024).

MA 26.5 Wed 16:00 H16

Ultrafast orbital Hall effect in metallic nanoribbons — •Oliver Busch, Franziska Ziolkowski, Börge Göbel, Ingrid Mertig, and Jürgen Henk — Institut für Physik, Martin-Luther-Universität, D-06099 Halle

The orbital Hall effect can generate currents of angular momentum more efficiently than the spin Hall effect in most metals. However, so far, it has only been understood as a steady-state phenomenon [1]. In this theoretical study, the orbital Hall effect is extended into the time domain [2]. We investigate the orbital angular momenta and their currents induced by a femtosecond laser pulse in a Cu nanoribbon.

Our numerical simulations provide detailed insights into the laser-driven electron dynamics on ultrashort timescales with atomic resolution. As we show, the ultrafast orbital Hall effect described here is consistent with the familiar pictorial representation of the static orbital Hall effect, but we also find pronounced differences between physical quantities that carry orbital angular momentum and those that carry charge. For example, there are deviations in the time series of the respective currents. This work lays the foundations for investigating ultrafast Hall effects in confined metallic systems.

[1] D. Go *et al.* Europhysics Letters **135**, 37001 (2021)
[2] O. Busch *et al.*, Physical Review Research **6**, 013208 (2024)

MA 26.6 Wed 16:15 H16

Ultrafast magnetization dynamics of magnetic garnet thin films — •Paul Herrgen[1], Christian Holzmann[2], Manfred Albrecht[2], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

The rare-earth iron garnets (REIG) are a class of magnetic oxide materials, known for their excellent magneto-optical properties, high magnetic permeability, and applications in photonics and spintronics. [1]

In our work we investigate the ultrafast magnetization dynamics of a gadolinium iron garnet (GdIG) thin film after an excitation with an ultrashort laser pulse. Our static characterization of the magnetic properties revealed hysteresis loops with opposite sign of the saturation magnetization for equal field directions depending on the probe photon energy. This points to a photon energy dependent magnetic response of both sublattices and allows us to disentangle their ultrafast response after optical excitation. We observe an ultrafast demagnetization of both sublattices within the first few hundred fs, after excitation with photon energies larger than the material's band gap. We find a different quenching for the signals of both sublattices despite the otherwise very similar demagnetization time. On longer timescales, we find another different behavior for the sublattices, with the iron sublattice starting to remagnetize much earlier than the gadolinium one.

[1]: C. Holzmann and M. Albrecht: Encyclopedia of Materials: Electronics 1, 777 (2023)

MA 26.7 Wed 16:30 H16

Accelerated ultrafast demagnetization of an interlayer-exchange-coupled Co/Mn/Co trilayer — •Jendrik Gördes[1], Ivar Kumberg[1], Chowdhury S. Awsaf[1], Marcel Walter[1], Tauqir Shinwari[1], Sangeeta Thakur[1], Sangeeta Sharma[2], Christian Schüssler-Langeheine[3], Niko Pontius[3], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Berlin — [2]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin

We studied the influence of the spin structure of an antiferromagnetic (AFM) layer at the interface to a ferromagnetic (FM) layer on the FM magnetization dynamics in epitaxial Co/Mn/Co/Cu(001) trilayers. The two FM layers are coupled indirectly by the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and directly by exchange through the AFM spin structure [1]. Deposition of Mn in a wedge allowed for access to different coupling regimes on the same sample. Magnetization dynamics were probed after excitation with 800 nm fs laser pulses by X-ray magnetic circular dichroism in reflectivity. A difference in demagnetization time between the two regimes for parallel and antiparallel alignment of FM is observed. We explain this by differences in the AFM spin structure leading to presence or absence of optically induced intersite spin transfer [2] between Mn and Co. [1] B. Zhang *et al.*, J. Appl. Phys. 115, 233915 (2014). [2] J. K. Dewhurst *et al.*, Nano Letters 18, 1842 (2018)

15 min. break

MA 26.8 Wed 17:00 H16

Development of planar micro optics for ultrafast in-situ measurements in the TEM — •Max Herzog[1], Johannes Schultz[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]IFMP, TU Dresden, Haeckelstraße 3, 01069 Dresden

The miniaturization of magnetic electron optics has been a goal for at least the past decade, because it will not only allow for smaller and easier to build electron optics, but will also result in other favorable scaling effects. Namely, the small scale allows for magnetic flux densities in the hundreds of millitesla with a significantly reduced power consumption and lower overall complexity regarding vacuum, cooling and power supply. More important for this work, however, is the small inductance that follows from the small size, which in turn allows the optics to be switched with radio frequencies (RF). The aim of this work is to lithographically produce planar micro optics (e.g. deflectors, focusing quadrupoles, vector magnets, etc.), that are capable of utilizing this RF switching to image ns-scale processes (e.g. the movement of magnetic domain walls) stroboscopically in a transmission electron microscope. The optics were characterized using differential phase contrast (DPC) to determine the spatial distribution of the magnetic field and by measuring the optical power (e.g. deflection, focusing behaviour) at varying switching frequencies. Using an acceleration voltage of 80 kV, the optics show a promising performance with a deflection power of up to 330 μrad at an excitation frequency of 7.5 MHz and still 120 μrad at 2 GHz with a very homogeneous magnetic field as determined by DPC.

MA 26.9 Wed 17:15 H16

Ultrafast energy-resolved spin dynamics in nickel — Christopher Seibel, Tobias Held, Markus Uehlein, •Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau

Magneto-optical methods were used when ultrafast magnetization dynamics were discovered and are still used intensively. Recent experiments show a strongly energy-dependent magneto-optic response and indicate spin transfer processes on the timescale of the pulse duration in a pure metallic ferromagnet [1].

We investigate the non-equilibrium spin dynamics on these early timescales by full spin-resolved Boltzmann collision integrals [2]. We trace the temporal evolution of the individual distribution functions of up and down electrons, where spin-flips due to electron-electron and electron-phonon collisions are taken into account.

From the dynamics of the distributions, we extract the spin-resolved densities of both, electrons and holes, at various energies. The energy-resolved spin polarization can vary significantly depending on the considered energy range. It can deviate from the overall magnetization dynamics, both in terms of the qualitative behavior and the timescales involved. Additionally, we present results on the non-equilibrium magneto-optic response calculated from the distribution functions.

[1] H. Probst et al., *Phys. Rev. Res.* **6**, 013107 (2024)
[2] B. Müller et al., *Phys. Rev. Lett.* **111**, 167204 (2013)

MA 26.10 Wed 17:30 H16

Differentiating mechanisms that drive ultrafast magnetization precession — •Fried-Conrad Weber[1,2], Maximilian Mattern[3], Jasmin Jarecki[3], Marwan Deb[1], Dieter Engel[3], Daniel Schick[3], Alexander von Reppert[1] und Matias Bargheer[1,2] — [1]Universität Potsdam — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin — [3]Max-Born-Institut, Berlin

We use the time-resolved polar magneto-optical Kerr effect to measure the laser-induced magnetization precession of a 20 nm and 200 nm thin nickel film for different external magnetic field angles. We identify the role of quasi-static strain,

strain pulses, and demagnetization for driving the precession in these samples. The magnetization response is modeled using the udkm1Dsim toolbox, which calculates the temperature, strain, and subsequent magnetization response with a modified Landau-Lifshitz-Gilbert equation that incorporates demagnetization. Contributions from the demagnetization-induced change in anisotropy, quasi-static strain, and propagating strain pulses are included in the time-dependent effective field. In the case of nickel, the quasi-static strain drives the effective field in the opposite direction to the demagnetization-induced change in anisotropy. For the samples and fluences measured, we identify the laser-induced strain and the subsequent change in the magnetoelastic field as the dominant mechanism controlling the precession. In a subsequent double-pulse excitation experiment, we balance the effect of the demagnetizationinduced change in anisotropy and the magnetoelastic contribution in a non-conventional coherent control scheme.

MA 26.11 Wed 17:45 H16

Temperature and Magnetic Field Dependence of Ultrafast Magnetization Dynamics — •Leon Seidel[1], Clemens von Korff Schmising[2], Tino Noll[2], Wolfgang-Dietrich Engel[2], Simon Gaebel[2], Daniel Metternich[2], and Stefan Eisebitt[1,2] — [1]Technische Universität Berlin — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie

In this work, we present a wide-field optical microscope designed to study the temperature and magnetic field dependence of ultrafast magnetization dynamics with femtosecond temporal and micrometer spatial resolution. The compact device integrates xyz, yaw and tilt adjustments as well as a motorized sample manipulation. The sample temperature is controlled by a continuous flow cryostat in a temperature range between 20 K / 80 K and 500 K using either LN2 or LHe. An inbuilt electromagnet provides an external magnetic field of up to one Tesla. We show first results of ultrafast all-optical magnetization switching (AOS) in ferrimagnetic rare earth-transition metal alloys. We characterize two CoTbGd films with different stochiometries and systematically examine the role of the magnetization and angular momentum compensation for AOS.

MA 26.12 Wed 18:00 H16

Heterogenity of the laser-induced magneto-structural phase transition in FeRh revealed by ultrafast x-ray diffraction — •Maximilian Mattern[1], Jan-Etinne Pudell[2], Vojtech Uhlir[3], Jon Ander Arregi[3], Angel Rodriguez-Fernandez[2], Roman Shayduk[2], Wonhyuk Jo[2], Anders Madsen[2], and Daniel Schick[1] — [1]Max-Born-Institut, Germany — [2]European XFEL, Germany — [3]CEITEC BUT, Czech Republic

Laser-induced heterogeneities play an important role for ultrafast dynamics especially of first-order phase transitions due to the phase co-existence during nucleation. However, their probing on picosecond time and nanometer length scales is challenging.

We use time-resolved x-ray diffraction to reveal the transient nanoscale heterogeneity of the laser-induced first-order antiferromagnetic (AFM) to ferromagnetic (FM) phase transition in FeRh that is accompanied by a lattice expansion. Utilizing the good reciprocal space and femtosecond time-resolution of the MID instrument at the European X-ray Free-electron laser, we individually track the picosecond shifts of the structural AFM and FM Bragg peak. The integral of the latter quantifies the transient fraction of the FeRh layer that is in the FM phase, and the signatures of the propagating picosecond strain pulses in the shift of both Bragg peaks reveal its spatial distribution. Our results can distinguish between different nucleation scenarios and reveal that the FM phase nucleates as laterally separated columns through the photoexcited near-surface region, finally forming a closed FM layer at the surface of the inhomogeneously excited FeRh film.

MA 26.13 Wed 18:15 H16

Ultrafast electron dynamics in altermagnetic materials — Marius Weber[1,2], •Kai Leckron[1], Luca Haag[1], Libor Šmejkal[2], Jairo Sinova[2], and Hans Christian Schneider[1] — [1]Department of Physics, University of Kaiserslautern-Landau, Germany — [2]Institut für Physik, Johannes Gutenberg University Mainz, Germany

One of the intriguing properties of altermagnetic materials is that a linearly polarized optical pulse can induce a spin polarization of the electrons depending on the direction of the linear polarization [1]. This contribution investigates the impact of the polarization direction and fluence of the optical excitation on the ultrafast magnetization dynamics in the prototypical altermagnetic band structure of KRu4O8. We explicitly consider electron-electron scattering and electron-phonon scattering contributions to the light-driven carrier dynamics. The optical excitation is computed using ab initio dipole transition rates in the whole Brillouin zone. Our momentum-dependent calculation of the subsequent scattering dynamics fully includes the anisotropies of the altermagnet, which leads to unique k-resolved electron dynamics at ultrashort times and a long-lived spin polarization [2]. We present a numerical study of the influence of the excitation conditions on the lifetime of this spin polarization.

[1] M. Weber et al., arXiv:2408.05187 (2024) [2] M. Weber et al., arXiv:2411.08160 (2024)

MA 26.14 Wed 18:30 H16

The dynamics of a memory-enhanced LLG equation — •Felix Hartmann[1] and Janet Anders[1,2] — [1]University of Potsdam, Institute of Physics and Astronomy, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

Recently, Anders et al. [1] have proposed a stochastic Landau-Lifshitz-Gilbert (LLG) equation which takes into account memory effects and colored thermal fluctuations, with either a classical, semi-classical or quantum thermostat. In this talk we will present some recent results that characterize the spin dynamics in different parameter regimes. We show how the proposed stochastic LLG equation has a well-described white-noise and Markovian limit of the spin dynamics. Further, going beyond the white-noise and Markovian limit, we present numerical results that show strong ultrafast and inertial effects in the spin dynamics, such as a faster relaxation and the appearance of nutation oscillations.

[1] J. Anders et al., New J. Phys. 24 033020 (2022)

MA 27: Focus Session: Magneto-Transport and Magneto-Optics of Higher Orders in Magnetization II

Magneto-transport and magneto-optic effects linear in the magnetization M (e.g. anomalous Hall effect (AHE), Faraday effect or magneto-optic Kerr effect (MOKE)) are important magnetic phenomena in spintronics and magneto-optics for the characterization of magnetic samples by vectorial magnetometry, microscopy, spectroscopy and pump probe experiments. However, already some time ago, it has been shown that the angular dependence of the anisotropic magnetoresistance and of magneto-optic effects contains higher-order-in-M terms. In the last decade, these effects beyond the linear dependence on M, e.g. quadratic effects proportional to M^2, have been mainly utilized to investigate antiferromagnetic materials.

Recently, the third-order MOKE proportional to M^3, so-called cubic MOKE, was reported to be sensitive to the structural domain twinning in thin-film samples of (111) orientation. By investigating AHE and MOKE of higher orders in M, the multipolar structure of the Berry curvature in magnetization space can be probed. These additional higher-order contributions in standard Hall or polar MOKE setup geometries are able to trace the in-plane magnetization while the linear effect keeps sensitive to the out-of-plane magnetic moment. This can be utilized, for example, to detect spin-orbit torques magneto-optically.

This Focus Session introduces the main magneto-transport and magneto-optic effects of higher orders in magnetization, draws connections between both research fields, distinguishes between already known and new higher-order effects and presents first applications beyond the study of antiferromagnets by quadratic effects.

Coordinators: Timo Kuschel, Bielefeld University, tkuschel@physik.uni-bielefeld.de;
Jaroslav Hamrle, Charles University, Prague, jaroslav.hamrle@matfyz.cuni.cz

Time: Wednesday 15:00–15:45 Location: H18

MA 27.1 Wed 15:00 H18

Quantifying magnetization multipole of Berry curvature in ferromagnets — •Wenzhi Peng, Zheng Liu, Bin Xiang, Qian Niu, Yang Gao, and Dazhi Hou — University of Science and Technology of China

The anomalous Hall effect, originating from the Berry curvature in momentum space, typically manifests as a dipole behavior in magnetization. This implies that the anomalous Hall conductivity is parallel to the magnetization in most transport measurements. However, even in iron, the in-plane magnetization can also induce the anomalous Hall effect, which contradicts the predictions of the dipole term in a cubic lattice. This behavior can be understood within the framework of the Berry curvature multipole structure in magnetization space. In this work, we propose a paradigm to quantify the coefficients of the Berry curvature multipole by examining the angular dependence of the Hall resistivity, which matches well with first-principles calculations. Under certain conditions, the contribution of the magnetization multipole can even surpass that of the dipole term, dominating the AHE.

MA 27.2 Wed 15:15 H18

Orthogonal faraday effect in garnet — •Haolin Pan[1], Han Li[2], Qinhui Yang[2], and Dazhi Hou[1] — [1]University of Science and Technology of China, Hefei, China. — [2]University of Electronic Science and Technology of China, Chengdu, China.

Faraday effect, a transmissive magneto-optical phenomenon with a long history and diverse applications, has been be confined within parallel configuration between light and magnetization in experiments. This routine originates from the common assumption that the asymmetric components of dielectric tensor is in linear response to magnetization. However, our experiments in garnet materials reveal the nonlinear nature of Faraday effect with respect to magnetization orientation, which allows the orthogonal geometry between light and magnetization. The lattice angular dependence and spectroscopy results are in good agreement with theory of multipole structures of Berry curvatures in magnetization space. The observation of orthogonal Faraday effect provides new opportunities for magneto-optical studies and applications.

MA 27.3 Wed 15:30 H18

Strong anisotropy of quadratic magneto-optical Kerr effect in FeRh — •zeynab sadeghi, vladislav wohlrath, jozef kimák, peter kubaščík, eva schmoranzerová, tomas ostatnický, and petr němec — faculty of mathematics and physics, charles university, prauge, 121 16, czech republic

recently, we developed a technique that enables to measure magnetic anisotropy and anisotropy of quadratic magneto-optical Kerr effect (QMOKE) [1]. This technique is based on measurement of magneto-optical response in rotating magnetic field using series of incident light linear polarizations at normal incidence on the sample with a fixed position and, therefore, it can be applied also for samples placed in a cryostat. In this contribution, we report on measurements in FeRh, which is an interesting material with an antiferromagnetic (AFM) ordering at room temperature and a ferromagnetic (FM) phase at temperatures above 400 K. We show that in the FM phase QMOKE has a very strong wavelength-dependent anisotropy in the investigated spectral range from 460 nm to 1600 nm. We also discuss the possibility of investigation of the FeRh AFM phase using this technique. [1] wohlrath, w., sadeghi, z. et al. "quadratic magneto-optical Kerr effect spectroscopy: Polarization variation method for investigation of magnetic and magneto-optical anisotropies." arXiv:2409.20205 (2024).

MA 28: Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions

Time: Wednesday 15:00–17:30 Location: H19

MA 28.1 Wed 15:00 H19

Correlations of short-range environment and hyperfine parameters in disordered FeV thin-films — •Simon Rauls[1], Benedikt Eggert[1], Jürgen Fasbender[2], Kay Potzger[2], Rantej Bali[2], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

The binary alloy $Fe_{1-x}V_x$ shows a variety of interesting properties, ranging from antiparallel coupling of induced V magnetic moments up to 1 μ_B per V atom to the positive vibrational entropy in the disorder/order transition from the A2 to the B2 bcc-crystalline phase. Furthermore, around equiatomic composition, the structurally complex σ-phase might develop. To understand these effects, the local atomic environment as well as both structural and chemical disorder need to be considered. Using Mössbauer spectroscopy, the local environment of ^{57}Fe atoms and different aspects of disorder can be investigated through careful analysis of the distribution of hyperfine parameters, i.e.. the hyperfine field splitting and the isomer shift. In this talk, the conversion electron Mössbauer spectra of the entire concentration range of $Fe_{1-x}V_x$ thin film samples are presentedd. Enrichment with 95% ^{57}Fe results in a very high signal to noise ratio, which allows for comparison of Hesse-Rübartsch fits with a model, in which the hyperfine parameters are described by a binomial distribution of the first three nearest-neighbor shells. We acknowledge funding by the DFG through project No. 322462997.

MA 28.2 Wed 15:15 H19

Simulating magnetostriction in skyrmion-hosting $MnSc_2S_4$ — •Justus Grumbach[1], Mahmood Deeb[1], Sergey Granovsky[1], Lilian Prodan[2], Vladimir Tsurkan[2], Martin Rotter[3], and Mathias Doerr[1] — [1]Institut für Festkörper- und Materialphysik, TU Dresden, 01062 Dresden — [2]Experimentalphysik V, Universität Augsburg, 86135 Augsburg — [3]*McPhase* Projekt, 01159 Dresden

Measurements of neutron scattering on $MnSc_2S_4$ explored an antiferromagnetic skyrmion state [1]. We measured the magnetostriction and found curves with characteristic anomalies. To find out which is linked to skyrmions, we performed mean field Monte Carlo simulations with the *McPhase* program package using the hamiltonian introduced earlier [1].

We could resemble main properties of the experimental outcome. The exact location of the skyrmionic state in the phase diagram and the discovery of a new $2\boldsymbol{q}$ structure between the skyrmion state and saturation in field were new informations gained by these simulations.

Simulations and experimental results introduce a link of magnetostriction and skyrmions by a plateau-like non-distorted region, which could also be found in other compounds.

[1] S. Gao et al.: Fractional antiferromagnetic skyrmion lattice induced by anisotropic couplings. Nature, 586:37, 2020.

MA 28.3 Wed 15:30 H19

Tilted spin state near the spin reorientation of the topological kagome magnet Fe_3Sn_2 — •Lilian Prodan[1], Donald M. Evans[1,2], Aleksandr S. Sukhanov[1], Stanislav E. Nikitin[3], Alexander A. Tsirlin[4], Lukas Puntingam[1], Marein C. Rahn[1], Liviu Chioncel[1], Vladimir Tsurkan[1,5], and Istvan Kezsmarki[1] — [1]University of Augsburg, Augsburg, Germany — [2]Department of Sustainable Energy Technology, SINTEF Industry, Oslo, Norway — [3]Paul Scherrer Institut, Switzerland — [4]Leipzig University, Germany — [5]Moldova State University, Chisinau, Moldova

Spin reorientation due to competing magnetic anisotropies can have drastic effects on various physical properties in itinerant magnets with topologically nontrivial band structure. Therefore, understanding the mechanism of spin reorientation provides an efficient tool for engineering the properties of topological magnets [1]. Our target material is the topological kagome ferromagnet Fe_3Sn_2 [2], where we investigated the temperature-driven spin reorientation using a number of experimental techniques and numerical modeling. We reveal that the crossover from the high-temperature state with uniaxial easy-axis anisotropy to the low-temperature state with easy-plane anisotropy take place at ~120 K through an intermediate tilted easy-cone state. Our MFM study highlights significant changes in the magnetic patterns emerging on the mesoscale across all three states, including the formation of magnetic bubbles on the surface of bulk centrosymmetric Fe_3Sn_2 crystals. [1] A. Kimel et.al, Nature 429, 850-853 (2004). [2] F. Schilberth et al., Phys. Rev. B 106, 144404 (2022).

MA 28.4 Wed 15:45 H19

High-field/high-frequency Ferromagnetic Resonance Studies on the van-der-Waals ferromagnet Fe_3GeTe_2 — •Birte Beier[1], Martin Jonak[1], Eva Brücher[2], Reinhard K. Kremer[2], and Rüdiger Klingeler[1] — [1]Kichhoff Institute for Physics, Heidelberg University, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Long-range ferromagnetic order develops down to the monolayer in Fe_3GeTe_2 and is particularly robust both in the monolayer and in the bulk as compared to other van-der-Waals ferromagnets. In the bulk, T_C amounts to about 220 K as compared to, e.g., 61 K in CrI_3 and 65 K in $Cr_2Ge_2Te_6$. In order to elucidate the origin of robust long-range ferromagnetism, we have investigated low-energy magnon excitations in Fe_3GeTe_2 by high-field/high-frequency ferromagnetic resonance studies. Our data reveal the size and temperature dependence of the anisotropy gap and also show the evolution of short-range magnetic order well above T_C. The frequency- and field-dependence of magnon excitation is discussed and compared with our recent findings on CrI_3 [1].

[1] M. Jonak *et al.*, Phys. Rev. B **106**, 214412 (2022)

MA 28.5 Wed 16:00 H19

Derivation of spin-orbit generated relativistic symmetric and antisymmetric exchange interactions — •Hiroshi Katsumoto[1], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

It has become clear that the higher-order exchange interactions beyond the Heisenberg interaction can promote very complex magnetic structures. Moriya derived the Dyzaloshinskii-Moriya interaction (DMI) for spin-1/2 systems, including spin-orbit coupling (SOC). We derived an expression that generates the DMI according to a systematic algorithm for any higher-order antisymmetric exchange interaction. Applying this expression to particular spin models consistently provides all recently suggested DMIs extended to higher-order exchange interactions [1]. In addition, it is found that in the second-order perturbation of SOC, not only the antisymmetric higher-order terms but also the symmetric spin-nematic term is obtained. The spin-nematic term is known to produce electromagnetic effects [2], and in this study, its microscopic derivation is given. We acknowledge funding from the ERC grant 856538 (project "3D MAGIC") and DFG through SPP-2137 and SFB-1238 (project C1).

[1] A. Lászlóffy *et al.*, PRB **99**, 184430 (2019); S. Brinker *et al.*, NJP **21**, 083015 (2019); S. Grytsiuk *et al.*, Nat. Commun. **11**, 511 (2020); Mankovsky *et al.*, PRB **101**, 174401 (2020). [2] M. Soda *et al.*, PRL **112**, 127205 (2014)

MA 28.6 Wed 16:15 H19

magnetism and electronic dynamics in CuCr1-xSnxS4 — •Elaheh Sadrollahi[1], Cynthia P. C. Medrano[2], Magno A.V. Herling[2], Elisa M. Baggio Saitovitch[2], Lilian Prodan[3,4], Vladimir Tsurkan[3,4], and F. Jochen Litterst[5] — [1]IFMP, TU Dresden, 01069 Dresden, Germany — [2]CBPF, Rio de Janeiro, 22290-180, Brazil — [3]EKM, Inst. of Physics, University Augsburg, 86135 Augsburg, Germany — [4]IAP, Moldova State University, MD 2028, Chisinau, Republic of Moldova — [5]IPKM, TU Braunschweig, 38106 Braunschweig, Germany

Magnetization, muon spin rotation and relaxation(muSR), and 119Sn Mössbauer spectroscopy have been performed on the metallic ferromagnetic CuCr1-xSnxS4 (x=0.03-0.08) cubic spinel (Tc=360 K-343 K). Magnetization and muSR results reveal the same low-temperature magnetic transitions around 80 K and 40 K as found for the undoped material with a magnetic ground state deviating from a simple collinear ferromagnet [1] and proposed charge ordering [2]. The changes in Mössbauer hyperfine spectra are less pronounced and are discussed in view of the different positions of the local probes mu+ and 119Sn and their different magnetic coupling to the magnetic Cr lattice. Above 70 K, both muSR and Mössbauer spectra show temperature-dependent inhomogeneous broadening either due to structural or charge disorder and changing spin and charge dynamics that can be related to a precursor magnetic phase above the well-defined static low-temperature phase.

[1] E. Sadrollahi, et al., Phys. Rev. B 110, 054439 (2024).
[2] K. Oda, et al., J. Phys. Soc. Jpn. 70, 2999 (2001).

15 min. break

MA 28.7 Wed 16:45 H19

Ground state magnetization in superstable graphs — •Fabio Pablo Miguel Méndez-Córdoba[1,2,3], Joseph Tindall[4], Dieter Jaksch[1,2,5], and Frank Schlawin[1,2,3] — [1]Universität Hamburg, Luruper Chaussee 149, Gebäude 69, D-22761 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, Hamburg D-22761, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010 — [5]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, UK

Much of our understanding of ground state magnetic properties rests on analytical results on bipartite lattices. However, few exact results are known in non-bipartite graphs with frustrated couplings. We determine the ground state magnetization of strongly correlated systems on non-bipartite graphs displaying superstability. Superstability allows reinterpreting non-bipartite graphs as a collection of bipartite-connected components, providing magnetic properties of important lattices, such as the triangular ladder. Numerical evidence suggests further generalizations are feasible.

MA 28.8 Wed 17:00 H19

Magneto-optical spectroscopy on cubic noncollinear antiferromagnet HoCu — •Felix Schilberth[1,2], Marein Rahn[3], Andreas Bauer[4], Christian Pfleiderer[4], Sándor Bordács[2], and István Kézsmárki[1] — [1]Lst. für Experimentalphysik V, Universität Augsburg — [2]Dept. of Physics, BME Budapest — [3]Lst. für Experimentalphysik VI, Universität Augsburg — [4]Lst. für Experimentalphysik zur Topologie korrelierter Systeme, TU München

Giant anomalous Hall effect (AHE) and magneto-optical Kerr-effect (MOKE) can emerge in magnets with topologically non-trivial electronic bands. Besides extrinsic contributions from scattering of electrons by impurities, two intrinsic contributions are considered. In momentum space, the Berry curvature generated by non-trivial band features like Weyl points or nodal lines can produce resonances in the optical conductivity, leading to AHE in the static limit. On the other hand, noncollinear magnetic texture in the real space can induce topological Hall effect (THE). The separation of all three contributions is a remarkable experimental challenge which typically cannot be solved by magnetotransport experiments alone. Here, we address this question in the itinerant cubic antiferromagnet HoCu where a remarkably large AHE on the order of $10^6\ \Omega^{-1}\mathrm{cm}^{-1}$ was observed. By measuring reflectivity and MOKE, we determine the optical Hall effect spectrum, the finite frequency analog of the AHE. In this quantity, the energy scales provided by the scattering rate or the energy of band degeneracies allow to disentangle the AHE contributions by free carriers from interband resonances, decomposing this remarkable transport response.

MA 28.9 Wed 17:15 H19

Investigating the soft X-ray-induced spin-state switching in the room temperature regime of a Fe(II) spin-crossover complex — •Lea Kämmerer[1], Carolin Schmitz-Antoniak[2,3], Tobias Lojewski[1], Damian Günzing[1], Torsten Kachel[4], Florin Radu[4], Radu Abrudan[4], Katharina Ollefs[1], Senthil K. Kuppusamy[5], Mario Ruben[5,6], and Heiko Wende[1] — [1]University of Duisburg-Essen and CENIDE — [2]Forschungszentrum Jülich — [3]University of Applied Sciences Wildau, — [4]Helmholtz-Zentrum Berlin — [5]Karlsruhe Institute for Technology — [6]Institut de Science et d'Ingénierie Supramoléculaires

Spin-crossover complexes exhibit two distinct spin-states, designated as low-spin and high-spin, which are contingent upon the ligand field surrounding the central metal ion. It is possible to induce a switching of the spin state in these complexes through the use of soft X-rays. The complex $Fe(1-bpp-COOC_2H_5)_2(BF_4)_2CH_3CN$ exhibits an abrupt spin-state switching with an open thermal hysteresis around room temperature. Static X-ray absorption spectroscopy was performed at the synchrotron BESSY II, which allows for the analysis of the two spin states at the Fe $L_{2,3}$ absorption edges due to the presence of different fine structures. We gained insight into the cooperative mechanism that occurs during the soft X-ray-induced spin-state switching at room temperature. It was observed that once the effect was initiated in a thin film, a chain reaction led to further switching, even in the absence of soft X-rays. We thank the Deutsche Forschungsgemeinschaft for their financial support of the SFB 1242.

MA 29: Skyrmions II

Time: Wednesday 15:00–18:45 Location: H20

MA 29.1 Wed 15:00 H20

Emergent electromagnetic inductance of interface skyrmions in $SrRuO_3/SrIrO_3$ bilayers — •Ludwig Scheuchenpflug[1], Sebastian Esser[2], Robert Gruhl[1], Max Hirschberger[2,3], and Philipp Gegenwart[1] — [1]Universität Augsburg, Lehrstuhl für Experimentalphysik VI — [2]Department of Applied Physics, University of Tokyo, Japan — [3]RIKEN Center for Emergent Matter Science, Japan

Emergent electromagnetic induction (EEMI) by current-driven spin dynamics was proposed and observed in the spin helix magnet $Gd_3Ru_4Al_{12}$ [1], where the (current-nonlinear) imaginary impedance at kHz frequency was associated with the motion of helical spin structures. To explore the possibility of EEMI arising from current-driven skyrmion dynamics, we fabricated and microstructured epitaxial thin film bilayers of ferromagnetic $SrRuO_3$ and paramagnetic $SrIrO_3$ on $SrTiO_3$. This bilayer system is known to host DMI-stabilized Néel-skyrmions, indicated by the topological Hall-effect (THE) [2]. We reproduce the THE signatures and observe an accompanying large and current-linear imaginary impedance at low temperatures over broad current density and frequency ranges, signaling the EEMI from the low-energy dynamics of pinned interface skyrmions.

[1] Naoto Nagaosa, Jpn. J. Appl. Phys. 58, 120909 (2019), Yokouchi et al., Nature 586, 232 (2020).
[2] J. Matsuno et al., Science Adv. 2, e1600304 (2016), S. Esser et al., Phys. Rev. B 103, 214430 (2021).

MA 29.2 Wed 15:15 H20

Surface acoustic wave based movement of skyrmions — •Philipp Schwenke, Ephraim Spindler, Vitaliy Vasyuchka, Philipp Pirro, Abbass Hamadeh, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Magnetic skyrmions have significant potential for utilization in spintronic devices, primarily due to their stability and the ability to be manipulated by electric currents. However, when a current is applied, the skyrmions do not move in a direction parallel to the current flow due to the skyrmion Hall effect [1]. Consequently, the precise control of their movement is challenging. Recently, it has been demonstrated that a skyrmion can be moved using a surface acoustic wave (SAW) [2]. Here, we propose an alternative scheme for acoustic manipulation of magnetic skyrmions. Our approach is based on exploiting skyrmion pinning and non-sinusoidal SAWs. To demonstrate feasibility of our approach, we performed micromagnetic simulations using Mumax in a realistic pinning energy landscape.

[1] G.Chen *et. al*, Nature Phys. **13**, 112-113 (2017)
[2] Y.Yang *et. al*, Nat. Commun. **15**, 1018 (2024)

MA 29.3 Wed 15:30 H20

Quantum skyrmions and antiskyrmions in monoaxial chiral magnets — •Štefan Liščák, Andreas Haller, Andreas Michels, Thomas L. Schmidt, and Vladyslav Kuchkin — Department of Physics and Materials Science, University of Luxembourg

Classical monoaxial chiral magnets represent a unique magnetic system that allows for the stabilization of both skyrmions and antiskyrmions of equal energy. Unlike a similar situation in frustrated magnets, the energy landscape here is much simpler, consisting of four states: the saturated ferromagnetic state, spin-spiral, skyrmion, and antiskyrmion. This simplicity makes such systems interesting for potential applications that rely on manipulating these states. We study the quantum analog of the already established classical theory by investigating the low-excitation spectra of a spin-1/2 quantum Heisenberg model with monoaxial Dzyaloshinskii-Moriya interaction. We establish that such a model supports the existence of skyrmion and antiskyrmion states of equal energy using the density matrix renormalization group method (DMRG). This degeneracy allows for the existence of a mesoscopic Schrödinger cat state exhibiting properties of both skyrmion and antiskyrmion. To characterize this superposition, we calculate two-point correlation functions, which can be measured in neutron scattering experiments. Finally, we introduce a perturbation in the form of a magnetic field gradient to induce a non-trivial time evolution of the superposition state. We study this time evolution both using a numerical variational approach and the collective coordinates method.

MA 29.4 Wed 15:45 H20

Magnetometry on the low-temperature skyrmion state in Cu_2OSeO_3 — Christian Oberleitner[1], •Lukas Heindl[1], Johannes Friedrich[1], Andreas Bauer[1,2], Denis Mettus[1,3], Helmut Berger[4], and Christian Pfleiderer[1,2,3] — [1]Physik-Dep., TU Munich, D-85748 Garching — [2]ZQE, TU Munich, D-85748 Garching — [3]MLZ, TU Munich, D-85747 Garching — [4]Inst. de Phys., EPFL, CH-1015 Lausanne

In cubic chiral magnets, skyrmion lattice states emerge near the magnetic ordering temperature, stabilized by thermal fluctuations [1]. Recently, a distinct low-temperature skyrmion state (LTS) was observed in Cu_2OSeO_3 for magnetic fields along the ⟨100⟩ axes, emphasizing the role of cubic anisotropies [2, 3]. Nucleation of this state at low temperatures requires an intermediate phase, the tilted conical phase, and has been studied mainly along major crystallographic axes [4].

Here, we examine the nucleation dynamics of the LTS under field rotation away from high-symmetry directions. Magnetization and ac susceptibility measurements on spherical and cuboid samples reveal key geometry effects. Spherical samples, with uniform internal field distributions, show significant spontaneous LTS nucleation. In contrast, cuboid samples, with inhomogeneous internal fields, need external field pumping to achieve substantial LTS populations[5].

[1]: S. Mühlbauer et al., Science, 323 (2009) 915-919 [2]: S. Seki et al., Phys. Rev. B, 85 (2012) 220406(R) [3]: A. Chacon et al., Nat. Phys., 14 (2018) 936-941 [4]: M. Halder et al., Phys Rev., B 98 (2018) 144429 [5]: A. Aqeel et al., Phys. Rev. Lett., 126 (2021) 017202

MA 29.5 Wed 16:00 H20

Edge dislocations in helimagnets as mobile topological defects — •Maurice Colling[1], Manuel Zahn[1,2], Jan Masell[3], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]University of Augsburg (UniA), Augsburg, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Magnetic topological solitons, such as skyrmions and hopfions, represent fertile ground for emergent physical properties with potential applications in spintronics and unconventional computing. In my talk, I will present magnetic edge dislocations as intriguing nano-sized topological textures, which can serve as mobile information carriers. Edge dislocations naturally arise in the helimagnetic background of the B20-type material FeGe, which we study as a model system. Using micromagnetic simulations, we demonstrate how isolated dislocations can be initialized in a track-like geometry and how their movement can be controlled using spin-polarized currents and magnetic fields. Furthermore, we show how pinning sites can be introduced to achieve 'stop-and-go' motion, allowing to translate events (e.g. magnetic field or current pulses) into positional information. One key difference between dislocations and other topological solitons is their relaxation motion which is driven by the system's intrinsic tendency to revert toward the helimagnetic ground state. This feature makes them interesting candidates for sensing and computing applications and low-energy device technologies in general.

MA 29.6 Wed 16:15 H20

Cubic magnetic anisotropy in *B*20 magnets: Interplay of anisotropy and magnetic order in $Fe_{1-x}Co_xSi$ — •Gilles Gödecke, Julius Grefe, Stefan Süllow, and Dirk Menzel — Insitut für Physik der Kondensierten Materie, TU Braunschweig, D-38106 Braunschweig, Germany

The itinerant systems MnSi and $Fe_{1-x}Co_xSi$ are prominent members among the chiral *B*20 helimagnets. They are known to host chiral spin structures and magnetic skyrmions as a result from the competition of various magnetic interactions, one of which is magnetic anisotropy. Recently, a secondary skyrmion phase governed by cubic anisotropy was identified in the compound Cu_2OSeO_3 [1] raising the question wether such a phase also exists in MnSi and $Fe_{1-x}Co_xSi$. To aid the search for this phase, a better understanding of the cubic anisotropy in these systems would be beneficial.

Here, we report on the quantitative measurement of the cubic magnetocrystalline anisotropy constants in MnSi and $Fe_{1-x}Co_xSi$ ($0.08 \leq x \leq 0.70$) single crystals. Our work presents a systematic study regarding the cubic anisotropy at $T = 5\,K$ and $T = 10\,K$ by means of angle-resolved SQUID magnetization measurements. We observe that the cubic anisotropy is generally weaker than in familiar compounds and more pronounced in MnSi than in $Fe_{1-x}Co_xSi$. For $Fe_{1-x}Co_xSi$ the anisotropy gains at low Co-concentrations with increasing x, vanishes for $x = 0.50$, and is then finite for high x.

[1] A. Chacon et al., Nature Physics 14, 936-941 (2018)

MA 29.7 Wed 16:30 H20

Imaging Topological Defect Dynamics Mediating 2D Skyrmion Lattice Melting — •Raphael Gruber[1], Jan Rothörl[1], Simon Fröhlich[1], Maarten Brems[1], Fabian Kammerbauer[1], Maria-Andromachi Syskaki[1], Elizabeth Martín Jefremovas[1], Sachin Krishnia[1], Asle Sudbø[2], Peter Virnau[1], and Msthias Kläui[1] — [1]Institute of Physics, JGU Mainz — [2]QuSpin, NTNU Trondheim

Two-dimensional (2D) phase transitions are mediated by topological defects, as predicted by KTHNY theory. Using real-time Kerr microscopy, we image the two-step melting of a 2D skyrmion lattice with high spatial and temporal resolution. Skyrmions in low-pinning thin-film systems offer tunability of their size and effective temperature [2,3], allowing us to controllably drive the phase transitions.

Our results reveal the emergence of an intermediate hexatic phase and identify topological defects as the key feature of the melting. We provide new insight into 2D melting dynamics and measure a dislocation diffusion coefficient orders of magnitude higher than skyrmion diffusion. This work highlights skyrmions as a versatile platform for studying phase behavior in 2D systems

[1] Kosterlitz & Thouless, J. Phys. C: Solid State Phys. 5, L124 (1972). [2] Zázvorka et al., Nat. Nanotechnol. 14, 658-661 (2019). [3] Gruber et al., Adv. Mater. 35, 2208922 (2023).

15 min. break

MA 29.8 Wed 17:00 H20

Imaging Topological Defect Dynamics Mediating 2D Skyrmion Lattice Melting — Maarten A. Brems[1], Tobias Sparmann[1], •Simon M. Fröhlich[1], Leonie-C. Dany[1], Jan Rothörl[1], Fabian Kammerbauer[1], Elizabeth M. Jefremovas[1], Oded Farago[2], Mathias Kläui[1], and Peter Virnau[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Ger many — [2]Biomedical Engineering Department, Ben Gurion University of the Negev, Be'er Sheva 84105, Israel

We demonstrate fully quantitative Thiele model simulations of magnetic skyrmion dynamics on previously unattainable experimentally relevant large length and time scales by ascertaining the key missing parameters needed to calibrate the experimental and simulation time scales and current-induced forces. Our work allows us to determine complete spatial pinning energy landscapes that enable quantification of experimental studies of diffusion in arbitrary potentials within the Lifson-Jackson framework. Our method enables us to ascertain the time scales, and by isolating the effect of ultra-low current density (order 10^6 A/m^2) generated torques we directly infer the total force acting on the skyrmion for a quantitative modelling. [2]

[1] S. Lifson and J. L. Jackson, J. Chem. Phys. 36, 2410 (1962). [2] M. A. Brems et al., Phys. Rev. Lett., (2024) (accepted for publication)

MA 29.9 Wed 17:15 H20

The dynamics of skyrmion shrinking — •Frederik Austrup[1], Wolfgang Häusler[2], Michael Lau[1], and Michael Thorwart[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Institut für Physik, Universität Augsburg

When magnetic skyrmions decay, their size in real space decreases in a finite time before they eventually collapse. We derive a continuum model to describe the shrinking behavior of skyrmions before they collapse. Using the Landau-Lifshitz-Gilbert equation and the time derivative of the vectorfield, we find a set of coupled nonlinear ordinary differential equation for the time dependent skyrmion radius and helicity. In particular, we use a triangular-shaped skyrmion profile of its polar angle. Contrary to the commonly expected simple exponential decrease in size, we reveal a more complicated time dependence, where the time-dependent radius crosses over from an exponential decay towards a square root decrease, $\sim (t - t_c)^{1/2}$, near a critical time t_c at which it collapses. This critical time is found to depend logarithmically on the lattice constant. Additionally, we present studies examining the interplay between the shrinking and a transformation through different skyrmion configurations, depending on the various system parameters. The findings are accompanied by numerical studies, supporting the predictions from the theoretical continuum model.

MA 29.10 Wed 17:30 H20

Effects of chiral polypeptides on skyrmion stability and skyrmion diffusion — Fabian Kammerbauer[1], Yael Kapon[2], •Theo Balland[1], Shira Yochelis[2], Sachin Krishnia[1], Yossi Paltiel[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Institute of Applied Physics, Faculty of Sciences, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

CISS, chirality-induced spin selectivity is a phenomenon that has raised significant interest due to the large spin polarizations generated by organic molecules and other effects such as magnetic switching of ferromagnets induced by chiral molecules [1]. In hybrid systems, these chiral molecules have been observed to influence magnetic properties such as changes in the magnetization [2]. In this study, we investigate how chiral molecules of α-helix polyalanine interact with chiral spin structures, namely magnetic skyrmions, which are stabilized in ferromagnetic/heavy metal multilayers due to Dzyaloshinskii-Moriya interaction [3]. Using magneto-optic Kerr effect imaging, we show that chiral polypeptides can influence the stability of skyrmions by modifying the ranges of temperature and applied magnetic field in which they are stable. We also show that the chiral molecules affect the skyrmion dynamics, in particular the thermal diffusion of the skyrmions [4].

[1] R. Naaman et al. Nat. Rev. Chem. 3, 250 (2019)
[2] Y. Kapon et al. J. Chem. Phys. 159, 064701 (2023)
[3] K. Everschor-Sitte et al. J. Appl. Phys. 124, 240901 (2018)
[4] Y. Kapon et al. (under review)

MA 29.11 Wed 17:45 H20

Interactions between Skyrmions with various topological charges — •László Udvardi and Mátyás Török — Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary

Magnetic Skyrmions exhibit intriguing and novel phenomena due to their topologically non-trivial spin textures. Their exceptional stability makes them possible candidates for information carriers for future spintronic devices.

We have determined the parameters appearing in a classical spin model from first principle for a FePd bilayer on Ir(111) and $Pt_{95}Ir_{05}$/Pd(111) overlayer. Optimizing the energy of the spin model several local minima have been identified as a Skyrmion with various topological charges. We demonstrate that the frustration of the isotropic exchange interactions is responsible for the creation of these various types of skyrmionic structures. We focused on objects with topological charge of Q=-1 (Skyrmion) and Q=1 (anti Skyrmion) and explored the interactions between them. We found that although the interaction between Skyrmions with Q=-1 is always repulsive it has attractive part between anti Skyrmions. The excitation of an isolated Skyrmion and a lattice has been also investigated.

MA 29.12 Wed 18:00 H20

RC circuit based on magnetic skyrmions — •Ismael Ribeiro de Assis, Ingrid Mertig, and Börge Göbel — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Skyrmions are nano-sized magnetic whirls attractive for spintronic applications due to their innate stability. They can emulate the characteristic behavior of various spintronic and electronic devices such as spin-torque nano-oscillators, artificial neurons and synapses, logic devices, diodes, and ratchets. Here, we show that skyrmions can emulate the physics of an RC circuit*the fundamental electric circuit composed of a resistor and a capacitor*on the nanosecond time scale. The equation of motion of a current-driven skyrmion in a quadratic energy landscape is mathematically equivalent to the differential equation characterizing an RC circuit: the applied current resembles the applied input voltage, and the skyrmion position resembles the output voltage at the capacitor. These predictions are confirmed via micromagnetic simulations. We show that such a skyrmion system reproduces the characteristic exponential voltage decay upon charging and discharging the capacitor under constant input. Furthermore, it mimics the low-pass filter behavior of RC circuits by filtering high-frequencies in periodic input signals. Since RC circuits are mathematically equivalent to the Leaky-Integrate-Fire (LIF) model widely used to describe biological neurons, our device concept can also be regarded as a perfect artificial LIF neuron.

MA 29.13 Wed 18:15 H20

Intrinsic non-reciprocity in skyrmion dynamics in synthetic antiferromagnet — •Mona Bhukta[1], Takaaki Dohi[1], Fabian Kammerbauer[1], Maria-Andromachi Syskaki[1,2], Duc Minh Tran[1], Markus Weigand[3], Sebastian Wintz[3], Simone Finizio[4], Jörg Raabe[4], Robert Frömter[1], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany — [2]Singulus Technologies AG, 63796 Kahl am Main, Germany. — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [4]Paul Scherrer Institut, Swiss Light Source, Forschungsstrasse 111 5232 PSI Villigen, Switzerland.

In this work, we investigate the dynamics of isolated AFM skyrmion tubes in synthetic antiferromagnetic (SyAFM) multilayers composed of 30-50 ferromagnetic (FM) layers, antiferromagnetically coupled via the interlayer exchange interaction. Using element-specific time-resolved scanning transmission X-ray mi-

croscopy (STXM), we demonstrate the current-induced dynamics of the resulting AFM skyrmions. In uncompensated SyAFM, we observe a current-polarity-dependent, non-reciprocal skyrmion Hall effect of individual AFM skyrmions, arising from the unique intrinsic properties of the hybrid chiral skyrmion tubes in the flow regime. This nonreciprocity can be tuned by the degree of magnetic compensation and vanishes in highly compensated SyAFM [1]. References [1] T. Dohi, M. Bhukta, et al., Observation of a non-reciprocal skyrmion Hall effect of hybrid chiral skyrmion tubes in synthetic antiferromagnetic multilayers,arxiv (2024).

MA 29.14 Wed 18:30 H20

Hybrid magnonic crystal based on skyrmions — •Krzysztof Szulc[1,2], Mateusz Zelent[2], and Maciej Krawczyk[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland — [2]ISQI, Faculty of Physics and Astronomy, Adam Mickiewicz University, Poznań, Poland

We study a hybrid magnonic crystal consisting of a Py waveguide over which the periodic chain of Co/Pt dots is placed [K. Szulc et al. arXiv:2404.10493]. In the dots, the Dzyaloshinskii-Moriya interaction is present, thus it is possible to stabilize the single-domain state and the skyrmion state. We show that the dispersion relation changes with the change of the magnetization configuration of the dot. The sizes of bandgaps significantly differ in these systems. Due to different character of excitation of the both states, the system with skyrmions in dots can interact with the waveguide at lower frequencies or even be excited below the frequencies of the waveguide. Furthermore, I show that one part of the skyrmion modes hybridize with the waveguide modes, sometimes inducing additional band gaps in the spectrum, while the second part does not interact, forming bound states. Such a system of waveguide coupled to the chain of dots forms a reconfigurable spin-wave platform which can be used in spin-wave filtering and artificial neural networks.

This work was supported by the National Science Centre, Poland, grant no. UMO-2021/41/N/ST3/04478 and EU Research and Innovation Programme Horizon Europe (HORIZON-CL4-2021-DIGITAL-EMERGING-01) under grant agreement no. 101070347 (MANNGA).

MA 30: Bulk Materials: Soft and Hard Permanent Magnets

Time: Wednesday 16:00–18:00 Location: H18

Invited Talk MA 30.1 Wed 16:00 H18

Boosting Coercivity in Additively Manufactured Magnets Through Nano-Functionalization of NdFeB Powder — •Anna Ziefuss — Technical Chemistry I and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, 45141 Essen, Germany

Permanent magnets are indispensable in the 21st century, powering applications in energy generation, transportation, and telecommunications. However, the high cost of rare-earth magnets, their supply, and availability represent critical factors, and novel technologies that avoid or minimize the use of such rare elements in permanent magnets need to be developed immediately. Additive manufacturing (AM) offers a promising solution by enabling complex structures with minimal material waste, reducing rare-earth usage. Yet, the successful printing of magnetic powders remains challenging, as printed magnets often exhibit brittleness and low magnetic properties. This contribution highlights how nanotechnology-driven innovations address limitations in additive manufacturing, unlocking the potential of printed magnets for sustainable, high-performance applications. Nano-functionalization emerges as a crucial approach to enhancing coercivity in additively manufactured magnets, emphasizing the importance of understanding the entire process chain - from nanoparticle production and feedstock modification to evaluating printed magnet properties.

MA 30.2 Wed 16:30 H18

Strategies for Nd-Fe-B Magnet Recycling in a Circular Economy — •Aybike Paksoy[1], Amrita Khan[1], Abdullatif Durgun[1], Mario Schönfeldt[1,2], Mahmudul Hasan[2], Iliya Radulov[2], Jürgen Gassmann[2], Imants Dirba[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Department of Materials and Geosciences, Functional Materials, Peter-Grünberg-Str. 16, 64287 Darmstadt, Germany — [2]Fraunhofer IWKS, Fraunhofer Research Institution for Materials Recycling and Resource Strategies, Aschaffenburger Str. 121, 63457 Hanau, Germany

Nd-Fe-B magnets have the highest energy product (BH)max at room temperature, making them the preferred material for various applications. However, their reliance on critical rare earth elements raises significant environmental, economic, and geopolitical challenges, particularly due to China's dominance as the primary global supplier. Both industry and academia are increasingly focusing on recycling end-of-life Nd-Fe-B permanent magnets.For an environmentally friendly product, it is necessary to reduce the criticality and increase the sustainability of rare earth permanent magnets [1]. We compare three advanced recycling routes to produce sustainable Nd-Fe-B magnets without sacrificing their performance. Scrap magnet material is processed via the hydrogen-assisted magnet-to-magnet route as well as the nanocrystalline hot pressing route and spark plasma sintering. The resultant magnetic properties and microstructure are systematically studied comparing the advantages and disadvantages of each process. [1] M. Schönfeldt et al., J. Alloys and Compounds (2023)

MA 30.3 Wed 16:45 H18

3D magnetic of interaction domains in nanostructured Nd-Fe-B using X-ray imaging techniques — •P. Klassen[1], D. Günzing[2], A. Aubert[3], T. Feggeler[4], B. Eggert[1], J. Neethirajan[5], L. Schäfer[3], F. Maccari[3], M. Guizar-Sicairos[6,7], V. Scagnoli[8,6], M. Holler[6], D. Shapiro[2], A. Ditter[2], E. Bruder[3], H. Wende[1], K. Skokov[3], O. Gutfleisch[3], C. Donnelly[5], and K. Ollefs[1] — [1]Fac. of Phys., UDE, Duisburg GER — [2]LBNL, ALS, CA US — [3]Mat. Sc., TU Darmstadt GER — [4]BNL, NSLS-II, NY US — [5]MPI CPfS, Dresden GER — [6]PSI, SLS, Villigen CH — [7]Inst. of Physics, EPFL, Lausanne CH — [8]Dep. of Mat., ETH Zürich CH

Nd-Fe-B magnets play a key role in sustainable energy conversion, for example in wind turbines or electric motors, due to their superior magnetic performance and high energy density. Here, we provide insights into the 3D magnetic domain structure of (therm.) demagnetized nanostructured Nd-Fe-B magnets obtained by X-ray ptychography and tomography at room temperature. We have imaged the magnetic interaction domains inside a hot-deformed, anisotropic, nanocrystalline Nd2Fe14B magnet to correlate the crystal and microstructure and the configuration of the magnetic moments. The combination of hard and soft X-rays enables the comparison of the domain structure between bulk and lamellae and provides detailed insights into the complex magnetic structure in deeper sections of the magnet and down to individual grains, which can be shown to partly exhibit a single-domain state. We gratefully acknowledge funding from the DFG via CRC/TRR 270.

MA 30.4 Wed 17:00 H18

Combined theoretical and experimental study of magnetic properties of Fe-Sn intermetallics — •Martin Friák[1], Petr Čípek[1,2], Pavla Roupcová[1], Oldřich Schneeweiss[1], Jana Pavlů[2], Dominika Fink[3], Šárka Msallamová[3], and Alena Michalcová[3] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Rep. — [2]Dept. Chem., Masaryk Uni., Brno, Czech Rep. — [3]Dept. Metal Corr. Eng., Uni. Chem. Technol. Prague, Czech Rep.

There are conflicting literature reports related to Fe-Sn intermetallic phases, when, for example, the $FeSn_2$ phase is theoretically predicted to be dynamically unstable due to imaginary phonon modes (see, e.g, C.-J. Yu et al., New J. Chem. 44 (2020) 21218, DOI:10.1039/d0nj04537c). We have, therefore, performed a combined theoretical and experimental study of both $FeSn_2$ and FeSn intermetallics. The theoretical part consists of quantum-mechanical calculations of ground-state properties, including structural, vibrational and magnetic properties. Computing phonon modes allowed for testing the dynamic stability and the thermodynamic properties were subsequently assessed using quasi-harmonic approximation (QHA). The $FeSn_2$ phase is computed stable, i.e., free of imaginary phonon modes. We have also characterized Fe-Sn phases using Mössbauer measurements of magnetic properties, including a temperature-dependent Mössbauer factor, which we compared with theoretical results based on quantum-mechanical calculations of thermal vibrations.

MA 30.5 Wed 17:15 H18

Pr-Fe-B hot deformed magnets for low-temperature applications — •Priyatosh Sahoo[1], Alex Aubert[1], Fernando Maccari[1], Yuye Wu[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Technische Universität Darmstadt, Germany — [2]Beihang University, China

Nd-Fe-B based PMs are the most prevalent in various applications due to their high coercivity and remanence, which result in exceptional energy product values near room temperature. However, their performance significantly diminishes below 135 K due to Spin Reorientation Transition (SRT). In contrast, when Nd is substituted by Pr, these magnets do not exhibit such transitions at low temperatures, making them preferable for cryogenic applications such as space industry. In our study, we compared the low-temperature performance of Pr17Fe76.5Cu1.5B5 and Nd17Fe76.5Cu1.5B5 hot deformed (HD) magnet. The microstructure of HD magnets consists of grains in the range of the critical single domain particle size of these systems, i.e., 200-300 nm, which enhances coercivity without the necessity of adding heavy rare earth elements. We conducted a comprehensive analysis that examined intrinsic magnetic properties based on single crystal studies and the transition to extrinsic properties through microstructure engineering along the hot deformation process. Additionally,

we explored the effect of doping Pr-Fe-B with Cu in the hot deformation process and correlated its influence on the magnetic properties and microstructure. We acknowledge Deutsche Forschungsgemeinschaft's (DFG) funding within the CRC/TRR 270 (Project-ID 405553726).

MA 30.6 Wed 17:30 H18

Peculiar low-temperature properties in the ferromagnetic pyrochlore metal $LuInCo_4$ — •Taiki Shiotani[1], Hiroyuki Nakamura[1], and István Kézsmárki[2] — [1]Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan — [2]Experimental Physics V, Institute of Physics, University of Augsburg, D-86159, Augsburg, Germany

The pyrochlore lattice, a network of corner-sharing tetrahedra, is attracting attention due to geometrical frustration as well as nontrivial topology of the band structure. $LuInCo_4$ is C15b-type laves phase compound with a Co-based pyrochlore sublattice. We have successfully synthesized single crystals of $LuInCo_4$ and found strong ferromagnetism with the T_C = 306 K [1]. The ferromagnetic nature was reproduced by density functional theory calculations, suggesting that Co-3d flat bands near the fermi level induce the spin polarization. The magnetization has no detectable anisotropy down to ≈100 K, below which the anisotropy gradually becomes stronger with the cubic 100-type axes being the easy-axes. For fields applied along the cubic 111-type directions the material goes through a metamagnetic transition.

Here, we will focus on the low-temperature phase of $LuInCo_4$ to discuss the origin of the anomalous behavior of the magnetization.

[1] T. Shiotani *et al*., Phys. Rev. Mater. 8, 114409 (2024)

MA 30.7 Wed 17:45 H18

Laser powder bed fusion of hard magnetic composites — •Kilian Schäfer — Functional Materials, Institute of Material Science, Technical University of Darmstadt

Hard magnetic materials are essential for advancing carbon-neutral technologies and medical devices. While traditional manufacturing methods suit large, simple magnets, there is increasing demand for resource-efficient processes to create intricate small magnetic components. Additive manufacturing offers a promising solution, enabling the production of complex, tailored magnetic components with improved efficiency. This study explores composites made via laser powder bed fusion, combining hard magnetic powders with polyamide and thermoplastic polyurethanes. It examines how the magnetic powder*s fraction, morphology, and particle size impact performance. Results show that anisotropic magnetic properties can be achieved with specific powder particle shapes. Additionally, localized mechanical properties were achieved by adjusting laser parameters, enabling the production of magnetically controllable actuators for applications like biomedical devices. These findings provide guidelines for optimizing hard magnetic composite performance using laser powder bed fusion.

MA 31: Poster II

Time: Wednesday 17:00–19:30 Location: P1

MA 31.1 Wed 17:00 P1

Near-Room-Temperature Compensation Temperature In Terbium Iron Garnet Thin Films — •Mehak Loyal, Akashdeep Akashdeep, Mathias Kläui, and Gerhard Jakob — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Rare-earth iron garnets (REIGs) with perpendicular magnetic anisotropy (PMA) have emerged as promising materials for spintronic applications. The compensation temperature (T_{comp}), where the net magnetization for the ferrimagnet becomes zero, plays a crucial role in determining potential application. While bulk REIGs have a T_{comp} well below room temperature, researchers have shown that it can be tuned in thin films. $Tb_3Fe_5O_{12}$ (TbIG) with bulk compensation temperature ~240 K, in particular has gained interest as recent report shows a near-room-temperature T_{comp} for TbIG thin films.

We investigate the factors that tune the compensation temperature (T_{comp}) of TbIG thin films to near-room-temperature. This would have significant implications for the development of spintronics applications, potentially enabling more efficient and stable operation at ambient conditions. PMA TbIG thin films are deposited on (111)-oriented $Gd_3Ga_5O_{12}$ (GGG) substrates using pulsed laser deposition (PLD). The magnetization reversal of TbIG thin films at different temperatures are probed using transverse magneto-resistance measurement. The study contributes to the broader understanding of REIGs and paves the way for integration into practical spintronic applications.

MA 31.2 Wed 17:00 P1

Polarized inelastic neutron scattering studies on magnetic excitations in the SDW ordered state of qasi 2D $Sr_{1.5}Ca_{0.5}RuO_4$ — •Felix Wirth[1], Yvan Sidis[2], Paul Steffens[3], and Markus Braden[1] — [1]II. Physic. Inst., Univ. Cologne, Germany — [2]LLB, CEA Saclay, France — [3]ILL, Grenoble, France

Superconductivity in the layered ruthenate Sr_2RuO_4 emerges near competing magnetic fluctuations. The different d orbitals of Ru^{4+} give rise to the multiband structure causing spin fluctuations with incommensurate (IC) propagation vector due to fermi-surface nesting. These antiferromagnetic fluctuations are anisotropic and condensate to static spin density wave (SDW) order with moments oriented along c when Sr is replaced by 25 % of isovalent Ca. Only a few realizations of SDW in metals have been studied concerning their magnetic excitations. Cr exhibits strong anisotropy as well as new excitations like the Fincher-Buke mode, while the spin-orbit coupling (SOC) is much smaller than in $Sr_{1.5}Ca_{0.5}RuO_4$. This renders it an ideal material for studying SDW state in the presence of SOC. Our contribution presents inelastic polarized neutron scattering measurements on the IC SDW signal. With scattering vector within the layer, we discriminated between transversal and longitudinal excitations. We see longitudinal or c-polarized spectral weight enhancement at low energy. At the same time, the transversal or in-plane response is suppressed over a broad temperature range and exhibits single-relaxor behavior like in the pure compound. SOC induces strong anisotropy in the magnetic fluctuations in $Sr_{1.5}Ca_{0.5}RuO_4$.

MA 31.3 Wed 17:00 P1

Structural and magnetic properties of Bi-bonded Mn-Al-C-Ti magnets — •Semih Ener, Fernando Maccari, Konstantin P. Skokov, and Oliver Gutfleisch — Functional Materials, Technical University of Darmstadt, Peter-Grünberg-Str. 16, D-64287, Darmstadt, Germany

In this study, the influence of Ti doping on the phase formation and magnetic properties of Mn-Al-C-Ti alloys is investigated. The alloys were synthesized by melt spinning followed by thermal treatment to obtain the ferromagnetic τ-phase, which was determined to be 20 min at 550 °C for all Ti compositions.

However, the Ti-doped samples exhibited β-phase formation due to partial phase decomposition, with TiC precipitates observed at higher Ti concentrations. Doping resulted in an increase in the Curie temperature from 557 K in the undoped sample to 600 K in the Ti-doped samples.

In order to increase the coercivity, a combination of ball milling and hot compaction was used along with the introduction of Bi as a metallic binder. This resulted in an increase in coercivity, from 0.18 T to 0.33 T, as the addition of Bi facilitated the formation of a grain boundary phase, which aided in densification. This work demonstrates how compositional and processing modifications can be used to improve the magnetic properties of Mn-Al based magnets.

[1] J.S. Trujillo Hernández, F. Maccari, J.A. Tabares, K.P. Skokov, G.A. Pérez Alcázar, O. Gutfleisch and S. Ener, J. Magn. Magn. Mater. 610 (2024) 172573.

MA 31.4 Wed 17:00 P1

Comparative study on magenetical and structural properties Mn_3XC (X=Sn,Ga,In,Zn) antiperovskites — •Lennart Endler, Benedikt Eggert, Katharina Oleffs, Mehmet Acet, and Heiko Wende — Faculty of Physics and CENIDE, University of Duisburg-Essen

The family of Mn_3XC antiperovskites shows a wide variety of properties ranging from large magnetocaloric effects, giant magnetoresistance to negative thermal expansion [1], which makes them an interesting material class for researchers and industry. Starting with ternary compounds, we also investigate the effect of multiple elements on the X-site, as done for perovskite oxides in the past, revealing a correlation between Neel temperature and Goldschmidt tolerance factor and therefore the chosen elements [2]. For the chemical, structural and magnetic characterisation, we have used EDX, X-ray diffraction, magnetometry and if possible ^{119}Sn Mössbauer spectroscopy. Based on the analysis of the ternary compounds prepared by solid state reaction, the foundation for a comparison to medium and high entropy Mn-antiperovskites is held to further explore and potentially control their properties.

We acknowledge the financial support through the Deutsche Forschungsgemeinschaft wihtin the framework of the CRC/TRR270 HoMMage (Project 405553726-TRR270).

[1] Y. Wang, Adv. Mater. 32, 1905007 (2020)
[2] R. Witte, Phys. Rev Mat. 3, 034406 (2019)

MA 31.5 Wed 17:00 P1

Effect of Ni addition to Fe-B-Si-Nb alloy on magnetic and thermal properties — •Purbasha Sharangi[1], Uma Rajput[2], Amirhossein Ghavimi[2], Ralf Busch[2], Isabella Gallino[3], Gabriele Barrera[1], Enzo Ferrara[1], and Paola Tiberto[1] — [1]INRIM, Istituto Nazionale di Ricerca Metrologica, Strade delle Cacce, 5, 10135 Torino, Italy. — [2]Saarland University, Chair of Metallic Materials, Campus C6.3 66123, Saarbrücken, Germany — [3]Technical University of Berlin, Chair of Metallic Materials, Ernst-Reuter Platz 1, 10587 Berlin, Germany

The next generation of electrical equipment, such as motors and generators, and power electronics, depend heavily on soft magnetic materials. It has been reported that the addition of Ni to Fe-Si-B-Nb BMGs has shown significant improvements in both their soft magnetic properties and plasticity. Fe-based BMGs that incorporate Ni exhibit a good glass forming ability (GFA), reasonable soft magnetic properties and improved mechanical performance. In this work we have investigated the effect of Ni addition and annealing on the microstructural, thermal and magnetic properties of Fe-B-Si-Nb alloy. It has been observed that the GFA is improved from 800 μm to almost 1000 μm upon the addition of 2 to 5 at. % Ni. A slight increment in saturation magnetization and reduction in coercive field have been observed with increasing the Ni% for the as cast ribbons. Further, the soft magnetic properties improve significantly in the form of reduced coercivity and energy losses after annealing the ribbons at 320 $^{\circ}$C for 2 hours due to the relief of frozen-in stresses.

MA 31.6 Wed 17:00 P1

A materials library for cryogenic magnetocaloric cooling — •T. Gottschall, E. Bykov, M. Strassheim, T. Niehoff, C. Salazar-Mejía, and J. Wosnitza — Helmholtz-Zentrum Dresden-Rossendorf, Dresden High Magnetic Field Laboratory (HLD), Dresden, Germany

Magnetic cooling is a refrigeration technique that is based on the so-called magnetocaloric effect, the change of temperature caused by a magnetic field. It can be utilized to construct environmentally friendly cooling devices, air conditioners, and heat pumps. Originally, magnetic cooling was used to achieve ultra-low temperatures near absolute zero. Recently, low temperatures have once again become the focus of attention as an area of application for magnetocaloric cooling namely for efficient hydrogen liquefaction. In this contribution, we will present our materials library for cryogenic applications. The basis for this is our research infrastructure at the Dresden High Magnetic Field Laboratory, which includes both static and pulsed fields. Our aim is to gain a better understanding of the magnetocaloric materials required for the cooling process, to provide consistent data sets for simulations, and to drive magnetic hydrogen liquefaction forward making it an energy efficiency alternative to conventional technology.

MA 31.7 Wed 17:00 P1

Inverse magnetocaloric effect in Tb_3Ni: So hot right now — •T. Niehoff[1,2], B. Beckmann[3], K. Skokov[3], A. Herrero[4], A. Oleaga[5], M. Strassheim[1,2], T. Wosnitza[1,2], and T. Gottschall[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [3]Institut für Materialwissenschaft, TU Darmstadt, Darmstadt, Germany — [4]Departamento de Física Aplicada, UPV/EHU, Vitoria-Gasteiz, Spain — [5]Departamento de Física Aplicada, UPV/EHU, Bilbao, Spain

The magnetocaloric effect (MCE) is a cornerstone of promising, environmentally friendly cooling technologies, particularly for cryogenic applications. In this presentation, we use Tb_3Ni as a case study, previously reported to exhibit a strong inverse MCE at very low temperatures based on magnetization measurements. By comparing these findings with other techniques, we show that neither Tb_3Ni nor similar materials with metamagnetic transitions from antiferromagnetic to ferromagnetic exhibit the predicted inverse effect. To support our claims and further investigate the MCE, we conducted specific-heat measurements and direct T_{ad} in pulsed-field experiments. These reveal no effects, while the pulsed-field data even show a significant positive effect, which we attribute to dissipative heating. Our findings highlight the importance of using complementary measurement techniques to accurately characterize the MCE and fully understand the behavior of these materials.

MA 31.8 Wed 17:00 P1

Design of $Cr_xFe_{1-x}MnCoNiGeSi$ high-entropy alloy with large barocaloric effect — •Yong Guo[1,2], Yuanyuan Gong[1], Tingting Zhang[1], Zhishuo Zhang[1], Bin Chen[1], Fenghua Chen[3,4], Zhengyi Jiang[4], Feng Xu[1], and Luana Caron[2,5] — [1]MIIT Key Laboratory of Advanced Metallic and Intermetallic Materials Technology, School of Materials Science and Engineering, Nanjing University of Science and Technology , Nanjing 210094, PR China — [2]Faculty of Physics, Bielefeld University, Bielefeld 33501, Germany — [3]School of Materials Science and Engineering, Taiyuan University of Science and Technology, Taiyuan 030024, PR China — [4]School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, Wollongong, NSW 2522, Australia — [5]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany

This paper presents a high-entropy system exhibiting a large barocaloric effect. Experimental results confirm that equiatomic FeMnCoNiGeSi and CrMnCoNiGeSi are high-entropy solid-solutions with hexagonal and orthorhombic structures at room temperature, respectively. Further tuning Fe/Cr ratio in $Cr_xFe_{1-x}MnCoNiGeSi$ establishes a thermal-induced hexagonal-orthorhombic structural transformation. For the alloy with $x = 0.44 - 0.50$, the structural transformation occurs at room temperature and can be induced by hydrostatic pressure. The barocaloric effect reaches -30.6 J/kgK for a pressure change from 5 to 0 kbar, and the entropy change per kbar is comparable to widely studied intermetallic compounds.

MA 31.9 Wed 17:00 P1

Collective out-of-plane stripe domain magnetization reversal via a single point of irreversibility — •Peter Heinig[1,2], Ruslan Salikhov[2], Fabian Samad[1,2], Lorenzo Fallarino[2,3], Attila Kákay[2], Nikolai S. Kiselev[4], and Olav Hellwig[1,2] — [1]Chemnitz University of Technology — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]CIC energiGUNE — [4]Forschungszentrum Jülich

Periodic stripe domain structures in thin films with perpendicular magnetic anisotropy are well-studied, however, the detailed field reversal of such systems in the transition regime between in-plane (IP) and out-of-plane (OOP) magnetization remains intriguing, with unexpected effects. In particular, the $[Co(3.0\ nm)/Pt(0.6\ nm)]_X$ multilayer system undergoes this transition[1]. We examine samples with $X = 10$ and $X = 11$ repetitions, which display a remanent state with both significant OOP as well as IP magnetization components, here referred to as the "tilted" stripe domain state[1,2]. Using vibrating sample magnetometry, magnetic force microscopy, and micromagnetic simulations, we analyze the unusual OOP field reversal behavior, which is characterized by a single point of irreversibility and parallel stripe domains at remanence. While these two characteristics seem at first sight mutually exclusive, we will reveal how they still can evolve simultaneously. In addition to the unusual OOP reversal, we also observe a significant IP angular dependence of the susceptibility around remanence induced by the parallel stripe domain alignment.

[1] [L. Fallarino et al., Phys. Rev. B 99, 024431 (2019)]
[2] [P. Heinig et al., Phys. Rev. B 110, 024417 (2024)]

MA 31.10 Wed 17:00 P1

Epitaxy and Magnetic Properties of Fe films on GaAs(001) in Dependence of the Electrodeposition Procedure — •Danny P. Quint[1], Raphael Kohlstedt[2,3], Olav Hellwig[2,3], and Karin Leistner[1] — [1]Institute of Chemistry, TU Chemnitz — [2]Institute of Physics, TU Chemnitz — [3]Research Center MAIN, TU Chemnitz

Epitaxial Fe/GaAs heterostructures are of great interest for spintronic devices.[1] The quality of the epitaxial growth is crucial for the functionality. While MBE is traditionally used to fabricate Fe/GaAs structures, electrodeposition (ED) offers a cost-efficient alternative. [2,3] We systematically examined the impact of an initial voltage pulse during ED of Fe films (approx. 20 nm thick) on GaAs(001) on their epitaxy and magnetic behavior. We compare depositions without a pulse (A), with a pulse after immersion in the electrolyte (B), and with a pulse during immersion in the electrolyte (C). The angle-dependent ferromagnetic resonance field, remanence and coercivity of the deposited films were analyzed by in-plane FMR and MOKE, respectively. The results show an enhanced fourfold anisotropy for the films prepared with the pulsed routines, with method C approaching the expected behavior for dominating cubic magnetocrystalline anisotropy in epitaxial Fe(001) films. The quality of epitaxial growth is investigated by X-ray diffraction. This work highlights the importance of optimizing the ED procedure to achieve epitaxial Fe films on GaAs and opens pathways for the broader application of ED in spintronic materials research.

[1] Wastlbauer et al., Adv. Phys., 54, 2005, 137.
[2] Liu et al., ESL, 7, 2004, D11.
[3] Guo et al., Nano Lett., 22, 2022, 4006.

MA 31.11 Wed 17:00 P1

Pt-catalyzed hydrogen magneto-ionics in Co/Pd multilayers — •Felix Engelhardt[1,2], Rico Ehrler[1,2], Olav Hellwig[1,2], Karin Leistner[1,2], and Markus Gössler[1] — [1]Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Research Center MAIN, D-09126 Chemnitz, Germany

Magneto-ionics, which is the electrochemical reconfiguration of magnetic materials at low gating voltages, offers a highly energy-efficient method to control magnetism. One major issue of this mechanism, however, is its response time, which is limited by the timescale of the electrochemical reactions. Here, we demonstrate that the hydrogen-based magneto-ionic effect in sputtered Co/Pd multilayers [1] can be accelerated catalytically via an additional Pt layer at the surface.

We investigate how the thickness of such a Pt overlayer affects the magneto-ionic effect strength and hydrogen insertion kinetics in the Co/Pd multilayer system. To analyze these effects, we use in-situ MOKE microscopy to monitor the magneto-ionic behavior, while flow-cell coulometry measurements are carried out to quantify the hydrogen concentration in the multilayers.

Our findings reveal that a Pt overlayer with a thickness of 0.5-2 nm significantly enhances the strength of the magneto-ionic effect by a factor of 2, while also reducing the time required for hydrogen insertion by a factor of 10. Our results highlight a route towards faster switching speeds in magneto-ionic devices, which is crucial for future magnetic memory applications.

[1] M. Bischoff et al., Adv. Funct. Mater., **34**, 2405323 (2024)

MA 31.12 Wed 17:00 P1

Investigating Micromagnetic Structures in Dy-Fe Ferrimagnetic Thin Films — •Pranati Parui[1], Tamer Karaman[1], Felix Büttner[1,2], and Manfred Albrecht[1] — [1]University of Augsburg, Augsburg, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

Ferrimagnetic thin films present a unique platform for studying emergent spin textures and magnetic phenomena due to the interplay between the transition-metal and rare-earth sublattices. Here, we investigate ferrimagnetic Dy-Fe alloy thin films, which exhibit a broad spectrum of magnetic properties that are highly sensitive to composition and temperature. Despite their potential, a systematic investigation of Dy-Fe thin films remains unexplored. This work focuses on the sputter deposition of thin films with varying compositions and employs comprehensive characterization techniques, including SQUID magnetometry, magneto-optical Kerr effect (MOKE) measurements, magnetic force microscopy (MFM), and Lorentz transmission electron microscopy (LTEM), to unravel their micromagnetic structures, domain patterns, and domain wall chirality.

MA 31.13 Wed 17:00 P1

Detecting correlation between surface and interface magnetism of Mn/Fe thin film heterostructures on the atomic scale — •Toshio Miyamachi[1,2], Shuhei Nakashima[1], Yasumasa Takagi[3], Toshiohiko Yokoyama[3], and Fumio Komori[1] — [1]ISSP, The University of Tokyo, Japan — [2]IMaSS, Nagoya University, Japan — [3]Institute for Molecular Science, Japan

The magnetic coupling between ferromagnetic (FM) and antiferromagnetic (AFM) layers has been the focus of interest for magnetic multilayer devices. The fundamental magnetic properties of FM/AFM magnetic multilayers, e.g., magnetic moment, magnetic anisotropy rely much on their interfacial structural and electronic properties. In this work, we investigated structural, electronic and magnetic properties of AFM/FM Mn/Fe thin film heterostructures grown on Cu(001) by spin-polarized scanning tunneling microscopy (Sp-STM) and x-ray absorption spectroscopy/x-ray magnetic circular dichroism (XAS/XMCD) [1]. With the help of surface sensitivity of SP-STM and element specificity of XAS/XMCD, electronic and magnetic properties of surface Mn and interface Fe layers were separately investigated. Sp-STM measurements revealed a new type of surface magnetic structures of Mn layers, which could be interpreted in term of the magnetic coupling with underlying Fe layers.

[1] S. Nakashima et al., Adv. Funct. Mater. 29, 1804594 (2019).

MA 31.14 Wed 17:00 P1

Integration of a dual broadband characterization setup for time-resolved magneto-optical spectroscopy — •Richard Leven, Sophie Bork, David Gutnikov, Umut Parlak, and Mirko Cinchetti — Department of Physics, TU Dortmund, 44227 Dortmund, Germany

We present a recently developed setup for broadband ultrafast magneto-optical pump-probe spectroscopy, optimized for operation at low temperatures and high magnetic fields. The setup utilizes a broadband supercontinuum (white light) probe beam, spanning wavelengths from the near UV to the near IR region. Two independent CMOS detector arrays enable simultaneous data acquisition across all available wavelengths, providing comprehensive insights into transient reflectivity ($\Delta R/R$) and polarization rotation ($\Delta\theta$) measurements in a single experiment. The system operates at variable repetition rates, ranging from <10 kHz to ~100 Hz, combining the precision of a femtosecond laser source with high sensitivity for low-light conditions. To validate the setup, we conduct experiments on the semiconducting antiferromagnet CrSBr, ensuring the spectrum encompasses the material's bandgap and exciton excitation energies. This poster will detail the technical specifications of the setup, its characterization results, and its performance benchmarks, highlighting its potential for studying ultrafast dynamics in a variety of magnetically ordered systems.

MA 31.15 Wed 17:00 P1

Element-resolved study of antiferromagnetic/ferromagnetic magnetization dynamics in epitaxial CoO/Fe bilayer — •Chowdhury Shadman Awsaf[1], Sangeeta Thakur[1], Markus Weissenhofer[2], Jendrik Gördes[1], Marcel Walter[1], Niko Pontius[3], Christian Schüssler-Langeheine[3], Peter Oppeneer[2], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Department of Physics and Astronomy, Uppsala University — [3]Helmholtz-Zentrum Berlin für Materialien und Energie

We examine the transient AFM spin structure in an epitaxial Fe/CoO bilayer on an Ag(001) single-crystal substrate after excitation by 60 fs laser pulses of 800 and 400 nm wavelength, below and above the CoO band gap, respectively, by evaluating the time-resolved x-ray magnetic linear dichroism in reflectivity at the Co L2 edge. The findings are compared to time-resolved x-ray magnetic circular dichroism measurements at the Fe L3 edge. Both layers exhibit a fast drop in magnetic order within 300 fs. Simulating an atomistic two-temperature model, coupled with the stochastic Landau Lifshitz-Gilbert equation for the spin degrees of freedom, indicates a direct energy transfer from hot Fe electrons to CoO spins in the case of 800 nm excitation. For demagnetization at 400 nm pump, above-band-gap excitation in CoO has to be assumed in the simulation to reproduce the experimental result [1]. [1] C. S. Awsaf et al., arXiv:2408.14360.

MA 31.16 Wed 17:00 P1

Laser-induced magnetostriction in Gd, Tb and Dy probed by UXRD — •Florian Baltrusch[1], Alexander von Reppert[1], Steffen P. Zeuschner[1], Maximilian Mattern[1], Matthias Rössle[2], Florin Boariu[2], Karine Dumesnil[3], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Institut Jean Lamour, Universite Lorraine, Nancy, France

In ultrafast X-ray experiments, we compare the laser-induced magnetostriction in Gd, Tb and Dy upon femtosecond laser excitation at temperatures above and below the magnetic ordering temperatures. These rare earths exhibit giant spontaneous magnetostriction and consequently negative thermal expansion (NTE). The coupling between magnetic order and the lattice below the Curie temperature leads to a competition between the expansive stresses from electrons and phonons and the contractive stress due to magnetic order. Thus, upon femtosecond laser excitation, the ultrafast dynamics show a variety of interesting results, such as transforming a typical bipolar strain wave into a unipolar pulse. By comparing equilibrium thermal expansion and heat capacities, we separate electronic, phononic, and magnetic stress contributions using an extended Grüneisen model based on energy densities in each of the three subsystems. This enables fitting ultrafast strain dynamics and identifying subsystem coupling constants.

MA 31.17 Wed 17:00 P1

Towards ultrafast time-resolved SHG imaging of ferroic materials — •Andrin Caviezel, Gerrit Horstmann, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

Ferroic materials enable the storage and manipulation of information within their domain structures, a fundamental property underpinning their technological potential. Second-harmonic generation (SHG) imaging is a well-established method for probing ferroic domain patterns at equilibrium, while optical excitation with femtosecond laser pulses holds promise for achieving ultrafast domain switching. However, studying the non-equilibrium dynamics of ferroic domains demands an imaging technique that offers both high temporal and spatial resolution. In this work, we present an ultrafast time-resolved SHG imaging setup designed specifically to investigate non-equilibrium dynamics in ferroic materials. By utilizing the high pulse energies of an amplified laser system, our setup enables direct wide-field imaging of ferroic structures. Additionally, the ability to tune the laser wavelength and employ sequences of pump pulses provides precise control over optical excitation conditions. This approach allows us to study ultrafast processes both in bulk ferroics with microscopic domain structures and micrometer-sized flakes of van der Waals ferroics under cryogenic conditions, advancing our understanding of their dynamic behavior.

MA 31.18 Wed 17:00 P1

Influence of defects on the ultrafast orbital Hall effect in metallic nanoribbons — •Theresa Albrecht, Franziska Ziolkowski, Oliver Busch, Börge Göbel, Ingrid Mertig, and Jürgen Henk — Institut für Physik, Martin-Luther-Universität, D-06099 Halle

The time-dependent orbital Hall effect, which is generated by a femtosecond laser pulse, called the ultrafast orbital Hall effect (UOHE) is investigated. We present the influence of different types of defects on the UOHE in a Cu nanoribbon. The laser-driven electron dynamics is numerically calculated by our theoretical framework Evolve based on a real-space tight-binding approach for finite systems and the solution of the von Neumann equation for the calculation of the occupation numbers [1]. As a result we discuss charge redistribution and charge currents as well as orbital angular momenta and their currents with atomic resolution in the time domain. The role of defects is analysed quantitatively which is particularly important to compare with experiments.

[1] O. Busch *et al.*, Physical Review Research **6**, 013208 (2024)

MA 31.19 Wed 17:00 P1

Ultrafast magneto-elastic phenomena in highly magnetostrictive materials with systematic variation of anisotropy — •Constantin Walz[1], Fried Weber[1], Karine Dumesnil[2], Alexander von Reppert[1], and Matias Bargheer[1,3] — [1]Institut für Physik und Astronomie, Universität Potsdam, Germany — [2]Institut Jean Lamour, Université Lorraine, Nancy, France — [3]Helmholtz-Zentrum Berlin, Germany

Highly magnetostrictive Rare Earth-Iron compounds ($REFe_2$ with RE = Tb, Dy, $Tb_{0.3}Dy_{0.7}$) are well known for their giant (inverse) magnetostriction, with more than 10^{-3} lattice constant change when applying a magnetic field. Because of that they are widely used as ultrasonic transducers in the MHz regime. Their

laser-induced magnetization dynamics are less explored, though they have potential as field-tunable magneto-acoustic transducers in the GHz regime or even for strain driven magnetization switching. Here we compare polar transient magneto-optical Kerr effect (trMOKE) data on three (110)-oriented $REFe_2$. The rare-earth ion influences the cubic magnetocrystalline anisotropy energy, leading to nontrivial demagnetization and precession responses with opposing signs for Dy and Tb. We discuss non-resonant strain-driven magnetization dynamics that follow the lattice deformation with a delay. Glass-capped $TbFe_2$ films help to disentangle signal contributions from unipolar strain pulses, quasi-static strain and spin disorder.

MA 31.20 Wed 17:00 P1

Controlling Spin periodicity in a Helical Heisenberg Antiferromagnet — •Hyein Jung[1,2], Abeer Arora[2], Deeksha Gupta[3], Franziska Walther[4], Kristin Kliemt[4], Victoria C. A. Taylor[2], Túlio de Castro[2], Hanqian Lu[1,2], Christian Schüssler-Langeheine[3], Niko Pontius[3], Urs Staub[5], Cornelius Krellner[4], Laurenz Rettig[2], Ralph Ernstorfer[1,2], and Yoav W. Windsor[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Goethe-Universität Frankfurt, Frankfurt, Germany — [5]Paul Scherrer Institut, Villigen, Switzerland

Manipulating antiferromagnetic spin structures is a promising route to new spintronics functionality. This is particularly desirable on ultrafast time scales due to the growing demands for device speeds. Here we investigate the chiral antiferromagnet EuCo2P2 using resonant X-ray diffraction and manipulate the periodicity of its spins under three distinct conditions: (a) femtosecond laser pulse excitation, (b) applied magnetic fields, and (c) heating. These represent fundamentally distinct microscopic routes for manipulation, and their combination can provide an essential basis for achieving precise control of antiferromagnetic spin structures.

MA 31.21 Wed 17:00 P1

Ultrafast demagnetization via 4f-multiplet excitations in Terbium investigated by tr-ARPES — •Timo Dully, Gaurav Kshetry, Xinwei Zheng, Christian Strüber, and Martin Weinelt — Freie Universität Berlin

The magnetic properties of rare earth metals are governed by the localized electrons in the partially filled 4f electron shell and the interaction with the itinerant 3d electrons. Spin polarization of the 4f electrons decreases much faster in Terbium than in Gadolinium [1]. This has been attributed to enhanced coupling to the lattice caused by the anisotropic shape of the electronic wavefunction in Terbium. However, recent XMCD and RIXS experiments demonstrate an additional excitation pathway that is involved in drastically increasing the response of the magnetic system to optical excitation [2]. Scattering of optically excited 5d electrons with the 4f-subsystem allows for an efficient excitation of the 4f-multiplet.

In our time- and angle-resolved photoemission spectroscopy (tr-ARPES) setup using a hemispherical energy analyzer we measure the demagnetization of Tb as a function of time and fluence. We observe transient changes to the 4f photoemssion signal indicating a substantial excitation of the 4f-multiplet by energy transfer from the 5d valence electrons.

[1] B. Frietsch et al. Sci. Adv. 6(2020) eabb1601

[2] Nele Thielemann-Kühn et al., Sci. Adv. 10 (2024) eadk9522

MA 31.22 Wed 17:00 P1

Probing magnetic dimensional crossover in CrSiTe3 through picosecond strain pulses — •Anjan Kumar Naralapura Manohara[1,2], Soumya Mukherjee[2], Abhirup Mukherjee[2], Ajinkya Punjal[3], Shubham Purwar[4], Thirupathaiah Setti[4], Shriganesh Prabhu[3], Siddhartha Lal[2], and Natarajan Kamaraju[2] — [1]Institute of Solid State and Materials Physics, TUD Dresden University of Technology, Dresden, Germany, 01069 . — [2]Department of Physical Sciences, Indian Institute of Science Education and research, Kolkata, West Bengal, India, 741246. — [3]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental research, Mumbai, Maharashtra, India, 400005. — [4]Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Kolkata, West Bengal, India, 700 106.

Two-dimensional van der Waals materials provide a unique platform to investigate the evolution of magnetic order from short-range 2D intraplanar to long-range 3D interplanar configurations. Employing non-degenerate pump-probe spectroscopy, we have generated and detected picosecond acoustic strain pulses in CrSiTe3. By analysing the distinct signatures of these pulses, we have elucidated a multi-stage pathway for the magnetic dimensional crossover. Furthermore, our study reveals novel insights into the intricate interplay between spin dynamics and lattice vibrations, as manifested in both picosecond strain pulses and ultrafast carrier dynamics.

MA 31.23 Wed 17:00 P1

Low-temperature XPEEM to study functional properties of magnetic 2D materials — •Shubhada Patil[1], Alevtina Smekhova[2], and Florian Kronast[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany

Two-dimensional (2D) magnetic van der Waals materials are particularly promising for electronic and spintronic devices. They exhibit novel electronic and magnetic properties that are ideally suited for investigation with surface-sensitive X-ray photoemission electron microscopy (XMCD-PEEM). In this poster, the experimental capabilities of the low-temperature PEEM facility at BESSY II are presented, including the possibility to study responses to optical excitations of a femtosecond laser system.

The results presented will focus on investigations of the magnetic properties of 2D heterostructures prepared by mechanical exfoliation of FexGeTe2 crystals (x=3, 4 or 5) with a thickness of up to a few monolayers on gold-coated Si/SiO2 substrates with h-BN capping layer in an inert atmosphere. Element-specific low-temperature imaging in XPEEM with a special sample environment is used to identify the magnetic domain configurations and their dynamic response to optical excitation with fs laser pulses.

MA 31.24 Wed 17:00 P1

Magnon-phonon scattering on ultrafast timescales — •Nabil Makadir, Kai Leckron, and Hans Christian Schneider — Physics Dept, University of Kaiserslautern-Landau (RPTU), Kaiserslautern, Germany

In the ultrafast demagnetization of ferromagnets, electron-magnon scattering likely plays an important role. Recently it has been shown in the framework of a two-band Stoner model (arXiv:2304.14978) that electron-magnon scattering processes lead to the creation of non-equilibrium magnons at large wave vectors on ultrafast time scales. In this contribution, we investigate how a large density of high-q magnons, as it is created during the demagnetization process, relaxes due to magnon-phonon and magnon-electron interactions. Treating phonons as bosons, we solve the dynamical equations for the magnon and phonon distributions including the relevant interactions at the level of Boltzmann scattering integrals. From the numerical results, we draw conclusions for the remagnetization process.

MA 31.25 Wed 17:00 P1

Ultrafast spin flop in Fe/Gd bilayers — Dominic Lawrenz[1], Tim Amrhein[1], Jonathan Weber[1], Wibke Bronsch[1], Niko Pontius[2], Christian Schüssler-Langeheine[2], Nele Thielemann-Kühn[1], and •Martin Weinelt[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Using time-resolved X-ray magnetic circular dichroism in reflection (XMCD-R) at the femtoslicing facility of BESSY II (Helmholtz-Zentrum Berlin) we studied ultrafast magnetization dynamics in an Fe(5 nm)/Gd(11 nm) bilayer on W(110). Structural and magnetic depth profiles of the bilayer were characterized by static $\Theta/2\Theta$ XMCD-R scans. The magnetization $\vec{M}$ lies in-plane with antiparallel alignment of $\vec{M}_{Fe}$ and $\vec{M}_{Gd}$ at the Fe/Gd interface. At 300 K, Gd is magnetized only at the interface. Upon optical excitation Gd demagnetizes within 2 ps reaching a transient ferromagnetic state for $\sim$ 20 ps, comparable to simulations for Co/Gd in [1]. Close to the compensation temperature of 235 K, $\vec{M}_{Fe} = -\vec{M}_{Gd}$ are oriented nearly perpendicular to the external field and twisted into the field direction with increasing distance to the interface. Upon optical excitation we observe a transient spin flop by 6° of the Gd magnetization within 300 fs. This is attributed to spin-transfer torque caused by ultrafast spin currents [2] and may hint to spin vacuum switching [3].

[1] M. Beens et al., Phys. Rev. B **100**, 220409(R) (2019).

[2] B. Liu, H. Xiao, M. Weinelt, Sci. Adv. **9**: eade0286 (2023).

[3] E. I. Harris-Lee et al., Sci. Adv. **10**: eado6390 (2024).

MA 31.26 Wed 17:00 P1

Setting up current-induced spin-wave Doppler shift experiments — •Linda Nesterov, Julian Strassburger, Johannes Demir, Karsten Rott, and Timo Kuschel — Universität Bielefeld, Germany

The coupling of coherent spin waves with incoherent spin transport, such as spin-polarized electrons, results in the transfer of angular momentum via spin-transfer torque, enabling the so-called spin-wave Doppler shift [1]. Our research aims to deepen the understanding of this fundamental process, which plays a significant role in the development of next-generation memory devices and other spintronic applications. Propagating spin-wave spectroscopy is used to detect a possible Doppler shift in spin waves generated by charge currents in a 20 nm thick $Ni_{81}Fe_{19}$ strip. The experiments are conducted using a vector network analyzer with both in-plane and out-of-plane magnetic fields applied perpendicular to the direction of the propagating spin wave, which is excited with the use of a coplanar waveguide design. In contrast to published works [1,2], this study uses Ta_2O_5 as an insulating material, chosen for its high permittivity, leading to

a different impedance matching within the system.

[1] V. Vlaminck, M. Bailleul, Science 322, 410 (2008)
[2] J. Lucassen et al., Appl. Phys. Lett. 115, 012403 (2019)

MA 31.27 Wed 17:00 P1

Angle-dependent pumping of magnon Bose-Einstein condensates — •Franziska Kühn[1], Matthias R. Schweizer[1], Georg von Freymann[1,2], Alexander A. Serga[1], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Fraunhofer Institute for Industrial Mathematics ITWM, Fraunhofer Platz 1, 67663 Kaiserslautern, Germany

Our work focuses on the generation and behavior of magnon Bose-Einstein condensates (BEC) in yttrium-iron-garnet films. To create a magnon BEC, the magnon gas must be populated above the thermal level by external injection of magnons. Conventionally, this is done by parallel parametric pumping, where magnons are injected into spin-wave modes at half the pumping frequency. This work aims to optimize the pumping configuration by changing the direction of the microwave pumping field relative to the external magnetic field. This concept of oblique pumping promises higher efficiency and easier manipulation of the magnon BEC. The measurements are performed using a vector magnet for the rotation of the external magnetic field and Brillouin light scattering spectroscopy as an optical detection method for magnons. First results promise lower thresholds for the pumping power and thus easier excitation of magnons leading to a magnon BEC. This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-TRR 173/3-268565370 Spin+X (Project B04)

MA 31.28 Wed 17:00 P1

Towards Aharonov–Casher effect based nonreciprocal electrical control of the magnon phase in a perpendicularly magnetised YIG film — •Gabriel Schwöbel[1], Alexander A. Serga[1], Vitaliy I. Vasyuchka[1], Rostyslav O. Serha[2], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszen- trum OPTIMAS, RPTU, 67663 Kaiserslautern — [2]Faculty of Physics, University of Vienna, 1090 Vienna

Modulation of phase and amplitude of spin waves plays a crucial role in the realization of ultra-low power magnon-based computing. Therefore, we study the magnon phase change, induced by an applied electric field, in yttrium iron garnet (YIG), which has favourable magnetic properties such as a very low spin wave damping.

Recent studies [1] performed in in-plane magnetized single crystal YIG films have allowed us to evaluate different contributions to this phase change and to provide experimental evidence for the theoretically predicted magnonic Aharonov–Casher effect. This effect describes the accumulation of a geometric phase when a magnon passes through an electric field. In our new setup, which provides a more homogeneous and stable magnetic field, we investigate the nonreciprocal effects of magnon phase accumulation when a tangential electric field is applied to an out-of-plane magnetized YIG film.

[1] R.O. Serha et al., *Towards an experimental proof of the magnonic Aharonov–Casher effect*, Phys.Rev. B **108**, L220404 (2023)

MA 31.29 Wed 17:00 P1

Towards magnetically controlled phononic crystals — •Philipp Knaus, Maximilian Alexander Thiel, Kaya Gauch, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum Optimas, RPTU Kaiserslautern, Germany

Phononic crystals (PnCs) are materials with periodic modulations in their elastic properties that allow precise tuning of the phonon dispersion relation, enabling control of phonon propagation, including bandgaps, waveguiding and confinement. Recent advances have focused on 2D PnCs, which support innovative applications such as nanoscale information processing, optomechanical systems and thermal management [1]. This work represents a first step towards magnetically controlled PnCs based on surface acoustic waves, where the phononic properties of the material can be tuned. We study a magnetically controlled PnC based on Lithium Niobate $LiNbO_3$/CoFeB heterostructure. We characterize our prototype by electrical transmission measurements using a vector network analizer and optical measurements based on Brillouin Light Scattering and the time-resolved magneto-optic Kerr effect. Based on our results, we discuss potential applications and device optimization.

[1] M. Sledzinska et. al, Adv. Funct. Mater. 8, 30 (2020)

MA 31.30 Wed 17:00 P1

Spin Hall driven spin-wave emission in Ga:YIG/Pt heterostructures — •Moritz Bechberger[1], David Breitbach[1], Björn Heinz[1], Carsten Dubs[2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]INNOVENT e.V. Technologieentwicklung, Jena, Germany

The development of a DC driven and scalable spin-wave source that exhibits a self-adaptive frequency is desirable. In particular, spin currents can be used for these spin-wave sources, but instead of radiating energy in the form of propagating spin waves, localized oscillations occur in most systems due to the underlying negative nonlinear frequency shift. Here, a heterostructure consisting of an yttrium iron garnet thin film substituted with gallium atoms (Ga:YIG), which exhibits a perpendicular magnetic anisotropy, and a thin layer of platinum is employed. The heterostructure allows studies in the positive nonlinear frequency shift regime for in-plane magnetization. A spin current is locally injected into the Ga:YIG film via the spin Hall effect by applying a direct current to the platinum pad. This allows for the study of the spin-wave emission into the adjacent Ga:YIG waveguide. The emission of spin waves was found to be partially decoupled from the auto-oscillation and is restricted to a narrow frequency and wave-vector range. This work provides a proof-of-concept and the fundamental basis for the development of spin-wave emitters utilizing this mechanism. This research is funded by the DFG - Project No. 271741898, TRR 173-268565370 (B01), and the ERC Grant No. 101042439 CoSpiN.

MA 31.31 Wed 17:00 P1

Controlling the Bi/Fe ratio in bismuth iron garnet thin films deposited by confocal magnetron sputtering for enhanced Faraday rotation — Gajendra L. Mulay[1,2], •Shraddha Choudhary[3], Bhagyashree A. Chalke[1], Rudheer D. Bapat[1], Jayesh B. Parmar[1], Manish B. Ghag[1], Vilas J. Mhatre[1], Shriganesh Prabhu[1], Ashwin A. Tulapurkar[2], and Venu Gopal Achanta[1,4] — [1]TIFR, Mumbai, 400005, India. — [2]IIT Bombay, Mumbai, 400076, India. — [3]Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, Münster, 48149, Germany. — [4]On lien at CSIR-NPL, New Delhi, 110012, India.

Among all known garnet films bismuth-iron-garnet (BIG;$Bi_3Fe_5O_{12}$) films not only demonstrate the highest Faraday rotation in visible light but also exhibit minimal optical losses. We have successfully deposited high-quality BIG epitaxial thin films on single-crystal gadolinium-gallium-garnet (GGG; $Gd_3Ga_5O_{12}$) (111) substrates via Radio frequency confocal sputtering, utilizing separate bismuth and iron oxide sputtering targets and optimized thermal treatments. The Bi/Fe ratio in the deposited BIG thin films can be varied by controlling the sputter process parameters. These deposited thin films exhibit homogeneity and surface root mean square roughness of less than 2 nm. The epitaxial film quality is confirmed by X-ray diffraction and Transmission electron microscopy. Moreover, the films demonstrate low optical loss and a magneto-optical Faraday rotation as high as $-34^o \pm 1^o/\mu$m at a wavelength of 535 nm for a BIG thin film with a Bi/Fe ratio of 0.7 and an annealing temperature of 510^oC.

MA 31.32 Wed 17:00 P1

Ultrafast dynamics in photoexcited antiferromagnets — •Katja Sophia Moos[1], Yun Yen[2], Arnau C. Romaguera[3], Hiroki Ueda[3], and Michael Schüler[1,2] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [3]PSI Center for Photon Science, 5232 Villigen PSI, Switzerland

State-of-the-art time-resolved probes provide unprecedented access to the dynamics of interacting quasiparticles in solids on their natural time scales. Although a significant body of work exists on the dynamics of electrons and phonons, much less is known about the ultrafast response of magnetic moments. Here, we study pump-induced out-of-equilibrium magnetism in the Mott insulator CuO, combining measurements of resonant magnetic X-ray scattering with quantum-kinetic simulations. In particular, the diffuse scattering reveals time-dependent magnetic correlations, which we interpret in terms of interacting magnons. For quantitative insights, we solve the time-dependent quantum Boltzmann equation to study magnon-magnon scattering. The calculations are consistent with experimental observations and provide a detailed picture of magnetic dynamics in terms of non-thermal magnons and their subsequent thermalization.

MA 31.33 Wed 17:00 P1

Investigating Spin Cherenkov Radiation in Magnetic Materials Using MuMax3 Simulations — •Kawa Noman, Matthias Schweizer, Vitaliy Vasyuchka, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Spin Cherenkov Radiation (SCE) is a groundbreaking mechanism that enables the emission of spin waves (magnons) in ferromagnetic materials when an external perturbation surpasses the minimum phase velocity of these spin waves. In this study, we employ MuMax3 micromagnetic simulations to investigate SCE induced by high-amplitude Surface Acoustic Waves (SAWs) in Yttrium Iron Garnet (YIG) thin films. Our simulations reveal that SAWs propagating at velocities exceeding the spin wave phase velocity efficiently excite coherent spin wave modes, exhibiting characteristic Cherenkov like conical wavefronts. Through comparative analysis with Cobalt Iron Boron (CoFeB), we affirm the universal nature of SCE across diverse ferromagnetic materials, thereby highlighting its significant potential for advanced applications in magnonic and spintronic devices. This study not only establishes spin Cherenkov Radiation as a fundamental physical phenomenon but also paves the way for innovative technologies that leverage controlled spin wave emission.

MA 31.34 Wed 17:00 P1

Excitation of spin waves via surface acoustic waves in complex magnetic domain structures — •Mohammad Javad Kamali Ashtiani[1], Alexandre Abbass Hamadeh[2], Ephraim Spindler[1], Mathias Weiler[1], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Center de Nanosciences et de Nanotechnologies, CNRS, Universite Paris-Saclay, 91120, Palaiseau, France

We investigated the interaction of surface acoustic waves (SAWs) with spin waves (SWs) in micrometer-sized cobalt-iron-boron (CoFeB) dots on a piezoelectric – ScAlN– substrate. These dots exhibit particular domain structures leading to complex magnon-phonon coupling. SAWs, generated using interdigital transducers across a broad GHz frequency range, were observed to excite SWs in the CoFeB structures. The dynamics were characterized using micro-focused Brillouin light scattering (*BLS) spectroscopy, allowing direct detection of SAW and SW excitations. Nitrogen-vacancy magnetometry provided high-resolution insights into the magnetic domain arrangement. Also, Mumax3 simulations confirmed the complex domain textures. The response of SWs at specific resonance magnetic fields was observed and shifted across different frequencies. Our findings highlight the potential of hybrid phonon-magnon systems for tunable magnonic devices, advancing wave-based information processing technologies.

This research was supported by DFG under TRR 173/3 - 268565370 Spin+X (Project B01).

MA 31.35 Wed 17:00 P1

All-Magnonic Frequency Multiplication in Ferromagnetic Microstructures — •Alexandra Schrader[1], Chris Körner[1], Rouven Dreyer[1], Niklas Liebing[2], and Georg Woltersdorf[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz

We have observed all-magnetic frequency multiplication and a six-octave frequency comb in polycrystalline NiFe thin films [1]. At low bias fields, magnetic ripples cause local magnetization tilting, and MHz-range excitation induces rapid switching and high-harmonic spin wave emission. To enable practical applications, it is essential to miniaturize active components and optimize the frequency multiplication efficiency, aiming to generate GHz-range spin waves using MHz rf excitation in minimal-sized elements.

Recently, frequency multiplication has also been observed in extended CoFeB layers [2]. This motivates us to investigate the effect in both thin films as well as microstructures of CoFeB. Using micromagnetic simulations, we analyze how various parameters - such as saturation magnetization, anisotropy, static bias field and the shape, size and thickness of micrometer-sized CoFeB elements - influence generation efficiency. These numerical results are then compared to experimental measurements performed via NV magnetometry and SNS-MOKE techniques on actual samples.

[1] Koerner et al., Science 375, 6585 (2022)

[2] Wu et al., npj Spintronics 2, 30 (2024)

MA 31.36 Wed 17:00 P1

Magnetoacoustic coupling in Yttrium Iron Garnet / Aluminium Scandium Nitride heterostructures — •Kevin Künstle[1], Kaya Gauch[1], Yannik Kunz[1], Agne Žukauskaite[2,3], Stephan Barth[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Fraunhofer Institute for Electron Beam and Plasma Technology FEP, 01277 Dresden, Germany — [3]Institute of Solid State Electronics, Technische Universität Dresden, 01062 Dresden, Germany

The magnetoelastic coupling between surface acoustic waves (SAWs) and spin waves (SWs) has garnered significant attention in recent years. Magnetoelastic excitation of SWs is particularly appealing in ferrimagnets with low magnetic damping, such as yttrium iron garnet (YIG). To enable the electrical excitation of SAWs, a piezoelectric layer is required. We have demonstrated that ZnO is a suitable choice [1]. In this study, a novel heterostructure comprising a YIG/GGG bilayer covered by a piezoelectric AlScN thin film is investigated to explore this coupling. The interaction of SAW and SW is characterized using micro-focused Brillouin light scattering (BLS) spectroscopy and vector network analyzer (VNA) measurements. Additionally, the observed magnetoelastic coupling is benchmarked against the coupling in the more established ZnO/YIG/GGG heterostructure.

[1] Ryburn et al., arXiv 2403.030006 (2024)

MA 31.37 Wed 17:00 P1

Efficient all-magnonic frequency multiplication in nano-scale devices — •Chris Körner[1], Anna Kiefel[1], Rouven Dreyer[1], Alexandra Schrader[1], Niklas Liebing[2], and Georg Woltersdorf[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von Danckelmann Platz 3, 06120 Halle (Saale) — [2]Fraunhofer-Institut für Elektronische Nanosysteme ENAS, Technologie-Campus, 3 09126 Chemnitz

We recently have observed all-magnonic frequency multiplication and the generation of a 6-octave spanning frequency comb within an extended polycrystalline NiFe layer [1]. At low bias fields the magnetization locally tilts due to a magnetic ripple effect in the film. Driving the magnetization with frequencies far below ferromagnetic resonance, i.e. in the MHz range, causes rapid synchronous switching and leads to high harmonic spin wave emission. To make use of this effect in an actual device it is necessary to shrink the dimensions of the active components and to enhance the efficiency of the frequency multiplication process. The aim is to generate spin waves in the range of up to 10 GHz most efficiently in elements as small as possible, just from r.f. excitation with MHz frequencies. We employ micromagnetic simulations to investigate how the generation efficiency is influenced by external parameters, such as bias field and the shape, size, and thickness of micrometer sized NiFe elements. We find that the comb generation process can still be efficient even if we scale down the elements to just a few microns and compare these results to NV-center and SNS-MOKE measurements.

[1] Koerner et al. Science, 375 (6585) 2022.

MA 31.38 Wed 17:00 P1

Realization of Inverse-Design Magnonic Logic Gates — •Fabian Majcen[1,2], Noura Zenbaa[1,2], Claas Abert[1,3], Florian Bruckner[1,3], Norbert Mauser[3,4], Thomas Schrefl[3,5], Qi Wang[6], Dieter Süss[1,3], and Andrii Chumak[1,3] — [1]University of Vienna, Faculty of Physics, Vienna 1090, Austria — [2]University of Vienna, Vienna Doctoral School in Physics, Vienna 1090, Austria — [3]Research Platform MMM "Mathematics-Magnetism-Materials", University of Vienna, Vienna 1090, Austria — [4]Faculty of Mathematics, University of Vienna, Vienna 1090, Austria — [5]Center for Modelling and Simulation, Donau-Universität Krems, Wiener Neustadt, 2700, Austria. — [6]School of Physics, Hubei Key Laboratory of Gravitation and Quantum Physics

The field of Magnonics, which utilizes magnons, the quanta of spin waves, for energy-efficient data processing, has made significant advancements through the application of inverse design. A universal magnonics processor has been developed, utilizing a 7x7 array of independent current loops to generate local inhomogeneous magnetic fields, thereby scattering spin waves in an Yttrium-Iron-Garnet film to achieve various functionalities. In this system, binary data ('0' and '1') is encoded in the spin-wave amplitude, and by making use of the nonlinearity of spin waves and applying the inverse-design process, logic gates including NOT, OR, NOR, AND, NAND, and a half-adder have been successfully created.

MA 31.39 Wed 17:00 P1

Yttrium iron garnet nanostructures for spin-wave computing — •Jannis Bensmann[1], Ahmad El Kadri[1], Dmitrii Raskhodchikov[1,2], Kirill O. Nikolaev[3], Robert Schmidt[1], Johannes Kern[1], Shraddha Choudhary[1], Vladislav E. Demidov[3], Steffen Michaelis de Vasconcellos[1], Wolfram H. P. Pernice[1,2,4], Sergej O. Demokritov[3], and Rudolf Bratschitsch[1] — [1]University of Münster, Institute of Physics and Center for Nanotechnology, 48149 Münster, Germany — [2]University of Münster, Center for Soft Nanoscience, 48149 Münster, Germany — [3]University of Münster, Institute of Applied Physics, 48149 Münster, Germany — [4]Heidelberg University, Kirchhoff-Institute for Physics, 69120 Heidelberg, Germany

The ever-increasing demand for computing power, particularly driven by the recent advances in the field of artificial intelligence, has triggered research into novel system architectures to improve the performance of current computing technology. Here, spintronics appears as a promising candidate, as spin waves are energy-efficient, broadband (up to THz), and can have wavelengths down to the nanometer scale. In order to realize hardware-based spin-wave computing, we employ nanofabrication techniques to create devices from 100-nm-thick films of yttrium iron garnet (YIG), a material well known for its exceptional low-damping. We evaluate the performance of individual building blocks using optical measurements such as Brillouin light scattering, which provides detailed insights into the spin-wave propagation.

MA 31.40 Wed 17:00 P1

Manipulation of spin waves in YIG/FM heterostructures — •Julien Schäfer, Akira Lentfert, Björn Heinz, and Philipp Pirro — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

The concept of using spin waves as data carriers is a promising alternative to existing communication standards with the potential for energy efficient data transfer. In magnonics, communication building blocks, such as time-delay lines for phase modulation, can be realized by exploiting the magnetic field-dependent spin-wave group velocities in e.g. yttrium-iron-garnet (YIG). In particular, the spin wave propagation in Damon-Eshbach geometry can be modified by the deposition of an additional ferromagnetic layer, leading to a strong frequency nonreciprocity induced by dipolar interaction. Here, we report an on-chip configurable magnonic frequency filter/phase shifter device consisting of a YIG transmission line with iron stripes deposited on top. These stripes act as Fabry-Pérot (FP) resonators due to the spin-wave reflections at the boundaries. Destructively interfering spin waves are filtered by such a resonator, while the transmitted spin

waves accumulate an additional phase due to the altered dispersion relation in the bilayer region. We present micromagnetic studies investigating the tunability of these FP resonators by means of external parameters such as local magnetic fields and the stripe magnetization configuration. This research is funded by the European Union within HORIZON-CL4-2021- DIGITAL-EMERGING-01 (No.101070536, MandMEMS).

MA 31.41 Wed 17:00 P1

Mapping of the Morin Transition in alpha-Fe2O3 using Surface Acoustic Waves — •Katharina Lasinger[1,2], Florian Kraft[1], Yannik Kunz[1], Kevin Künstle[1], Finlay Ryburn[2], John F. Gregg[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, Germany — [2]Clarendon Laboratory, Department of Physics, University of Oxford, United Kingdom

Antiferromagnets (AFMs) hold great potential for applications due to their insensitivity to external magnetic fields, the absence of associated stray fields and and their ability to host fast spin dynamical phenomena [1,2]. While AFMs interact only weakly with external magnetic fields, their magnetic order couples to elastic deformation. We investigate the manipulation of AFMs using magnetoelasticity and demonstrate both the possibility to probe changes in the static magnetization as well as map out the Morin transition of alpha-Fe2O3 through concurrent modification of its elastic properties. To achieve this, surface acoustic waves (SAWs) are launched in an alpha-Fe2O3 | ZnO heterostructure while magnetic field sweeps are performed. We observe significant changes in SAW group velocity and amplitude depending on the angle of the external magnetic field relative to the crystallographic c-axis and the SAW propagation direction. A temperature-dependent study around the Morin transition reveals the critical fields at each temperature required for the antiferromagnetic phase transition to occur.

[1] A. V. Chumak, et al., Nature Physics 11, 453 (2015).
[2] S. M. Rezende, et al., J. Appl. Phys. 126, 151101 (2019).

MA 31.42 Wed 17:00 P1

Interlayer coupling in Co/Pd multilayers with perpendicular magnetic anisotropy — •Raphael Kohlstedt[1,2], Rico Ehler[1,2], Peter Heinig[1,2], and Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Research Center MAIN, D-09126 Chemnitz, Germany — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany

Antiferromagnetically (AF) coupled perpendicular magnetic anisotropy (PMA) multilayers (MLs) are widely utilized in magnetic devices. In Co/Pd MLs with PMA, the coupling is implemented via non-magnetic spacer layers like Ru or Ir. Using Pd itself as a spacer would be beneficial, since purely-Pd-based systems are promising candidates for applications in magneto-ionics, as demonstrated in recent reports [1-3]. In sputtered Co/Pd/Co trilayers, aging under ambient conditions induces a transient coupling effect, leading to a transition from ferromagnetic to antiferromagnetic coupling [4]. Building onto these experiments, we investigate the coupling behavior in Co/Pd/Co trilayers and Co/Pd MLs separated by a thicker Pd spacer. In our samples, we observe AF coupling as well as distinctly time-dependent effects, differing from those reported previously.

[1] A. E. Kossak et al., Sci. Adv., 9(1), 2023
[2] A. E. Kossak et al., Adv. Funct. Mater., 34(46), 2024
[3] M. Gößler et al., Adv. Funct. Mater., 34(40), 2024
[4] F. S. Wen et al., J. Appl. Phys., 110(4), 2011

MA 31.43 Wed 17:00 P1

Magnetometry of Buried Co-based Nanolayers by Hard X-ray Photoelectron Spectroscopy — •Andrei Gloskovskii[1], Christoph Schlueter[1], and Gerhard Fecher[2] — [1]Photon Science / DESY, Hamburg — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

Magnetic circular dichroism (MCD) effect has a cos (θ) dependence where θ is the angle between light polarization and sample magnetization. This yields direct information about the magnetization direction with respect to the polarization of the synchrotron X-ray beam for both ferromagnetic and antiferromagnetic materials. In the hard X-ray regime, the beam polarization can be conveniently modified utilizing the phase shift produced by a diamond phase plate in the vicinity of a Laue or Bragg reflection. Extracting quantitative information about absolute values of local magnetic moments is very challenging, because of the complicated structure of photoelectron spectra. For example, the 4eV Co satellite cannot be explained by the solid-state calculations. The satellite obviously exhibits strong dichroism.

The electronic and magnetic properties of CoFe, CoFeB and Co-based Heusler nanolayers were studied using MCD. Both the polarization-dependent spectra and the dichroism indicate that the lines of the multiplet extend over the entire spectral range. It is demonstrated that MCD in HAXPES is an effective and powerful technique to perform element- and depth-specific magnetometry of deeply buried ferromagnetic and antiferromagnetic magnetic materials.

MA 31.44 Wed 17:00 P1

Kerr Microscopy Studies of Magnetic Domains in proximity-coupled 3d FM-EuO Heterostructures — •Katharina Wehrstein, Seema Seema, Pia Maria Düring, and Martina Müller — FB Physik, Universität Konstanz

Europium monoxide (EuO) is a promising material for future spintronic applications as it is an insulator with a similar band gap to silicon, is ferromagnetic (FM) up to a Curie temperature (T_c) of 69 K and shows good spin-filter qualities. Since the low T_c is limiting for applications, methods to increase T_c are actively investigated. For this purpose, it is important to understand the magnetic behavior of EuO below, near and above T_c. One possible option to increase T_c is the proximity coupling of EuO with room temperature (RT) FM such as Fe or Co. Here, the temperature- and thickness-dependent magnetization of EuO thin films and 3d FM coupled EuO heterostructures synthesized by molecular beam epitaxy was investigated using magneto-optical Kerr microscopy. Systematic temperature- and thickness-dependent investigations on one hand revealed that the magnetic domain structure in Fe undergoes significant modifications in the presence of EuO, compared to Co. On the other hand, coercivity gets more affected due to the presence of Co than Fe. Such observations could lead to tuning thickness of EuO and overlayer choice in proximity-coupled heterostructures with T_c close to RT for applications.

MA 31.45 Wed 17:00 P1

Phase Modulation of Spin Waves via Surface Acoustic Waves — •Tim Vogel, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau

The interaction of spin waves and surface acoustic waves (SAWs) offers promising opportunities for advanced spintronic and magnonic applications. This study investigates the feasibility of using low-frequency SAWs in the MHz range to modulate the phase of high-frequency spin waves in the GHz range. Using micromagnetic simulations with mumax3, we investigate the dynamic coupling mechanisms and conditions necessary for effective phase manipulation of propagating spin waves.

While the primary focus is theoretical, this work also provides a framework for potential experimental validation to elucidate key factors such as coupling efficiency, propagation dynamics and system geometry. These results will contribute to a deeper understanding of magnon-phonon interactions.

We acknowledge funding by the European Union via Horizon Europe project MandMEMS, Grant No. 101070536.

MA 31.46 Wed 17:00 P1

Antiferromagnetic coupling in Co/Au/Co tri-layers — Lokesh Rasabathina[1], Rico Ehrler[1], Markus Gössler[1], Karin Leistner[1], Georgeta Salvan[1,2], and •Olav Hellwig[1,2,3] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology,Chemnitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Magnetic thin film systems are of great interest for many applications, such as magnetic memory, storage, sensor devices, etc. Specifically synthetic antiferromagnets (SAFs) with perpendicular magnetic anisotropy are of interest in the fabrication of nanomagnetic and spintronic devices[1]. In reference to earlier studies[2], we fabricate thin films consisting of $Au_{seed}/Co_{(1)}/Au_{interlayer}/Co_{(2)}/Au_{cap}$ layer stack using magnetron sputtering in ultra-high vacuum conditions. Varying the $Au_{interlayer}$ thickness the $Co_{(1)}$ and $Co_{(2)}$ layers either reverse separately at different switching fields or jointly at the same switching field. We investigate if the interaction between the two cobalt layers originates from RKKY coupling, orange-peel coupling or through growth induced asymmetry between the two cobalt layers[3]. The Au_{seed} layer thickness also seems to affect the observed reversal behaviour. For our sample characterization, we use different types of magnetometry and magnetic microscopy techniques.

[1] R.A.Duine, et al., Nat. Phys. 14, 217 (2018)
[2] M. Matczak et al., J. Appl. Phys., vol. 114, no. 9 (2013)
[3] V. Grolier et al, Phys. Rev. Lett. 71, 3023 (1993)

MA 31.47 Wed 17:00 P1

Site-selective substitution effects on the magnetic phase diagram of multiferroic $Fe_2Mo_3O_8$ — Lilian Prodan[1], •Dorina Croitori[2], Irina G. Filippova[2], Sergiu Shova[3], Vladimir Tsurkan[1,2], and Istvan Kezsmarki[1] — [1]University of Augsburg — [2]Moldova State University — [3]Romanian Academy

Antiferromagnetic materials hold great promise for the design of ultra-fast and energy-efficient spintronic devices. Therefore, understanding the robustness of crystals, their magnetic structures, and their manipulation is of high importance. Here, we report the effect of site-selective substitution of Zn^{2+} for Fe^{2+} ions on the crystal structure, magnetic and thermodynamic properties of the multiferroic $Fe_2Mo_3O_8$. We found the strong preference of Zn to occupy the tetragonal positions for substitution concentrations $\mathbf{0} \geq \mathbf{x} \leq \mathbf{1.3}$. This contrasts the previously reported results for related system $Co_2Mo_3O_8$ [1]. Site-selective substitution affects the magnetic phase diagram of $Fe_2Mo_3O_8$ influencing both the intra and inter-layer exchange interactions. This leads to the stabilization of the FiM phase for $\mathbf{x} \geq \mathbf{0.2}$ and to the decrease of T_C with increasing the Zn content. [1]. L. Prodan, I. Filippova, et al. Phys Rev B 106 (2022) 174421.

MA 32: Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)

Time: Wednesday 17:30–19:00 Location: H19

MA 32.1 Wed 17:30 H19

Orbital torques and orbital pumping in two-dimensional rare-earth dichalcogenides — •Mahmoud Zeer[1,2,3], Dongwook Go[3], Mathias Kläui[3,4], Wulf Wulfhekel[5], Stefan Blügel[1], and Yuriy Yuriy Mokrousov[1,3] — [1]Peter Gr *unberg Institute, Forschungszentrum J *ulich, 52425 J *ulich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, German — [3]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [4]Centre for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway — [5]5Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The design of spin-orbit torque (SOT) properties in two-dimensional (2D) materials represents a key challenge in modern spintronics. We now explore ferromagnetic Janus H-phase monolayers of 4f-Eu rare-earth dichalcogenides EuSP, EuSSe, and EuSCl using first-principles calculations. Our findings reveal that these compounds exhibit substantial SOT, primarily driven by the colossal current-induced orbital response of Eu f-electrons. Additionally, the resulting orbital torques can generate strong in-plane currents of orbital angular momentum with non-trivial orbital polarization directions. These results establish f-based 2D materials as a highly promising platform for in-plane orbital pumping and SOT applications, positioning f-based 2D materials as a promising platform for next-generation orbitronic and spintronic technologies with 2D materials.

MA 32.2 Wed 17:45 H19

Orbital Topology of Chiral Crystals for Orbitronics — •Ying-Jiun Chen[1], Kenta Hagiwara[1,2], Dongwook Go[3], Xin Liang Tan[1,2], Sergii Grytsiuk[1], Kui-Hon Ou Yang[4], Guo-Jiun Shu[5], Jing Chien[4], Yi-Hsin Shen[4], Xiang-Lin Huang[5], Iulia Cojocariu[1], Vitaliy Feyer[1,2], Minn-Tsong Lin[4,6], Stefan Blügel[1], Claus Michael Schneider[1,2], Yuriy Mokrousov[1,3], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich — [2]University of Duisburg-Essen — [3]Johannes Gutenberg University Mainz — [4]National Taiwan University, Taiwan — [5]National Taipei University of Technology, Taiwan — [6]Academia Sinica, Taiwan

Chirality is ubiquitous in nature and manifests in a wide range of phenomena including chemical reactions, biological processes, and quantum transport of electrons. In quantum materials, the chirality of fermions, given by the relative directions between the electron spin and momentum, is connected to the band topology of electronic states. Here, we show that in structurally chiral materials like CoSi, the orbital angular momentum (OAM) serves as the main driver of a nontrivial band topology in this new class of unconventional topological semimetals, even when spin-orbit coupling is negligible. A nontrivial orbital-momentum locking of multifold chiral fermions in the bulk leads to a pronounced OAM texture of the helicoid Fermi arcs at the surface. Our findings highlight the pivotal role of the orbital degree of freedom for the chirality and topology of electron states, in general, and pave the way towards the application of topological chiral semimetals in orbitronic devices.

MA 32.3 Wed 18:00 H19

Vectorial flow of the Berry curvature and its relation to the transport and band structure — •Jaroslav Hamrle[1,2], Ondřej Stejskal[1], Milan Vrána[2,1], and Martin Veis[2] — [1]Czech Technical University, Prague, Czechia — [2]Charles University, Prague, Czechia

Berry curvature expresses the curvature of the reciprocal space, in a similar manner as magnetic field express curvature of the real space, resulting in a curved transport of electrons in solids. Therefore, Berry curvature is a base of various lossless transport phenomena such as anomalous Hall effect, anomalous Nerst effect, orbital magnetization or electric polarization. Here, in model materials bcc Fe and Fe_3Ga, we demonstrate details of the vectorial flow of the Berry curvature (monopole source, 1-dimensional flow, 2-dimensional flow), and its relations to the band structure, orbital magnetization as well as anomalous Hall and Nerst effects.

[1] O. Stejskal, M. Veis, J. Hamrle, Sci Rep **12**, 97 (2022) [doi: 10.1038/s41598-021-04076-z]

[2] O. Stejskal, M. Veis, J. Hamrle, Phys. Rev. Materials **7**, 084403 (2023) [doi:10.1103/PhysRevMaterials.7.084403]

MA 32.4 Wed 18:15 H19

Finite-temperature transport properties of magnetic/non-magnetic alloys: trends in the longitudinal and in the transverse charge and spin currents — •Alberto Marmodoro[1], Yang Wang[2], Yuqing Lin[3], and Ilja Turek[4] — [1]Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czech Republic — [2]Pittsburgh Supercomputer Center (PSC), Carnegie Mellon University, Pittsburgh, USA — [3]Mellon College of Science, Carnegie Mellon University, Pittsburgh, USA — [4]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

Alloys composed of magnetic and non-magnetic metals exhibit non-trivial transport trends as a function of composition and temperature. The stoichiometry controls not only the Curie point, but also the slope of resistivity vs. temperature. Beside affecting longitudinal currents, this has further implications also for transverse charge and spin currents, i.e. on anomalous Hall effects [1]. We report first-principles results based on density functional theory (DFT), relativistic linear response and Green function methods based on the multiple scattering Korringa-Kohn-Rostoker (KKR) or linear muffin tin orbitals (LMTO) frameworks.

[1] "Large anomalous Hall angle in the Fe(60),Al(40) alloy induced by substitutional atomic disorder" by J.Kudrnovsky et al. PRB 101, 054437 (2020); "Exploiting Spin Fluctuations for Enhanced Pure Spin Current" by P.Wu et al. PRL 128, 227203 (2022); "Critical enhancement of the spin Hall effect by spin fluctuations" by S.Okamoto et al. Quantum Materials 29, 9 (2024).

MA 32.5 Wed 18:30 H19

Impact of the substrate on angular momentum transport between separated ferromagnets — •Fiona Sosa Barth[1,2], Matthias Grammer[1,2], Richard Schlitz[3], Tobias Wimmer[1,2], Janine Gückelhorn[1,2], Luis Flacke[1,2], Sebastian T.B. Goennenwein[3], Rudolf Gross[1,2,4], Hans Huebl[1,2,4], Akashdeep Kamra[5], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]Department of Physics, University of Konstanz, Konstanz, Germany — [4]Munich Center for Quantum Science and Technology, München, Germany — [5]RPTU Kaiserslautern-Landau, Kaiserslautern, Germany

Spintronics relies on the transfer of angular momentum between electrons and solid state excitations such as magnons and phonons. In our recent work, we demonstrate angular momentum transfer between two ferromagnetic strips on diamagnetic substrates [1] by converting a DC current at one of the electrodes to a non-equilibrium magnon accumulation. Due to dipolar and potentially phononic coupling, angular momentum is transferred to the magnonic system of the second FM electrode and measured by the inverse processes. In this work, we investigate the substrate influence on the angular momentum transport by comparing our results for SiOx and SiN layers on Si substrates. As a next step, we investigate substrate-supported strips versus freestanding strings to separate phononic contributions from dipolar coupling. [1] R. Schlitz et al., Phys. Rev. Lett. 132, 256701 (2024)

MA 32.6 Wed 18:45 H19

Orbital Edelstein contribution to the spin-charge conversion in Germanium Telluride — •Sergio Leiva-Montecinos[1], Libor Vojáek[2], Jing Li[2], Mairbeck Chshiev[2], Ingrid Mertig[1], and Annika Johansson[3] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Université. Grenoble Alpes, CEA, CNRS, SPINTEC, Grenoble, France — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Edelstein effect (EE) is a promising mechanism for generating spin and orbital polarization from charge currents in systems without inversion symmetry. In ferroelectric materials, such as Germanium Telluride (GeTe), the combination of bulk Rashba splitting and voltage-controlled ferroelectric polarization provides a pathway for reversible spin-charge interconversion [1, 2].

In this work, we investigate current-induced spin and orbital magnetization in bulk GeTe using Wannier-based tight-binding models derived from DFT calculations and semiclassical Boltzmann theory. Employing the modern theory of orbital magnetization (MTOM), we demonstrate that the orbital Edelstein effect (OEE) entirely dominates its spin counterpart (SEE). This difference is visualized through the spin and orbital textures at the Fermi surfaces, where the orbital moment surpasses the spin moment by one order of magnitude. Moreover, the OEE remains largely unaffected when we suppress the spin-orbit coupling, highlighting its distinct physical origin compared to the SEE.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2012).

[2] C. Rinaldi *et al.*, Nano Lett. **18**, 2751 (2018).

MA 33: Non-Skyrmonic Magnetic Textures I

Time: Thursday 9:30–13:00 Location: H16

MA 33.1 Thu 9:30 H16

Anomalous quasielastic scattering in centrosymmetric helimagnets — N. D. Andriushin[1], J. Grumbach[1], A. A. Kulbakov[1], Y. V. Tymoshenko[2,1], Y. A. Onykiienko[1], R. Firouzmandi[3], E. Cheng[3], S. Granovsky[1], Y. Skourski[4], J. Ollivier[5], H. C. Walker[6], V. Kocsis[3], B. Büchner[3], M. Doerr[7], •D. S. Inosov[1], and D. C. Peets[1] — [1]IFMP, TU Dresden, Germany — [2]JCNS, FZ Jülich, Germany — [3]IFW Dresden, Germany — [4]HZDR, Dresden, Germany — [5]ILL, Grenoble, France — [6]ISIS, RAL, Didcot, UK — [7]MPI-FKF, Stuttgart, Germany

Centrosymmetric helimagnets which host spin helices or skyrmion-like topological spin structures comprise a distinct subclass of materials in which helical order is stabilized by bond frustration in contrast to the more common path of antisymmetric exchange interactions. Here we will present the spin-dynamical properties of the $SrFeO_3$ [1] and $Sr_3Fe_2O_7$ [2] perovskites. Inelastic neutron scattering reveals that with increasing temperature, high-energy magnons increasingly lose coherence, and the spin fluctuations become dominated by a distinct quasielastic component at low energies, concentrated at the ordering wave vectors. This quasielastic component likely originates from helical domain walls. We anticipate that this could be generic to all symmetric helimagnets in which the chiral symmetry is spontaneously broken by the magnetic order.

[1] N. D. Andriushin *et al.*, arXiv:2409.10214 (2024).
[2] N. D. Andriushin *et al.*, npj Quant. Mater. **9**, 84 (2024).

MA 33.2 Thu 9:45 H16

Characterising 3D Topological Magnetic Textures using the Hopf index: Hopfions, Fractional Hopfions and Screw Dislocations — •Maria Azhar, Sandra Chulliparambil Shaju, Ross Knapman, Alessandro Pignedoli, and Karin Everschor-Sitte — Faculty of Physics and CENIDE, University of Duisburg-Essen.

In magnetic systems, twisted, knotted, linked, and braided vortex tubes manifest as Skyrmions, Hopfions, Fractional hopfions, or screw dislocations [1]. These complex textures are characterized by topologically non-trivial quantities, such as a Skyrmion number, a Hopf index H, a Burgers vector (quantified by an integer), and linking numbers.

We address the common challenges and pitfalls associated with numerically calculating H using the traditional Whitehead integral [2]. We present an alternative analytical method for determining H, introducing a new discrete geometric formulation [3]. This approach separates H into contributions from the self-linking and inter-linking of flux tubes of the emergent magnetic field.

Our analysis reveals the natural emergence of fractional Hopfions or textures with non-integer H, which we interpret as "mixed topology" states. These states can smoothly transform into one of several possible topological sectors with integer H. We establish a robust physical foundation for the Hopf index to assume integer, non-integer, or specific fractional values, depending on the system's underlying topology. [1] M. Azhar, et al., PRL 128, 157204 (2022)
[2] R. Knapman, M. Azhar, et al., arxiv:2410.22058
[3] M. Azhar, et al., arXiv:2411.06929

MA 33.3 Thu 10:00 H16

Strain-induced spin spiral in Dy-doped Ferrite films — •Holger Meyerheim[1], Anupam Singh[1], Verena Ney[2], Andreas Ney[2], Arthur Ernst[2], Malleshwararao Tangi[1], Ilya Kostanovski[1], Manuel Valvidares[3], Pierluigi Gargiani[3], Jean-Marc Tonnerre[4], Stuart S. P. Parkin[1], and Katayoon Mohseni[1] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle — [2]Johannes Kepler University, A-4040 Linz (Austria) — [3]ALBA Synchrotron, E-08290 Cerdanyola del Valles (Spain) — [4]Institut Neel, CNRS & Univ. J. Fourier, F-38042 Grenoble (France)

Ferrites are known as textbook ferrimagnets. Recent interest in oxides as low-dissipation materials in spintronics has also focused interest on the modification of the spin texture of oxides in general [1]. Here we present a combined experimental and theoretical study which shows that in 5-40 nm thick Dy-doped Ni-ferrite films the local structural strain and the resulting concomitant symmetry reduction induced by the large Dy^{3+} ions incorporated in the percent concentration range into the octahedral sites of the spinel-type structure leads to the emergence of the chiral Dzyaloshinskii-Moriya interaction (DMI). The DMI is responsible for the onset of a non-collinar spin texture. Using soft x-ray resonant magnetic reflectivity and x-ray magnetic circular dichroism experiments in the vicinity of the Fe- and Ni-$L_{2,3}$- and the Dy-$M_{4,5}$ edges we develop a model in which the Fe and Ni magnetic moments are aligned in a spiral-like spin texture with a q-vector almost parallel to [001]. This work is supported by the DFG under grant MO 4198/2-1. [1] L. Caretta, et al., Nat. Comm. 11, 1090 (2020)

MA 33.4 Thu 10:15 H16

Quantum Bloch points in magnetic systems — •Vladyslav Kuchkin, Štefan Liščák, Andreas Haller, Andreas Michels, and Thomas Schmidt — University of Luxembourg

A Bloch point represents a three-dimensional hedgehog singularity of a magnetic vector field in which the magnetization vanishes at the center. Experimentally, the appearance of such points is well-established; at the same time, the standard micromagnetic theory is only suitable for fixed-length continuous magnetization vector fields and is thus not applicable to such singularities. To approach this problem, we study a Bloch point in a quantum Heisenberg model for the case of spin-1/2 particles. Such a state can be stabilized by adding a Zeeman term that imposes a boundary condition. We obtain the ground state and the corresponding magnetization profile by performing an exact diagonalization and using density matrix renormalization group techniques. Our findings show a smooth change of the spin length in the quantum model, leading to zero magnetization at the Bloch point. This behavior is generic for different system sizes. Our results indicate the necessity of generalizing the classical micromagnetic model, relying on a magnetization vector field of constant length, by adding a third degree of freedom of the spin: the ability to change its length. We achieve this by introducing a regularized $\mathbb{S}^3$ model that describes a four-dimensional order parameter of unit length. In contrast to earlier attempts to describe magnetization profiles of varying lengths, our approach satisfies the quantum mechanical constraints on spin operators.

MA 33.5 Thu 10:30 H16

Magnetic solitons in hierarchical 3D magnetic nanoarchitectures of nanoflower shape — •Olha Bezsmertna[1], Rui Xu[1], Oleksandr Pylypovskyi[1], David Raftrey[2,3], Andrea Sorrentino[4], Jose A. Fernandez-Roldan[1], Ivan Soldatov[5], Daniel Wolf[5], Axel Lubk[5], Rudolf Schäfer[5], Peter Fischer[2,3], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]University of California Santa Cruz, Santa Cruz CA, USA — [3]Lawrence Berkeley National Laboratory, Berkeley CA, USA — [4]Alba Light Source, Cerdanyola del Vallès 08290, Spain — [5]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Curvilinear magnetism is an emerging field that explores how magnetic properties and responses are modified in geometrically curved objects [1]. Here, we synthesize large-scale, highly-periodic 3D nanomembranes [2] of 50-nm-thick permalloy of a nanoflower shape interconnected by close-to-hemispherical indentations. Nanoflowers with a size of about 200 nm exhibit a variety of magnetic states, e.g. domain walls, flower, vortex and a state with two Bloch lines. The ground magnetic state is a vortex, which is shifted away from the geometric center of the nanoflower. Micromagnetic simulations show nonlocal symmetry breaking, which is specific to 3D curved geometries enabling interactions between surface and volume magnetostatic charges, responsible for the shift of the vortex [3]. [1] D. Makarov et al., Springer Nature, Vol. 146 (2022). [2] R. Xu et al., Nature Comm 2022. [3] O. Bezsmertna et al., Nano Lett., doi.org/10.1021/acs.nanolett.4c04584

MA 33.6 Thu 10:45 H16

Emergence of topological superconductivity in the presence of chiral magnetism in 2D $CrInTe_3$ — •Arnob Mukherjee[1], Fengyi Zhou[2], Soheil Ershadrad[1], Tanay Nag[3], Duo Wang[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden — [2]Faculty of Applied Sciences, Macao Polytechnic University, Macao SAR, 999078, China — [3]Department of Physics, BITS Pilani-Hyderabad Campus, Telangana 500078, India

We propose a framework for designing two-dimensional (2D) topological superconductors (TSCs) using a bilayer hybrid system of monolayer $CrInTe_3$ with noncoplanar magnetic textures coupled to a 2D s-wave superconductor. This hybrid system induces a topological superconducting phase, serving as a platform for realizing the 2D Kitaev model and supporting Majorana zero-energy modes via emergent p-wave pairing. Using Density functional theory calculations, we calculate the essential magnetic parameters, such as Heisenberg exchange and Dzyaloshinskii-Moriya interactions (DMI) using the LKAG approach. Large-scale Monte Carlo simulations reveal that the substantial DMI stabilizes a noncoplanar spiral magnetic state without external fields. In this phase, we observe a transition from dipolar to edge modes in the zero-energy local density of states as the chemical potential varies. Under finite magnetic fields, the system exhibits a mixed magnetic state with isolated skyrmions and spiral domain walls, leading to unique low-energy electronic states and insulating behavior.

MA 33.7 Thu 11:00 H16

Topological textures in antiferromagnetic thin-films stabilized by interfacial magnetostrictive destressing — •Lukas D Cavar[1], Julian Skolaut[2], Olena Gomonay[1], Simon J Sochiera[1], David Anthofer[1], Miela Gross[3], Evangelos Golias[4], Dirk Backes[5], Caroline A Ross[3], and Angela Wittmann[1] — [1]JGU, Mainz, DE — [2]IEAP, CAU, Kiel, DE — [3]MIT, Cambridge, USA — [4]MAX IV, Lund, SE — [5]DLS, Didcot, UK

Weakly-compensated antiferro- and ferrimagnets present us with ultrafast dynamics, along with a weak magnetization vector that is legible, accessible, and robust to external perturbations. This makes them ideal candidates for the next generation of computing materials, where information may be encoded in the form of topological magnetic textures. Conventional long-range interaction– namely, the stray field– is not sufficient to stabilize such textures on its own. Here we discuss the magnet-substrate interface, where a magnetostriction-dependent interfacial incompatibility gives rise to long-range destressing fields capable of stabilizing topological textures in easy-plane magnetic thin-films with nearly-compensating staggered spin ordering. We investigate two such materials– α-Fe_2O_3 (hematite) and dysprosium iron garnet (DyIG) near its compensation temperature– by x-ray magnetic linear dichroism microscopy and indeed observe a rich landscape of topological textures. Thereby we tread towards a rigorous understanding of the interfacial destressing field and begin to uncover a promising new source of topological mesostructure.

15 min. break

MA 33.8 Thu 11:30 H16

Towards stabilizing 360° domain walls in dysprosium iron garnet through magnetoelastic interactions — •Julian Skolaut[1,2], Lukas Cavar[1], Olena Gomonay[1], Miela Gross[3], Simon Sochiera[1], David Anthofer[1], Evangelos Golias[4], Dirk Backes[5], Caroline A. Ross[3], and Angela Wittmann[1] — [1]JGU, Mainz, DE — [2]present address: IEAP, CAU, Kiel, DE — [3]MIT, Cambridge, US — [4]MAX IV, Lund, SE — [5]DLS, Didcot, UK

Topologically protected magnetic textures, including 360° domain walls (DWs), are of considerable interest for next-generation data storage and computing technologies. Realizing such textures in ferri- and antiferromagnetic systems allows us to capitalize on these materials' intrinsic robustness to external perturbations and faster dynamics. However, well-established mechanisms, such as stray fields, cannot stabilize 360° DWs at zero magnetic field. Hence, we must turn to more exotic stabilization mechanisms. One promising candidate is magnetoelastic destressing mediated by the substrate/magnetic film interface. Here, we report the observation of 360° DWs in ferrimagnetic dysprosium iron garnet thin films. These topological DWs are present in applied magnetic fields from zero to above coercivity, suggesting topological protection, and can be manipulated using magnetic fields. Upon return to zero magnetic field, the initial state is not reproduced, indicating hysteresis. This hints toward stabilization via magnetoelastic interactions. Corroborating these results with insights from other materials and theory will further the understanding of exotic mechanisms, such as destressing fields, as a source of topological magnetic textures.

MA 33.9 Thu 11:45 H16

Computational studies of novel Dzyaloshinsky-Moriya interactions — •Samuel Holt[1,2], Martin Lang[1,2], Swapneel Pathak[1,2], and Hans Fangohr[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Faculty of Engineering and Physical Sciences, University of Southampton, Southampton SO17 1BJ, United Kingdom

The exploration of magnetic phases in chiral magnets has gathered significant interest due to the unique physics and potential applications of these materials. A key factor in these systems is the Dzyaloshinsky-Moriya interaction (DMI), which arises from the asymmetric environment of interacting magnetic spins and is linked to non-centrosymmetric crystallographic point groups. While a few point groups have had their DMI extensively studied, many remain unexplored.

In this talk, we systematically explore the multidimensional parameter space of these new DMI terms using micromagnetic simulations to identify and classify magnetic phases. Machine learning algorithms, such as clustering and autoencoders, are employed to automate this process, enabling the rapid identification and grouping of similar magnetic phases across extensive parameter spaces. Funded by EU Horizon 2020, grants 101152613 and 101135546.

MA 33.10 Thu 12:00 H16

Interplay between magnetic and charge order in an ultra-clean van der Waals material — •Priya Baral[1], Sun Okumura[1], Moritz Hirschmann[2], Sebastian Esser[1], Rinsuke Yamada[1], Shun Akatsuka[1], Jonathan White[4], Samuel M. Moody[4], Stanislav Niktin[4], Nina-juliane Steinke[5], Shang Gao[6], Yoshichika Onuki[2], Taka-hisa Arima[2,7], Taro Nakajima[3], and Max Hirschberger[1,2] — [1]Department of Applied Physics, The University of Tokyo, Tokyo, JP — [2]RIKEN Center for Emergent Matter Science (CEMS), Saitama, JP — [3]Institute for Solid State Physics, University of Tokyo, Chiba, JP — [4]PSI Center for Neutron and Muon Sciences, Villigen PSI, CH — [5]Institut Laue-Langevin, 71 avenue des Martyrs, Grenoble, FR — [6]Department of Physics, University of Science and Technology of China, CHN — [7]Department of Advanced Materials Science, The University of Tokyo, JP

The interplay between charge-density wave order and magnetism has been a prominent area of research for decades, encompassing unconventional superconductors to more recent Kagome metals. The cooperative or competitive nature of these two phenomena has been a fundamental aspect of many-body physics. Recently, it has been demonstrated that RTe3 (R = rare earth) van der Waals materials exhibit helimagnetic textures coupled to an unconventional charge-density wave order. Here, we review recent developments in one of the ultra-clean members of the series, DyTe3. We reveal further evidence for the unconventional spin-charge coupling in this material by combining magnetic, transport and neutron scattering measurements.

MA 33.11 Thu 12:15 H16

Magnetic Ordering Temperature for Spin Spiral materials — •Varun Rajeev Pavizhakumari and Thomas Olsen — CAMD, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby Denmark

Spin Spirals are the materials that show a helical arrangement of magnetic moments in the ground state. Thermal fluctuations from this state form collective excitations known as spin waves/magnons. As the thermal stability of a spin spiral is a decisive factor for its technological applications, there is considerable interest in the theoretical prediction of its critical temperature. This could be accomplished using two approaches - Holstein-Primakoff(HP) bosonization and the Green's function-Random Phase Approximation(RPA) where we can calculate the thermally renormalized magnon energies at each temperature. But these methods only exist for ferromagnetic and a few specific antiferromagnetic materials. In this work, we propose a single-Q spiral generalization of the HP bosonization and the Green's function-RPA to calculate the critical temperature. We benchmark these methods along with the classical Monte Carlo simulations and the Mean field theory, using their experimental exchange parameters for a diverse range of materials ; MnO and NiO(single site Neel state),MnF_2(altermagnetic),Cr_2O_3 and Fe_2O_3(two site Neel state) and $Ba_3NbFe_3Si_2O_{14}$(incommensurate). In all cases, we observe that the Green's function-RPA shows excellent agreement to the experiments and hence is as an ideal candidate to predict the critical temperature for any single-Q spirals.

MA 33.12 Thu 12:30 H16

Three-dimensional topological spin textures in curved chiral magnets — •Luke Turnbull[1,2], Max Birch[3], Marisel Di Pietro Martínez[1,2], Rikako Yamamoto[1,2], Jeffrey Neethirajan[1], Marina Raboni Ferreira[1,4], Rachid Belkhou[5], Simone Finizio[6], Dieter Suess[7], Geetha Balakrishnan[8], Claas Abert[7], Sebastian Wintz[9], and Claire Donnelly[3] — [1]MPI CPfS, Dresden, Germany — [2]WPI-SKCM2, Hiroshima, Japan — [3]RIKEN CEMS, Saitama, Japan — [4]Brazilian Synchrotron Light Laboratory, Sao Paulo, Brazil — [5]Synchrotron SOLEIL, Saint Aubin, France — [6]SLS, PSI, Villigen, Switzerland — [7]University of Vienna, Vienna, Austria — [8]Univeristy of Warwick, Coventry, UK — [9]HZB, Berlin, Germany

Nanoscale topologically non-trivial magnetization configurations generate significant interest due to both their fundamental properties, and their potential applications in ultra-efficient computing devices. While such textures have been widely studied in two dimensions, three dimensional (3D) ordering can yield more complex configurations, resulting in richer topologies and dynamic behaviours. However, reliably nucleating such 3D textures has proven challenging. Here, we achieve the controlled formation of a double helix ordering through the 3D nanopatterning of chiral single crystal helimagnets into nano-tori. We demonstrate that the interplay of intrinsic exchange interactions of the single crystal, with the extrinsic emergent effects of the patterned geometry, leads to the stabilisation of surface-localized topologically non-trivial double helices. Our approach has the potential to be applied to a wide range of quantum material systems.

MA 33.13 Thu 12:45 H16

Lifetime of toroidal Hopfions in bulk magnets with competing exchange interactions — •Moritz Sallermann[1,3], Hannes Jonsson[3], and Stefan Blügel[1,2] — [1]RWTH Aachen University, Germany — [2]PGI-1, Forschungszentrum Jülich, Germany — [3]University of Iceland, Iceland

Hopfions are three-dimensional topological solitons characterized by the Hopf invariant, which quantifies the pairwise linking number of constant magnetization pre-images. In simple models of bulk magnets with competing exchange interactions, Hopfions emerge as local energy minima in numerical simulations. However, to fully understand their stability against decay due to thermal fluctuations, merely identifying these local minima is insufficient. A more comprehensive understanding requires determining their expected average lifetimes. We employ the harmonic transition state theory framework, a computationally efficient yet approximate method, to estimate these lifetimes. This approach yields an Arrhenius-type expression comprising two key ingredients: the energy bar-

rier and an entropic prefactor. The energy barrier represents the minimal energy needed to initiate decay, while the entropic prefactor measures the relative entropy of the energy bottleneck, compared to the configuration space volume of the local minimum. We present our findings on the lifetimes of Hopfions in these systems and discuss technical challenges encountered, such as the treatment of Goldstone modes and the computation of sparse positive-definite determinants.

We acknowledge funding from the ERC grant "3D MAGIC".

MA 34: Molecular Magnetism

Time: Thursday 9:30–12:45 Location: H18

MA 34.1 Thu 9:30 H18

Handling higher order ligand field parameters of single molecule magnets using deep learning — •Zayan Ahsan Ali, Julius Mutschler, Preeti Tewatia, and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany

In recent decades, Single Molecule Magnets (SMMs) have sparked an interest not only due to their applications in quantum computing and spintronics, but also as an ideal platform for exploring fundamental principles of quantum magnetism. While substantial progress has been made towards the characterization of magnetic properties of 3d SMMs, the study of 4f SMMs remains challenging. This difficulty arises from the involvement of up to 27 ligand field parameters and the typically featureless nature of experimental magnetic data, leading to severe overparameterization. Moreover, the physically relevant regions in this parameter space are mostly unknown a priori. Although deep learning based inverse models, such as Conditional Variational Autoencoders and Invertible Neural Networks, have shown promise in addressing overparameterization, their performance degrades significantly when trained on uninformative parameter spaces, which dominate especially in high dimensional settings. This work investigates the use of Monte Carlo based parameter sampling for the higher order ligand field parameter space as a crucial precursor towards improving the deep learning inverse models. The resulting dataset represents a more informative prior, enabling insights into the effects of higher order ligand field parameters and the correlations between them.

MA 34.2 Thu 9:45 H18

Polarization of Electron Spin and Orbitals in Chiral Molecular Junctions on Semiconductors — •Peng Xiong[1], Yuwaraj Adhikari[1], Tianhan Liu[1,3], Hailong Wang[2], Zhenqi Hua[1], Haoyang Liu[1], Paul Weiss[3], Binghai Yan[4], and Jianhua Zhao[2] — [1]Florida State University, USA — [2]Institute of Semiconductors, Chinese Academy of Sciences, China — [3]University of California, Los Angeles, USA — [4]Weizmann Institute of Science, Israel

Electrical generation and transduction of polarized electron spins in semiconductors via nonmagnetic means are of broad interest in spintronics and quantum information science. One such pathway is chirality-induced spin selectivity (CISS), where real-space structural chirality induces spin polarization of electrons from a nonmagnetic electrode. We have studied the CISS effect through measurement of spin-selective transport in chiral molecular junctions comprising a nonmagnetic normal metal electrode and a self-assembled monolayer of chiral molecules on magnetic (GaMnAs) or nonmagnetic (n-GaAs) semiconductors, where the spin polarization is detected via the spin-valve conductance and Hanle effect, respectively. The results reveal several important characteristics of the CISS effect [1-3]: i) nontrivial linear-response magnetoconductance in two-terminal CISS spin valves, in apparent violation of the Onsager reciprocal relation; ii) crucial role of the spin-orbit coupling in the normal metal electrode, suggesting the importance of orbital polarization in the chiral molecules; iii) spin generation by CISS in semiconductors. 1. ACS Nano 14, 15983 (2020); 2. Nat. Commun. 14:5163 (2023) ; 3. Ad. Mater. 36, 2406347 (2024).

MA 34.3 Thu 10:00 H18

Effects of Boundary Condition on Quantization in the Spin-1/2 Heisenberg Chain — •Saketh Ravuri[1], Chenxiao Zhao[1], Pascal Ruffieux[1], and Roman Fasel[1,2] — [1]Empa, Dübendorf, Switzerland — [2]University of Bern, Bern, Switzerland

The spin-1/2 antiferromagnetic Heisenberg chain resides in a gapless spin liquid phase in the thermodynamic limit. In finite-length systems, however, quantization introduces a length-dependent excitation gap, which is further influenced by the boundary conditions. In this work, we investigate how open and periodic boundary conditions affect the quantization and gap behavior in spin-1/2 antiferromagnetic Heisenberg chains constructed by covalently linking magnetic nanographene units. For chains of fixed length, we demonstrate that open boundary conditions result in a smaller gap compared to periodic boundary conditions, as clearly evidenced by the inelastic electron tunneling spectra. This impact of boundary conditions diminishes with increasing chain length and vanishes in the thermodynamic limit. Moreover, in periodic rings with odd-numbered units, we investigated the scattering of a single spinon caused by J-fluctuations. These findings illuminate the role of boundary effects in finite-size quantum spin systems and contribute to the fundamental understanding of quantum magnetism and excitations in spin chains.

MA 34.4 Thu 10:15 H18

Approximate finite-temperature Lanczos modelling of dysprosium containing magnetic molecules — •Jürgen Schnack and Dennis Westerbeck — Bielefeld University, Faculty of Physics, 33615 Bielefeld

Dysprosium containing magnetic molecules are considered promissing building blocks of future quantum technology such as storage, quantum computing, quantum sensing, or magnetocalorics. The initial physical characterization includes measurements of magnetization or heat capacity as function of temperature and applied magnetic field.

A theoretical modelling of an approximate quantum spin model by means of exact diagonalization of multicenter systems is virtually impossible due to the large magnetic moment of dysprosium. We resort to the finite temperature Lanczos method which however converges rather slowly [1]. We explain the reasons, our solutions and results for recent Dy containing molecules [2].

[1] O. Hanebaum and J. Schnack, Eur. Phys. J. B, 87, 194, 2014.

[2] D. Westerbeck, Ph.D. thesis, Bielefeld University, 2025, in preparation.

MA 34.5 Thu 10:30 H18

Annealing Induced Ordered Structures of H2Pc Monolayer on γ'-Fe4N Thin Film — •Hiroki Ono[1], Yoshitaka Umeda[1], Kaito Yoshida[1], Kenzaburo Tsutsui[1], Kohei Yamamoto[2], Osamu Ishiyama[2], Toshihiko Yokoyama[2], Masaki Mizuguchi[1], and Toshio Miyamachi[1] — [1]Nagoya University, Nagoya, Japan — [2]Institute for Molecular Science, Okazaki, Japan

Organic-inorganic hybrid interface has been studied because its interfacial spin state can be controlled through proximity effect. Spin state depends on local interface structures as well as electronic interaction between organic molecules and magnetic substrates. Therefore, controlling the interface structure is essential but remains challenging because of strong interaction between organic and inorganic materials.

In this work, we fabricate organic-inorganic hybrid thin films using iron nitride as a ferromagnetic substrate and phthalocyanine(H2Pc) as an organic molecule. Iron nitride atomic layers with γ'-Fe4N stoichiometry uniformly grow and show weaker interaction than typical ferromagnetic substrate. Therefore, γ'-Fe4N is a candidate to create structurally controlled interface. We investigate interface structure by using scanning tunneling microscopy(STM) and low energy electron diffraction(LEED), and electronic/magnetic properties by using x-ray absorption spectroscopy/magnetic circular dichroism(XAS/XMCD). We confirm the magnetic coupling occurs at H2Pc/γ'-Fe4N bilayer interface from XAS/XMCD results. H2Pc monolayer on γ'-Fe4N bilayer do not have any long-range lattice manner. But, we find annealing induces well-ordered structure while preserving interface magnetic coupling.

MA 34.6 Thu 10:45 H18

CuCu4 metallacrowns on the Au(111) surface: A density functional study — •Ariyan Tavakoli[1], Stefan Lach[1], Benjamin Stadtmüller[2], Christiane Ziegler[1], Peter Puschnig[3], and Hans Christian Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, Augsburg University, Augsburg, Germany — [3]Department of Physics, University of Graz, Graz, Austria

Metallacrowns [1] combine chemical and structural features that make them a promising material system for single-molecule magnets. Here, we present a first-principles study of the electronic and magnetic properties of the metallacrown (HNEt3)2CuII [12-MCYN(Shi)-4] (Y=CuII), in short CuCu4, in the gas phase and on the Au(111) surface. First, we study the magnetic properties of CuCu4 metallacrown in the gas phase by applying the broken symmetry approach [2], where we benchmark the performance of various (range-separated) hybrid functionals compared to the computationally cheaper GGA+U approach. In the second step, we explore the magnetic configurations of CuCu4 metallacrown adsorbed on an Au(111) surface using density functional theory (DFT) with GGA+U framework. The analysis highlights the changes of the ligand structure and the density of state (DOS) around the metal centers by a comparison between the isolated molecule and the adsorbed one on the surface.

[1] B. R. Gibney et al., Inorganic Chemistry 33 (1994). [2] Pavlyukh, Y. et al., PhysRevB. 99, 144418 (2019).

15 min. break

MA 34.7 Thu 11:15 H18

Cooperative and Selective Redox Doping Switches Single-Molecule Magnetism — Fabian Paschke[1], Matteo Briganti[2], Vivien Enenkel[1], Tobias Birk[1], Jan Dreiser[3], Peter Schmitt[4], Rainer F. Winter[4], Federico Totti[2], and •Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Department of Chemistry 'Ugo Schiff' and INSTM Research Unit, University of Florence, 50019 Sesto Fiorentino, Italy — [3]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [4]Fachbereich Chemie, Universität Konstanz, 78457 Konstanz, Germany

The controlled manipulation of electronic and magnetic states in single-molecule magnets (SMMs) is crucial for their implementation in molecular spintronics. In typical SMMs, key properties like magnetic anisotropy and slow magnetic relaxation are imposed by complex ligand shells, whose bulky and three-dimensional structures hamper efficient manipulation of the molecular magnetism by chemical methods. Here, we demonstrate highly selective chemical doping of an Fe_4 nanomagnet on a Pb(111) surface using lithium atoms. Scanning tunneling microscopy, X-ray absorption spectroscopy, and ab initio calculations reveal the cooperative incorporation of three Li atoms per Fe_4 molecule, resulting in a selective, threefold reduction of its iron-based magnetic core. The doping modifies the intramolecular exchange interaction, turning from antiferromagnetic to ferromagnetic coupling, and changes the molecular magnetic anisotropy from easy-axis to easy-plane.

MA 34.8 Thu 11:30 H18

Tuning spin-injection into metallacrown/thin-metal film systems — •David Anthofer[1], Ashish Moharana[1], Dominik Laible[2], Fabian Kammerbauer[1], Alexander Hagenow[2], Eva Rentschler[2], and Angela Wittmann[1] — [1]Institut für Physik, Johannes-Gutenberg Universität Mainz, Deutschland — [2]Department Chemie, Johannes-Gutenberg Universität Mainz, Deutschland

Single-molecular magnets (SMMs) have recently gained significant interest due to their ability to retain magnetic information at the molecular level, offering potential applications in high-density data storage devices. A crucial challenge hindering their application in technology is the integration with thin-film devices. To tackle this challenge, we explore the spin-injection efficiency in hybrid molecule/non-magnetic metal thin film heterostructures to understand the impact of hybridization. For this, we utilize molecules based on the metallacrown system, chosen for their unique combination of synthetic versatility and structural stability. We inject a pure spin current at ferromagnetic resonance into the hybrid interface, allowing us to measure the magnetic damping of the system. We observe a notable increase in damping after adsorption of Dysprosium-based metallacrown SMMs. In contrast, no change in damping was observed after deposition of Copper-based metallacrowns indicating the significance of molecular composition on the spin-injection efficiency at the hybrid interface. Further optimization of the ferro- and nonmagnetic metal layer thicknesses proves to affect the observed change in damping, paving the path toward a sensitive framework to study hybridization at the molecule/metal interface.

MA 34.9 Thu 11:45 H18

Probing magnetic exchange interactions in cobalt-based molecular magnets using magneto-Raman spectroscopy — •Komalavalli Thirunavukkuarasu[1], David Hunger[2], Julia Netz[3], Duncan Moseley[4], Ziling Xue[4], Dmitry Smirnov[5], Andreas Koehn[3], and Joris van Slagaren[2] — [1]Department of Physics, Florida A & M University, Tallahassee, FL, USA — [2]Institute of Physical Chemistry, University of Stuttgart, Stuttgart, Germany — [3]Institute of Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany — [4]Department of Chemistry, University of Tennessee, Knoxville, USA — [5]National High Magnetic Field Laboratory, Tallahassee, USA

Combining spectroscopy with one or more external parameters such as low temperature, high pressure, and high magnetic fields, allows us to probe interplay between spin, charge, orbital, and lattice degrees of freedom. Spin exchange interactions play an important role in single-molecule magnets and molecular qubits that feature magnetic bistability. However, there have been few detailed studies to experimentally find the energy scale of these interactions such as spin-phonon coupling. Recently, we employed magneto-Raman spectroscopy together with theoretical work on single molecular magnets to reveal the signatures of spin-phonon interactions in these materials. In this talk, the magneto-Raman experimental results from mononuclear cobalt(II) and radical-bridged dinuclear cobalt(II) complexes and the outcome will be discussed.

MA 34.10 Thu 12:00 H18

The Role of Quantum Vibronic Effects in the Spin Polarization of Charge Transport through Chiral Molecular Junctions — •Samuel Rudge[1], Christoph Kaspar[1], Riley Preston[1], Joseph Subotnik[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg — [2]Department of Chemistry, Princeton University

The chirality-induced spin selectivity (CISS) refers to the experimentally observed phenomenon that the transport of spin-polarized electrons through chiral mediums can be highly asymmetric between the two spin orientations and enantiomers [1]. Although the exact mechanism underpinning the CISS effect is still unknown, one of the leading ideas is that it is connected to the coupling of transport electrons to molecular vibrations. In this contribution, we follow this theme by investigating CISS in the context of charge transport through a chiral molecular nanojunction via the numerically exact, fully quantum hierarchical equations of motion (HEOM) approach [2]. Specifically, we calculate charge currents through a two-site, two-mode model [3], focusing on the highly nonadiabatic regime of low-voltage charge transport, in which we find significant spin polarization.

[1] R. Naaman and D. H. Waldeck, Annu. Rev. Phys. Chem. **66**, 263-281 (2015)

[2] C. Schinabeck, A. Erpenbeck, R. Härtle2, and M. Thoss, Phys. Rev. B **94**, 201407(R) (2016)

[3] H.-H. Teh, W. Dou, and J. Subotnik, Phys. Rev. B **106**, 184302 (2022)

MA 34.11 Thu 12:15 H18

Chiral-induced unidirectional spin-to-charge conversion — •Ashish Moharana[1], Yael Kapon[2,3], Fabian Kammerbauer[1], David Anthofer[1], Shira Yochelis[2,3], Mathias Klaüi[1], Yossi Paltiel[2,3], and Angela Wittmann[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz 55128, Germany — [2]Institute of Applied Physics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel — [3]Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

The chiral-induced spin selectivity (CISS) effect has recently gained significant attention in the field of spintronics. The remarkably high efficiency of the spin polarizing effect has recently gained substantial interest due to the high potential for future sustainable hybrid chiral molecule magnetic applications. While so far research has predominantly focused on transport properties, in our work, we explore spintronic phenomena at hybrid chiral molecule magnetic interfaces to elucidate the underlying mechanisms of the chiral-induced spin selectivity effect. For this, we investigate the interfacial spin-orbit coupling in chiral molecule/metal thin film heterostructures by probing the chirality and spin-dependent spin-to-charge conversion. Our findings validate the central role of spin angular momentum for the CISS effect, paving the path toward the functionalization of hybrid molecule-metal interfaces via chirality.

MA 34.12 Thu 12:30 H18

Interplay between spin induced polarization and quantum entanglement in triangular magnetic molecules — •Zhirayr Adamyan[1,2], Vadim Ohanyan[1,2], and Ani Chobanyan[1] — [1]Laboratory of Theoretical Physics, Yerevan State University, 1 Alex Manoogian, 0025 Yerevan, Armenia — [2]CANDLE, Synchrotron Research Institute, 31 Acharyan Str., 0040 Yerevan, Armenia

The quantum entanglement of spin states in molecular magnets has important applications in quantum information technologies and quantum computing. Currently, qubit models based on magnetic molecules are being used to develop quantum computation and communication technologies. We consider two models of three-spin molecular magnets with additional features that allow one to manipulate and enhance their entanglement. The first model is a mixed-spin (1/2, 1, 1/2) triangle with two g-factors. The second model is a spin-1/2 triangle with the Katsura-Nagaosa-Balatsky (KNB) mechanism, providing the coupling between spin degrees of freedom and the external electric field. It is shown that non-conserving magnetization originated from the non-uniformity of g-factors leads to an essential increase of the entanglement of certain spin states along with the rich structure of zero-temperature phase diagrams. Whereas, the model with magnetoelectric coupling due to the KNB mechanism offers a wide possibility of manipulation of quantum entanglement by the electric field, both using its magnitude and direction.

MA 35: PhD Focus Session: Using Artificial Intelligence Tools in Magnetism

Over the last decade, the field of artificial intelligence (AI) has experienced significant growth and progressively offers applications across a wide range of topics, becoming an integral part of our daily lives. Its importance was also underscored by the 2024 Nobel Prize in Physics awarded to John J. Hopfield and Geoffrey E. Hinton 'for foundational discoveries and inventions that enable machine learning with artificial neural networks'. The application of AI methods is also becoming increasingly relevant in research for prediction and data analysis to enhance research, making it faster and more efficient. Typically, these AI tools come from the domain of machine learning, centered on deep learning architectures such as neural networks, convolutional neural networks, and transformer networks. To ensure young researchers, especially in the field of magnetism, can benefit from this progress, we organize the PhD Focus session 'Using Artificial Intelligence Tools in Magnetism'. In this session, experts will demonstrate in highly pedagogical presentations how AI tools can be applied in material science and magnetism. Additionally, there will be a direct, practical introduction to this area of AI tools in magnetism with a hands-on part, where each participant can engage and explore the fascinating world of AI tools for magnetism firsthand using a prepared repository. You can find the repository at https://github.com/kfjml/AI-Magnetism-Session-Regensburg-2025 , please follow the instructions in the Readme, ideally before the session. Alternatively, you can download the repository as a ZIP file, including the instructions in the Readme, from https://download.klaeui-lab.de/AI-Magnetism-Session-Regensburg-2025.

Organizers: Kilian Leutner, kileutne@students.uni-mainz.de; Thomas B. Winkler, thomas.winkler@ru.nl; Robin Msiska, robin.msiska@uni-due.de; Kübra Kalkan, kuebra.kalkan@uni-due.de, Jan Maskill, maskill@rptu.de

Time: Thursday 9:30–13:00 Location: H20

Introduction

Invited Talk MA 35.1 Thu 9:35 H20

Artificial Intelligence for Materials Science: Critical Importance of Rare Events, Active Learning, and Uncertainties — •Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, 14195 Berlin, DE

Materials properties are often governed by an intricate interplay of many processes. As a consequence, the description in terms of meaningful analytical equations is typically inappropriate, and we are promoting the concept of 'materials genes'. These are elemental materials features that 'correlate' with the materials property of interest. Thus, they address the full intricacy and describe (in a statistical sense) the material's property and function.[1]

AI and machine learning (ML) exhibit diminished reliability when entering uncharted data regions. When the training data are representative of the full population (or iid), extrapolation may work. However, for materials this requirement is hardly fulfilled. Still, materials scientists are searching for 'statistically exceptional' situations, and properties are often triggered by 'rare events' that are not or not well covered by the available data, or smoothed out by the ML regularization. This all implies caution when applying ML. In my talk I will explain these issues and routes toward solutions. Key issues are the 'range of applicability' of ML models, the awful overconfidence of prediction uncertainties, and the needs for active learning.

(**) In collab. with Lucas Foppa, Kisung Kang, and Akhil S. Nair.

1) Scheffler M AI guided workflows for screening the materials space. Coshare Science 02, 02 (2024); https://doi.org/10.61109/cs.202403.129

Invited Talk MA 35.2 Thu 10:05 H20

Physics meets data: decoding magnetic inhomogeneities through latent analysis — •Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

Physicists are trained to simplify complex problems into their fundamental components, often using effective minimal models to describe experimentally observed phenomena. This approach's standard challenges include the difficulty of directly measuring model parameters and the frequent oversimplification or neglect of sample inhomogeneities. As a result, models often fail to make accurate predictions when critical effects are overlooked or inadequately represented. In contrast, data-driven approaches focus on learning directly from the data, ideally without making restrictive assumptions about the data. This talk addresses the problem of hidden features in data and presents computationally efficient, physics-inspired data analysis tools - latent entropy and latent dimension [1,2] - that, for example, allow uncovering magnetic inhomogeneities from video data.

[1] I. Horenko, D. Rodrigues, T. O'Kane, K. Everschor-Sitte, Communications in Applied Mathematics and Computer Science 16, 2 (2021). [2] D. Rodrigues, K. Everschor-Sitte, S. Gerber, I. Horenko, iScience 24, 3 (2021).

Invited Talk MA 35.3 Thu 10:35 H20

AI used for micromagnetic simulations — •Thomas Schrefl[1], Felix Lasthofer[1], Qais Ali[1], Heisam Moustafa[2], Harald Oezelt[2], Alexander Kovacs[2], Masao Yano[3], Noritsugu Sakuma[3], Akihito Kinoshita[3], Tetsuya Shoji[3], and Akira Kato[3] — [1]Christian Doppler Laboratory for magnet design through physics informed machine learning, Wiener Neustadt, Austria — [2]University for Continuing Education Krems, Wiener Neustadt, Austria — [3]Advanced Materials Engineering Division, Toyota Motor Corporation, Susono, Japan

Micromagnetic simulations are an excellent means for prediction of magnetic properties. However, the required computational resources limit the use of micromagnetics for materials design. Machine learning models can serve as surrogate for evaluating target properties during optimization. Artificial intelligence can sort pictures based on content or create new images given keywords. Treating the magnetization distribution as an image, methodologies from image processing can be applied in magnetism. We used this approach to predict the magnetization dynamics of thin film elements. The magnetic states are encoded by a convolutional neural network. For bulk magnets a different approach is required. Their three-dimensional grain structure can be represented by a graph. The regular pixels are replaced by the nodes and edges of a graph. We applied graph neural networks to predict hysteresis properties of permanent magnets. Trained machine learning models can be used for inverse design. Given certain targets, optimized magnets are suggested.

10 min break

Invited Talk MA 35.4 Thu 11:15 H20

Future method for estimating parameters in magnetic films using machine learning — •Kenji Tanabe — Toyota Technological Institute, Nagoya, Japan

Estimating material parameters in fabricated materials is a crucial experiment in the field of materials science. Some parameters are difficult or time-consuming to measure. In spintronics, parameters such as the Dzyaloshinskii-Moriya exchange constant are good examples of this. If these parameters could be easily and quickly estimated, our research field would grow rapidly. Here, we present a new method for estimating parameters in magnetic films from a magnetic domain image using machine learning. A magnetic structure is well-known to be deeply related to magnetic parameters. Although a complicated magnetic structure, which often appears in an as-grown magnetic film, is considered random by human eyes, it is influenced by several magnetic energies. Thus, the characteristics of such parameters are probably hidden in the random magnetic structure. Such a relationship suggests that parameters can be estimated from a magnetic domain image by using pattern recognition. We collected a huge number of datasets of magnetic parameters and magnetic domain images made by micromagnetic simulation and/or taken by magnetic microscopes. The datasets were used as training and test data for the convolution neural network, which is a famous technique in machine learning for pattern recognition. We succeeded in the estimation of the parameters from the magnetic image using machine learning. This result may relieve future researchers from the difficulty of measuring parameters.

MA 35.5 Thu 11:45 H20

Hands-on workshop for using AI in magnetism research — •Kilian Leutner[1], Thomas B. Winkler[2], Jan Maskill[3], Kübra Kalkan[4], and Robin Msiska[4] — [1]Institute of Physics, Johannes Gutenberg-University Mainz — [2]Institute for Molecules and Materials, Radboud University — [3]Department of

Physics, University of Kaiserslautern-Landau — [4]Faculty of Physics, University of Duisburg-Essen

In this workshop, participants will receive a practical introduction to applying artificial intelligence (AI) in magnetism research. As a hands-on session, everyone can actively engage. We will demonstrate how to automatically analyze magneto-optical Kerr microscopy images of magnetic skyrmions using AI. The critical and significant step in the analysis involves segmenting the Kerr images using the Skyrmion U-Net, a convolutional neural network [1]. The participants will use their own devices to explore a repository, learning and executing the steps necessary to train and apply a skyrmion U-Net model. The required experimental Kerr data, pre-trained Skyrmion U-Net models, and code are available in a repository at https://github.com/kfjml/AI-Magnetism-Session-Regensburg-2025 or can be downloaded as a ZIP file from: https://download.klaeui-lab.de/AI-Magnetism-Session-Regensburg-2025. Please follow the instructions in the Readme file prior to the session, to make most use of it. This presented approach, is adaptable to other magnetic textures or imaging methods and can also be applied beyond magnetism.

[1] I. Labrie-Boulay et al., Phys. Rev. Applied 21, 014014 (2024)

MA 36: Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)

Superconducting monolayer transition metal dichalcogenides (TMDs) like $NbSe_2$, TaS_2, and gated WSe_2 or MoS_2, have attracted lot of interest in recent years. On the one hand Ising spin-orbit coupling pins the electron's spin out of plane, and hence is responsible for critical in-plane magnetic fields by far exceeding the Pauli limit. On the other hand, while the underlying pairing mechanism is still under debate, recent experiments provide strong evidence for its unconventional, multiband, nature. The Focus Session will feature experimental and theoretical advances on the superconductivity in monolayer TMDs, with focus on universal features, a possible Luttinger-Kohn mechanism, a nodal or even chiral nature of the gap functions, and their phase diagram.

Organizers: Milena Grifoni (Universität Regensburg), Julian Siegl (Universität Regensburg)

Time: Thursday 9:30–12:45 Location: H36

See TT 44 for details of this session.

MA 37: Magnetic Imaging Techniques

Time: Thursday 15:00–17:45 Location: H16

MA 37.1 Thu 15:00 H16

Magnetic particle spectroscopy of ferrite nanoparticles: Controlling the Néel to Brownian relaxations — •Ondřej Kaman[1], Tereza Voltrová[1,2], Lenka Kubíčková[1,2], Ali Hassan[1], Pavel Veverka[1], Kyo-Hoon Ahn[1], Karel Knížek[1], Denisa Kubániová[2], and Jaroslav Kohout[2] — [1]FZU - Institute of Physics, CAS, Praha, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic

The Fourier transform of the magnetization response of a suspension of magnetic particles to a sinusoidal AC magnetic field provides so-called magnetic particle spectrum, i.e., a series of higher harmonics that originate in the non-linear $M(H)$ dependence. This characteristic is crucial for magnetic particle imaging (MPI), which is an emerging technique employing magnetic particles, typically in the superparamagnetic state, as exogeneous tracers for medical imaging. The magnetization dynamics of such tracers is governed by two distinct mechanisms, the Néel relaxation of magnetic moments and the Brownian rotation of whole particles. The present study is based on a series of hydrothermally prepared and thoroughly characterized (XRD, XRF, TEM, SQUID magnetometry) samples of $Co_{1-x}Ni_xFe_2O_4$ particles with x=0–0.5 and the mean crystallite size of 8–9 nm. Their silica-coated clusters, forming colloidally stable aqueous suspensions, were prepared, and MPI study was performed by means of an in-house built system (interchangeable coils impedance-matched to ~10, 15, 25, 35, and 50 kHz; magnetic field up to 20 mT).

MA 37.2 Thu 15:15 H16

Nanoscale magnetic imaging with color centers in fiber-coupled diamond nanobeams — •Gesa Welker[1], Yufan Li[1], Richard Norte[2], and Toeno van der Sar[1] — [1]Delft University of Technology, Faculty of Applied Sciences, Lorentzweg 1, 2628 CJ Delft, the Netherlands — [2]Delft University of Technology, Faculty of Mechanical Engineering, Mekelweg 2, 2628 CD Delft, the Netherlands

Nitrogen vacancy centers (NV-centers) in diamond are powerful magnetic field sensors that are excited and read out optically. They are an established tool for imaging weak magnetic signatures of condensed matter samples such as skyrmions, spin waves or 2D magnetism [1]. We present a unique fiber-coupled approach to scanning probe magnetometry, where a diamond nanobeam with NV-centers at its apex is attached to a tapered optical fiber and scanned across a sample [2]. Fiber-coupling could enable a higher excitation and collection efficiency compared to traditional setups. It also simplifies measurements at low temperatures, because it eliminates the need for re-alignment of free-space optics. We demonstrate diamond nanobeam fabrication via quasi-isotropic etching and a robust nanobeam-fiber assembly using optical glue. With this setup, we performed a 2D scan of the magnetic stray field of a current-carrying wire with sub-micrometer resolution [3]. Our method is also promising for magnetic sensing with recently emerged color centers such as tin vacancy centers (SnV-centers) [4].

[1] Casola et al. Nat. Rev. Mater 3, 17088 (2018) [2] Y. Li et al. ACS Photonics 10, 1859-1865 (2023) [3] Y. Li, G. Welker et al., New J. Phys. 26, 103031 (2024) [4] T. Iwasaki et al. PRL 119, 253601 (2017)

MA 37.3 Thu 15:30 H16

Planar scanning probe microscopy enables nanoscale vector magnetic field imaging with nitrogen-vacancy centers — •Paul Weinbrenner[1,2], Patricia Klar[3], Christian Giese[3], Luis Flacke[4,5], Manuel Müller[4,5], Matthias Althammer[4,5], Stephan Geprägs[4], Rudolf Gross[4,5,6], and Friedemann Reinhard[1,2,6] — [1]Institute for Physics, University of Rostock, Rostock, Germany — [2]Department of Life, Light and Matter, University of Rostock, Rostock, Germany — [3]Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany — [4]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [5]Physics Department, Technical University of Munich, Garching, Germany — [6]Munich Center for Quantum Science and Technology, Munich, Germany

We present imaging of vector magnetic fields on the nanoscale using planar scanning probe microscopy with nitrogen-vacancy (NV) centers in diamond as magnetic field sensors. Instead of traditional tip-based scanning probes, we employ an extended bulk diamond doped with NV centers. Despite the probe's large lateral size, it can still be scanned in nanoscale proximity to a planar sample.

We perform repeated measurements with NV centers with different orientations to obtain a direct image of the three-dimensional vector magnetic field of magnetic vortices in a thin-film magnetic heterostructure. Our result opens the possibility of quantum sensing using multiple qubits within the same scanning probe, which can be used for entanglement-enhanced and massively parallel sensing schemes.

MA 37.4 Thu 15:45 H16

Nanostructure and Coercivity Mechanism of Single-Phase $Ce(Co_{0.8}Cu_{0.2})_{5.4}$ — •Tatiana Smoliarova[1], András Kovács[2], Nikita Polin[3], Esmaeil Adabifiroozjaei[4], Shangbin Shen[4], Xinren Chen[3], Leopoldo Molina-Luna[4], Oliver Gutfleisch[4], Konstantin Skokov[4], Michael Farle[1], Baptiste Gault[3], and Rafal E. Dunin-Borkowski[2] — [1]Faculty of Physics and Center for Nanointegration, Universität Duisburg-Essen, Duisburg, Germany — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany — [3]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf 40237, Germany — [4]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

$CeCo_5$ rare-earth RCo_5 permanent magnets achieve high coercivity (H_C = 1 T) upon the addition of Cu up to 20%, making Ce-based magnets an abundant R-alternative to Sm-based magnets. Here, we report a study that employs TEM

in conjunction with APT to investigate the $Ce(Co_{0.8}Cu_{0.2})_{5.4}$ magnet, prepared by induction melting followed by controlled heat treatment and water quenching. The process results in the formation of a cellular structure characterized by elongated along the *c*-axis, Cu-rich precipitates with a diameter of ~ 5 nm and a length of ~ 20 nm, surrounded by a Cu-poor matrix with a thickness of ~ 10 nm. The alignment of the Cu-rich precipitates creates a preferential direction for zigzag-shaped domain walls, yielding effective pinning and $H_C = 1 \pm 0.05$ T. Financial support by DFG, CRC/TRR 270 (project ID 405553726) is acknowledged.

MA 37.5 Thu 16:00 H16

Transport of Intensity Phase Retrieval in the Presence of Intensity Variations and Unknown Boundary Conditions — •Oleksandr Zaiets[1,2], Axel Lubk[1,2], Radmilla Kyrychenko[1], Daniel Wolf[1], Maximilian Wegner[1], Max Herzog[1], Moritz Winter[1,3,4], Praveen Vir[3], Johannes Schultz[1], Claudia Felser[3], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Dresden Center for Nanoanalysis, cfaed, Technical University Dresden, Dresden, Germany

Transport of Intensity Equation (TIE) phase retrieval technique is widely applied in light, X-ray and electron optics to reconstruct, e.g., refractive indices, electric and magnetic fields in solids. The TIE method reconstructs the phase from two or three mutually slightly defocused microscopy images by solving an elliptic partial differential equation - the TIE. Here, we present a largely improved TIE reconstruction algorithm, which properly considers intensity variations as well as unknown boundary conditions in a finite difference implementation of the TIE. That largely removes reconstruction artifacts encountered in state-of-the-art Poisson solvers of the TIE, and hence significantly increases the applicability of the technique. We demonstrate the improved performance of the TIE reconstruction algorithm at a set of simulated and experimental image intensities arising from magnetic structures investigated in TEM.

MA 37.6 Thu 16:15 H16

Fast spectroscopic imaging using extreme ultraviolet interferometry — •Hannah C. Strauch[1], Fengling Zhang[2], Stefan Mathias[1], Thorsten Hohage[3], Stefan Witte[2,4], and G. S. Matthijs Jansen[1] — [1]University of Göttingen, 1st Institute of Physics, Göttingen, Germany — [2]Advanced Research Center for Nanolithography, Amsterdam, The Netherlands — [3]University of Göttingen, Institute of Numerical and Applied Mathematics, Göttingen, Germany — [4]Imaging Physics department, TU Delft, The Netherlands

Extreme ultraviolet (EUV) pulses generated by high harmonic generation (HHG) offer element-specificity in spectroscopic applications [1], and an excellent platform for nanoscale coherent diffractive imaging. Thus, the combination of time-resolved spectroscopy and microscopy using HHG light is highly promising, but it is only hardly explored due to the challenge of extracting full spectroscopic and microscopic information from measurements of reasonable duration.

We will present FTSH, an interferometric solution that combines Fourier-transform spectroscopy (FTS) and holography [2], employing a pair of phase-locked EUV pulses. This combination explicitly encodes the EUV spectral information in the diffraction pattern. Compared to traditional FTS, FTSH dramatically reduces the interferometric sampling requirements. This enables full spectroscopic images in less than two minutes and makes our approach particularly promising for femtosecond time-resolved spectroscopic imaging.

[1] Möller et al., Commun. Phys. 7, 74 (2024)

[2] Strauch et al., Opt. Express 32(16), 28644-28654 (2024)

MA 37.7 Thu 16:30 H16

Magnetic vector field imaging with single domain magnetooptical indicator films — •Michael Path and Jeffrey McCord — Institute for Materials Science, Kiel University, Germany

Robust and fast magnetic vector field imaging is essential for the characterization of, e.g., electronic systems. We present a magnetooptical method for quantitative and spatially resolved magnetic vector field imaging based on the use of magnetooptical indicator films. Simultaneous magnetooptical temperature extraction ensures temperature independent quantification of the magnetic field amplitude and angle. Yttrium-iron-garnet indicator films with in-plane and out-of-plane magnetic anisotropy can be used for this method. In both cases, a magnetic bias field is applied to bring the indicator film into a single-domain state along four different directions. By measuring the out-of-plane tilt of the magnetization with four images using magnetooptical microscopy, the local magnetic vector field distribution and the local temperature are obtained. As an example, the magnetic vector field distribution generated by the current of an integrated circuit is observed and compared with the calculations. The accuracy of this method is verified by means of relative and statistical error analysis.

15 min. break

MA 37.8 Thu 17:00 H16

Characterization of the periodic stray field along ferromagnetic domain textures in synthetic antiferromagnets — •R. J. Peña Román[1], S. Maity[1], F. Samad[2,3], A. Kákay[2], O. Hellwig[2,3], K. Kern[1,4], and A. Singha[5,1] — [1]Max Planck Institute for Solid State Research — [2]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf — [3]Insititute of Physics, Chemnitz University of Technology — [4]Institute de Physique, École Polytechnique Fédérale de Lausanne — [5]Institute of Solid State and Materials Physics, Dresden University of Technology,

Magnetic imaging of domains and domain walls (DWs) composing the texture of any magnetic material is a crucial step toward understanding their properties and finding solutions to tailor the material properties to achieve new technology-driven functionalities. Synthetic Antiferromagnets (SAFs) are particularly interesting due to their highly tunable properties since their magnetic texture can be controlled by adjusting the design parameters during fabrication. Here, we use diamond Nitrogen-Vacancy Scanning Probe Microscopy (NV-SPM) to investigate and characterize ferromagnetic domains with periodic stray fields in SAFs. The magnetic field in the sample is sensed by measuring the Zeeman splitting that it produces on the NV electron spin states, while the magnetic noise is detected due to its impact on the NV spin relaxation time. NV-SPM allows us to explore the sample properties quantitatively with high magnetic sensitivity and non-invasively at the nanoscale. It is essential to identify the nature of the DWs and engineer them for potential applications in magnonics or spintronics.

MA 37.9 Thu 17:15 H16

Investigation of charge-state stability in shallow NV centers with surface treatments — •Atharva Paranjape[1], Olga Shevtsova[1], Lisa Ebo[1], Toni Hache[1,2], Rainer Stöhr[2], Jörg Wrachtrup[2], and Aparajita Singha[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]3rd Institute of Physics and Research Center SCoPE, University of Stuttgart — [3]IFMP, Technical University of Dresden

Nitrogen-vacancy (NV) centers in diamond are optically active defects which can be used for precise measurement of magnetic fields. While near-surface NV centers can provide high spatial resolution in magnetic imaging, they also face charge-state instability, which is aggravated in in ultra-high-vacuum (UHV). Here we aim to develop surface-treatment methods to reduce charge-state instability of shallow (< 10 nm from surface) NV centers in UHV conditions. We show that a TiO_2 coating using Atomic Layer Deposition (ALD) on nanostructured diamond stabilizes the charge state by modifying the local environment. These experiments are crucial for the development of a scanning NV magnetometer in UHV with a high spatial resolution.

MA 37.10 Thu 17:30 H16

Magnetic Force Microscopy: High Quality-Factor Two-Pass Mode — •Christopher Habenschaden[1], Sibylle Sievers[1], Alexander Klasen[2], Andrea Cerreta[2], and Hans Werner Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig — [2]Park Systems Europe GmbH, 68199 Mannheim

Magnetic Force Microscopy (MFM) is an effective technique for characterizing magnetic micro- and nanostructures, typically detecting interactions between a magnetically coated tip on an oscillating cantilever and the sample. MFM sensitivity is enhanced under vacuum conditions due to the higher cantilever quality factor (Q-factor), which significantly improves force sensitivity. However, the commonly used two-pass mode in MFM faces challenges under vacuum, as the high Q-factor can lead to tip crashing when surface forces overpower the restoring force during topography imaging.

Here, we present a novel approach for high-sensitivity vacuum MFM measurements while maintaining stable topography detection. Implemented on a Park Systems NX-Hivac AFM, this method modifies the two-pass mode to create a high Q-factor two-pass mode [1]. In the first pass, the cantilever's Q-factor is artificially lowered to ensure stable non-contact topography imaging. In the second pass, a phase-locked loop (PLL) measures the frequency shift, maintaining the maximum Q-factor for optimal sensitivity in magnetic field measurements. This approach prevents tip crashes during the first pass and eliminates non-linear phase response in the second pass, ensuring robust and precise measurements.

[1] Rev. Sci. Instrum. 95, 113704 (2024).

MA 38: Magnetic Particles / Clusters & Biomagnetism

Time: Thursday 15:00–18:00 Location: H18

Invited Talk MA 38.1 Thu 15:00 H18

Liquid-mediated surface-surface interactions investigated by close-to-surface magnetic particle transport — •Rico Huhnstock, Yahya Shubbak, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Studying phenomena at the liquid-solid interface has tremendous significance for the physical, chemical, biological, and nanostructure sciences [1]. Experimental access to the underlying interactions is a non-trivial task, demonstrated for instance by the difficulties connected with performing atomic force microscopy measurements in liquids. In this talk, we propose a novel technique to inspect liquid-mediated surface-surface interactions based on guiding magnetic microparticles (MPs), surrounded by a quiescent fluid, along defined trajectories in the vicinity of a solid interface. The MP motion is induced by harnessing engineered magnetic stray field landscapes (MFLs) emerging from customized magnetic domain patterns imprinted into a topographically flat substrate. We will give an overview of the MFL fabrication process and discuss the influence of MP [2], liquid, and MFL [3] properties on the MP motion. Finally, we highlight, that the MP motion dynamics can be studied to identify changes in liquid-mediated DLVO interactions between surfaces of the MP and the underlying substrate.

[1] Chen *et al.* (2022), Advanced Materials Interfaces, 9(35):2201864.
[2] Huhnstock *et al.* (2021), Scientific Reports, 11(1):21794.
[3] Huhnstock *et al.* (2024), Small, 20(10):2305675.

MA 38.2 Thu 15:30 H18

Exploring iron nitrides: Insights from Mössbauer spectroscopy — •Lenka Kubíčková[1,2], Jaroslav Kohout[1], Tomáš Kmječ[1], Karel Knížek[2], Štefan Hricov[2,3], Ondřej Kaman[2], Yevhen Ablets[4], Robin Kidangan Paul[4], Stanislav Mráz[5], Jochen Schneider[5], Oliver Gutfleisch[4], and Imants Dirba[4] — [1]Faculty of Mathematics and Physics, Charles University, 180 00 Praha 8, Czechia — [2]FZU - Institute of Physics of the CAS, 162 00 Praha 6, Czechia — [3]Faculty of Science, Charles University, 128 00 Praha 2, Czechia — [4]Functional Materials, Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [5]Materials Chemistry, RWTH Aachen University, 52074 Aachen, Germany

Mössbauer spectroscopy, a powerful tool for probing the local electronic and magnetic properties of materials containing Mössbauer isotopes, will be employed to investigate selected examples of iron nitrides. First, we will show spectra of air-sensitive Fe_3N nanoparticles, which exhibit a high degree of structural disorder. Moreover, we will discuss formation of an oxide layer by their passivation, whose nature and extent is difficult to assess from other methods but is crucial for medical applications. Second, conversion-electron Mössbauer spectroscopy (CEMS) of $Fe_{4-x}Ge_xN$ (x = 0, 0.5 and 1) crystalline thin films allows us to determine not only the direction of magnetization in the film of the undoped phase, but also, together with the DFT calculations, position of the Ge atoms in the Fe_4N structure. Such local insights are valuable for designing and optimizing iron-based films, e.g., for their magnetic or thermoelectric applications.

MA 38.3 Thu 15:45 H18

Tunable magnetic behavior in $[CoFe_2O_4]_n$@Pt hybrid nanoparticles — •Joachim Landers[1], Moritz Raphael[2], Soma Salamon[1], Heiko Wende[1], and Annette Schmidt[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Chemistry, Institute of Physical Chemistry, University of Cologne

$[CoFe_2O_4]_n$@Pt hybrid nanoparticles were prepared by growing monodisperse $CoFe_2O_4$ (CFO) nanocubes epitaxially on the corners of 6 nm cubic Fe/Co-doped Pt seeds. The hybrid particles display a defined configurational order, in which the CFO cubes cover the corner positions, allowing the formation with a variable number n of CFO cubes in reproducible geometries. Thereby, the hybrid particles represent a system of tunable intraparticular magnetic dipolar interaction, acting in superposition to the high cubic magnetocrystalline anisotropy of the CFO nanocubes. This competition creates a complex temperature-dependence of the shape of the magnetic hysteresis curves, dependent on the size and number of attached CFO nanocubes. In the future, this could facilitate the production of high-anisotropy and -magnetization hybrid particles of widely controllable magnetic behavior. To analyze the acting mechanisms and resulting magnetic properties, in-field Mössbauer spectroscopy and different magnetometry protocols were employed. The experimental observations are compared to micromagnetic simulations utilizing MuMax3. Funding by the DFG projects SCHM1747/16-1 and LA5175/1-1 is gratefully acknowledged.

MA 38.4 Thu 16:00 H18

Inductive Heating of ZnFe Nanoparticles — •Esra Uz[1], Yohei Fujita[2], Marina Spasova[1], Tatiana Smaliarova[1], Ivan Tarasov[1], Michael Farle[1], Yuko Ichiyanagi[2], and Ulf Wiedwald[1] — [1]Universität Duisburg Essen — [2]Yokohama National University

Hyperthermia is a novel medical treatment that uses magnetic fields in combination with specially designed magnetic nanoparticles for the non-invasive elimination of pathological cells. The ZnFe nanoparticles (6-19 nm) have been chemically synthesized and analyzed with a focus on applications in magnetic hyperthermia. The structure and morphology of the nanoparticles have been investigated using X-ray diffraction (XRD) and transmission electron microscopy (TEM). The results confirm the cubic spinel structure of the nanoparticles. Vibrating sample magnetometry (VSM) revealed a ferromagnetic character of the 19 nm particles with a saturation magnetization of 79.8 Am*m/kg. The smaller particles, however, have shown superparamagnetic behavior. For two distinct particle sizes, 11 nm and 19 nm, agarose gel electrophoresis was applied to experimentally measure the heating power in an alternating magnetic field (100-250 kHz, 0-50 mT). For the specific loss power (SLP), determined by calorimetry, our experiments show a maximum value of 71 W/g at a frequency of 247 kHz and B = 40 mT. These findings demonstrate that ZnFe nanoparticles are a promising candidate for applications in the context of magnetic hyperthermia.

MA 38.5 Thu 16:15 H18

Simulation of Dynamics and Self-assembly of Magnetically Decorated Particles — •Maximilian Neumann, Sibylle Gemming, Oliver G. Schmidt, Daniil Karnaushenko, and Aaron Steinhäusser — TU Chemnitz, Chemnitz, Germany

Self-assembly allows for the aggregation of highly complex structures from simple components. Coupled with the highly tunable properties and susceptibility to external fields of magnetic particles this results in the potential to fashion systems with a plethora of applications. By decorating tubular particles with permanent magnets in specific patterns of up/down configuration we create different species of particles, whose behaviour is governed by a mix of attractive and repulsive interactions between individual magnets. This results in selective assembly between specific species, position and orientation. We show simulations of the interaction and dynamics of these particles with and without the influence of external fields and the surrounding medium.

MA 38.6 Thu 16:30 H18

Arranging dipoles on a ring to create homogenous fields — •Ingo Rehberg[1] and Peter Blümler[2] — [1]Experimental Physics, University of Bayreuth, D-95440 Bayreuth, Germany — [2]Institute of Physics, University of Mainz, 55128 Mainz, Germany

Homogeneous magnetic fields can be generated using appropriately arranged permanent magnets. Halbach rings serve as a prominent example of this approach [1], particularly effective when employing very long magnetic rods, often modelled as line dipoles. However, for shorter magnets, the optimal configuration of magnetic moments diverges from the traditional Halbach geometry [2]. In this talk, we present an experimental setup utilizing magnetic cubes and visualize the anticipated fields through an open-source animation of point dipole clusters [3].

[1] Peter Blümler and Helmut Soltner, Practical Concepts for Design, Construction and Application of Halbach Magnets in Magnetic Resonance. Appl. Magn. Reson. 54, 1701 (2023).
[2] Ingo Rehberg and Peter Blümler, submitted.
[3] Ingo Rehberg, From Concentric Halbach Rings to Tetraplex Cuts - Examine 540 Dipole Clusters with a Single Python Animation. https://zenodo.org/records/11214206 (2024).

15 min. break

MA 38.7 Thu 17:00 H18

Quantum Mechanical Analysis of Complex Ferrimagnetic States in Iron Oxide Nanoparticles — •Valentína Berecová[1,2], Martin Friák[1], Naděžda Pizúrová[1], and Jana Pavlů[2] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Republic — [2]Dept. Chem., Masaryk Uni., Brno, Czech Republic

Maghemite (γ-Fe_2O_3) is a biocompatible ferrimagnetic iron oxide that crystallizes in an inverse spinel lattice and can be viewed as magnetite (Fe_3O_4) with iron vacancies. Iron oxide nanoparticles related to maghemite have numerous applications in the biomedical field thanks to the combination of their magnetic properties, biocompatibility, low cytotoxicity and small size. Density functional theory calculations were employed to examine the local magnetic moments of individual atoms in two maghemite-related nanoparticles. Our calculations for the nanoparticles were inspired by bulk maghemite γ-Fe_2O_3, where tetrahedrally

and octahedrally coordinated Fe sublattices have opposing orientations of local magnetic moments. Importantly, our results show that the nanoparticle surfaces create far more complex magnetic states compared to the magnetic ordering found in bulk. These complex magnetic states were described as "nested" ferrimagnetism, which is characterized by local magnetic moments of Fe atoms with mutually opposite orientations appearing even within each of the two (tetrahedral or octahedral) sublattices. Financial support from the Czech Academy of Sciences (*Praemium Academiae* of M.F.) is gratefully acknowledged. Computational resources were provided by the e-INFRA CZ project and IT4Innovations National Supercomputing Center.

MA 38.8 Thu 17:15 H18

Iron Nitride Magnetic Nanoparticles for Biomedical Applications — •Sayar Das[1], Yevhen Ablets[1], Lenka Kubíčková[2], Imants Dirba[1], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Germany — [2]FZU, Praha, Czech Republic

With the urgent need for advanced materials in healthcare, magnetic nanoparticles (MNPs) have emerged to be helpful in versatile biomedical applications such as Hyperthermia for cancer treatment, contrast agents for Magnetic resonance Imaging, drug delivery, and others. For such applications, MNPs must be small in size and have high saturation magnetization (M_s) for better performance. Typically, iron oxide nanoparticles are used as they are inexpensive, chemically stable, and show low toxicity. Owing to the superior properties of iron nitride phases, it is considered a promising candidate over traditionally used iron oxides. This study systematically investigates the synthesis and characterization of iron nitride nanoparticles for intended biomedical applications. MNPs are synthesized via the thermal decomposition method using $Fe(CO)_5$ as a precursor, where nitriding is realized with ammonia as a carrier gas. Key findings demonstrate that surfactant-free synthesis yields ε-Fe_3N nanoparticles with M_s up to 122 Am^2/kg and a mean particle size of 14 nm. Synthesis with surfactants results in nanoparticles with higher yields and enhanced M_s. Moreover, using pure hydrogen as a reducing agent during synthesis significantly improves magnetic properties, with room temperature M_s reaching 162 Am^2/kg at a particle size of 15 nm, which is the highest M_s in iron nitride nanoparticles prepared by wet chemical routes up to date.

MA 38.9 Thu 17:30 H18

Magnetophoretic distinction of differently surface-functionalized magnetic microparticles by transport in a quiescent liquid — •Yahya Shubbak, Katharina Eichhorn, Nikolai Weidt, Arne Vereijken, Rico Huhnstock, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Magnetic particles (MPs) transported in a quiescent liquid close to the surface of a substrate with a periodic magnetic domain pattern is a promising Lab-on-a-chip technology for the detection of MP-bound analytes, even when their size is negligible compared to the MP size. As a proof of principle, we show an all-optical method to distinguish single MPs of the same nominal size that are surface-functionalized with two different chemical groups. More specifically, MPs measuring 2 micrometer in diameter with a polymer coating with only carboxyl end groups (COOH) or a mixture of carboxyl and amino (NH2) groups, respectively, have been studied. Harnessing a variation of liquid-mediated surface interaction forces in our close-to-substrate MP transport scheme, the different MP surface potentials lead to different magnetophoretic mobilities. Accordingly, transport of these MPs in double-distilled water showed a remarkable difference in the average velocity where the COOH MPs were almost twice as fast as the NH2 counterparts. A thorough investigation using external magnetic field pulses of varying durations revealed a significant distinction between both MP species using only moderate flux densities of a few mT.

MA 38.10 Thu 17:45 H18

Structural, magnetic properties and induction heating behavior studies of Mn doped cupper ferrite nanopowders synthesized using co-precipitation method — •Mahmoud Ismail[1] and Diaa EL-Rahman Rayan[2,3] — [1]Biophysics Branch and Physics Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo, Egypt — [2]Central Metallurgical Research and Development Institute (CMRDI), P.O. Box: 87 Helwan, 11421, Egypt — [3]Department of Physics, Deraya University, New Minia, Minya, Egypt

In this research synthesizes nanocrystalline CuFe2O4 spinel structure using co-precipitation method. The pure copper ferrite is substituted by manganese MnxCu(1*x)Fe2O4 nanopowders (x from 0.0 to 1.0). XRD, HR-TEM, UV-visible-Spectrophotometer and vibrating sample magnetometer (VSM) are utilized in order to study the effect of variation of Mn2+ ions substitution and its impact on crystalline size, lattice parameters, microstructure and optical and magnetic properties of the formed nanopowders. Indeed, heating properties of the MnxCu(1-x)Fe2O4 nanoparticles in an alternating magnetic field at 160 kHz were estimated. The results reveal that the sonochemical method for polyethylene glycol (PEGylated) MnxCu(1-x)Fe2O4 nanoparticles with size 5 nm leads to pseudo-single domain with smallest loop area. Of note, it is clear that the specific heat rate SAR values were in the range from 104.5 to 302.0 W/g at different synthesis conditions. Finally, large SAR values are obtained within 10*15 min using low magnetic field, making Cu-Mn ferrite appropriate for hyperthermia treatment of cancer.

MA 39: Magnetic Thin Films

Time: Thursday 15:00–17:00 Location: H19

Invited Talk MA 39.1 Thu 15:00 H19

Voltage control of magnetism using hydrogen — •Markus Gössler — Chemnitz University of Technology, Chemnitz, Germany

Voltage-controlled magnetic properties have entered the research spotlight as they hold great potential for future spintronic and magnetic memory devices. The use of electrochemistry in voltage-controlled magnetism, dubbed magneto-ionics,[1] promises a superior energy efficiency compared to many conventional mechanisms. Here, we present a versatile magneto-ionic concept based on the hydrogen-loading into [Co/Pd]-based bilayers and multilayer structures with perpendicular anisotropy. We show that the magnetic properties of [Co/Pd] multilayers sensitively depend on the absolute hydrogen concentration in the material and that this concentration can be set electrochemically via the applied voltage.[2] Reversibility and switching speed, as the two main limitations towards practical magneto-ionic devices, can be improved by a targeted multilayer engineering, exploiting synergies with hydrogen electrocatalysis. Funding from DFG-499361641 and ERC-101125178 is acknowledged. [1] Nichterwitz et al. APL Mater. (2021) 030903; [2] Bischoff et al., Adv. Funct. Mater. (2024) 2405323

MA 39.2 Thu 15:30 H19

Magneto-ionic control of coercivity in electrodeposited Ni_xFe_{1-x} films — •Anna Ullrich[1], Florin L. Hambeck[1], Francesca Sgarbi Stabbellini[1,2], and Karin Leistner[1,2] — [1]Institute of Chemistry, TU Chemnitz — [2]Leibniz IFW Dresden

Magneto-ionic effects provide a promising route for low-voltage, non-volatile control of magnetic materials, essential for next-generation, energy-efficient devices. Prior research has mainly focused on iron- or cobalt-based thin films and nanostructures.[1] So far only few works mention magneto-ionic effects for Ni-based alloys,[2,3] which are promising due to their unique magnetic properties. This study systematically investigates the magneto-ionic behavior of electrodeposited Ni_xFe_{1-x} films with thicknesses of (160 ± 30) nm as a material platform to enhance magneto-ionic functionality. Coercivities range from (0.4 ± 0.3) mT in $Ni_{80}Fe_{20}$ (permalloy) to (44.6 ± 0.6) mT in pure Fe, as measured by magneto-optical Kerr effect magnetometry. Magneto-ionic control upon electrolytic gating in 1 M KOH reveals a reduction of coercivity of up to 50 % (e.g., in $Ni_{70}Fe_{30}$) at −1.18 V versus Ag/AgCl. We discuss this modification in the context of a surface oxide reduction reaction, which can modify the domain wall pinning.[4] The observed effects highlight the potential of magneto-ionic Ni-Fe alloys, especially in thicker films, for sensing and actuation applications. [1] M. Nichterwitz et al., APL Mat. 2021, 9, 030903. [2] D. Murray et al., ACS Appl. Mater. Interf. 2021, 13, 38916. [3] De h-Ora et al., Zenodo 2021, doi:10.5281/zenodo.5769775. [4] J. Zehner et al., Adv. Electron. Mater. 2020, 6, 2000406.

MA 39.3 Thu 15:45 H19

Structural, magnetic and electrical properties of oxygen-deficient $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ thin films — Suqin He[1,2,3], •Oleg Petracic[1], Valeria Lauter[4], Lei Cao[1,5], Yunxia Zhou[5], Moritz Weber[2,3], Jürgen Schubert[6], Omar Concepción[6], Regina Dittmann[2,3], Rainer Waser[2,3], Thomas Brückel[1,3], and Felix Gunkel[2,3] — [1]JCNS-2, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — [2]PGI-7, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — [3]JARA-FIT, RWTH Aachen University, 52056 Aachen, Germany — [4]Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [5]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [6]PGI-9, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

In $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ (LSCO) the gradual oxygen release triggers a phase transition from the initial ferromagnetic perovskite to an oxygen vacancy layered antiferromagnetic brownmillerite structure. We have studied LSCO thin films fabricated by pulsed laser deposition. In situ x-ray diffraction and polarized neutron diffraction reveals the topotactic phase transition of the LSCO thin films, which can be attributed to the release of oxygen and ultimately the transition

to a coherently ordered BM phase. By comparing the magnetic and electronic properties of the sample at different oxygen deficient states, we demonstrate that the magnetic and electronic transitions are apart from the structural phase transition. S. He, O. Petracic, V. Lauter, L. Cao, Y. Zhou, M. L. Weber, J. Schubert, O. Concepción, R. Dittmann, R. Waser, T. Brückel, F. Gunkel, Adv. Funct. Mater. 2024, 34, 2313208.

MA 39.4 Thu 16:00 H19

Double Exchange Bias (EB) Effects in IrMn/CoFe/IrMn Systems — •Arne Vereijken, Varun Vanakalapu, Rico Huhnstock, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, Germany

The EB effect, characterized as an unidirectional anisotropy in a ferromagnet (FM) coupled to an antiferromagnet (AFM) through a shared interface[1], is utilized in Lab-on-Chip (LOC) systems[2], among other technologies. In LOC systems, it is combined with ion bombardment induced magnetic patterning (IBMP) to engineer magnetic stray field landscapes (MFLs)[2]. This work demonstrates that adding a second EB interface to the same FM adds a degree of freedom for tailoring MFLs, achieving stronger and steeper stray field gradients beneficial for LOC applications. Whether the two EBs are independent of each other, particularly when aligned parallel or at an angle, poses an intriguing question. Investigations using vibrating sample magnetometry and magneto-optical Kerr effect measurements and comparisons with advanced EB models tailored for polycrystalline systems and the specific measurement conditions[3], reveal that the EB strength in the employed Ir17Mn83/Co70Fe30/Ir17Mn83 systems slightly exceeds twice that of single EB systems. This is attributed to additive, mostly independent EBs, making the second EB a great candidate for refining MFL engineering. [1] Meiklejohn, W. H. et al. (1956). Phys. Rev. 102, 1413 [2] Holzinger, D. et al. (2015). ACS Nano 9 (7), 7323-7331 [3] Merkel, M. et al. (2022). Phys. Rev. B 106, 014403

MA 39.5 Thu 16:15 H19

Layer-resolved Vector Magnetometry using Generalized Magneto-optical Ellipsometry — •Carmen Martín Valderrama, Irene Prieto, Mikel Quintana, and Andreas Berger — CIC nanoGUNE BRTA, E-20018 Donostia-San Sebastián, Spain

For a detailed and quantitatively precise understanding of magnetic multilayers it is crucially important to determine their spatial magnetization configurations, particularly along the depth of their structures. Here, we demonstrate that it is possible to achieve layer-resolved vector magnetometry in nanoscale magnetic multilayer films by means of a single magneto-optical reflection experiment. We designed, fabricated, and measured a set of epitaxial ferromagnetic/non-magnetic/ferromagnetic multilayer samples that exhibit in-plane uniaxial anisotropy and a tunable ferromagnetic interlayer coupling strength through the non-magnetic interlayer. By means of Generalized Magneto-optical Ellipsometry measurements, we obtain the entire optical reflection matrix R of a given sample for each applied field value, which allows us to monitor the field evolution of the magnetization vector for the two ferromagnetic layers independently. Hereby, we observe that the magnetization switching of one layer can trigger a discontinuous change of the magnetization in the second layer even for weak ferromagnetic interlayer coupling. Moreover, we reproduce the obtained behavior using a model of two coupled macrospins, which corroborates even the unexpected aspects of our experimental results and thus reinforces the sensitivity and reliability of our experimental layer-resolved vector magnetometry.

MA 39.6 Thu 16:30 H19

Ferrimagnetic moment arrangement in the Ti-doped Barium hexaferrite revealed by EMCD — •Hitoshi Makino[1], Devendra Singh Negi[2], Ján Rusz[3], Bernd Rellinghaus[1], and Darius Pohl[1] — [1]DCN, TUD Dresden University of Technology — [2]Indian Institute of Technology Jodhpur — [3]Uppsala University

Barium hexaferrite is a well-known ferrimagnetic complex oxide with good durability at high temperatures and in erosive environments. Previous research has indicated that Titanium substitutions can enhance the coercivity at elevated temperatures. Our efforts aim at elucidating the underlying mechanism through measurements of electron energy loss magnetic chiral dichroism (EMCD) in the transmission electron microscope (TEM). We conducted EMCD experiments on three samples with different Titanium concentration ($BaFe_{12-x}Ti_xO_{19}$, x=0, 0.6, 1.0). We have deconvoluted the Fe L-edges as obtained from classical EMCD measurements into different oxidation states of iron ($Fe^{3+} \rightarrow Fe^{2+}$ generated by Titanium-substitution) to observe the changing of magnetic moment arrangement. High resolution EELS mapping revealed, that Ti^{4+} ion substitute mainly for the $4f_2$ site, an atomic site with parallel magnetic Fe moment. The EMCD signal of the Ti-rich sample ($BaFe_{12-x}Ti_xO_{19}$, x=1.0) indicate an antiparallel Fe^{2+} magnetic moment arrangement. This discrepancy will be discussed by using inelastic scattering simulations as well as DFT calculations. A detailed analysis of the underlying measurement errors and the involved limitations of the method will be presented.

MA 39.7 Thu 16:45 H19

Imaging Local Magnetic Moments with Atomic-Scale Electron Vortex Beams via EMCD in $BaFe_{11}TiO_{19}$ — •Darius Pohl[1], Hitoshi Makino[1], Bernd Rellinghaus[1], Rolf Erni[3], Devendra Singh Negi[5], Arthur Ernst[4], and Ján Rusz[2] — [1]DCN, TUD Dresden University of Technology, Dresden, Germany — [2]Uppsala University, Uppsala, Sweden — [3]Empa, Dübendorf, Switzerland — [4]JKU, Lenz, Austria — [5]Indian Institute of Technology Jodhpur

Electron magnetic circular dichroism (EMCD), the electron wave counterpart of X-ray magnetic circular dichroism (XMCD), enables element-specific measurement of spin and orbital magnetic moments with nanometer-scale resolution in transmission electron microscopy. Electron vortex beams (EVBs), recently discovered to carry quantized orbital angular momentum (OAM), are emerging as a promising tool for EMCD measurements, facilitating the analysis of magnetic properties in materials. Since EVBs can be tightly focused to sub-nanometer scales, this approach offers unprecedented potential for quantifying spin and orbital magnetic moments with exceptional spatial resolution. We employ specially designed condenser apertures to produce isolated, atomic-scale EVBs with user-defined OAM. As a proof-of-concept, we demonstrate vortex EMCD measurements on ferrimagnetic barium hexaferrite samples. For the first time, EVB-EMCD achieves the resolution necessary to resolve local ferrimagnetic order. The experimental findings are further corroborated by inelastic scattering simulations and density functional theory (DFT) calculations.

MA 40: Frustrated Magnets II

Time: Thursday 15:00–17:45 Location: H20

MA 40.1 Thu 15:00 H20

Magnetism of rare-earth A2Ir2O7 pyrochlore single crystals — •Filip Hájek[1], Daniel Staško[1], Kristina Vlášková[1], Jiří Kaštil[2], and Milan Klicpera[1] — [1]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics,Ke Karlovu 5, 121 16 Prague 2, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic

The rare-earth A2Ir2O7 pyrochlore iridates form a heavily studied series of materials revealing a plethora of complex properties. Geometrically frustrated lattice, strong spin-orbit coupling comparable to the strength of electron correlations, or f-d exchange between rare-earth and iridium sites lead to, e.g., spin ice state [1], spin liquid [2], topological Mott insulator [3], axion insulator [4] or Weyl semimetal [4,5].

Among the A2Ir2O7 series, we focus on the previously less studied heavy rare-earth members, namely Ho2Ir2O7, Er2Ir2O7, and Lu2Ir2O7 single crystals. In these materials, the Ir sublattice magnetically orders above 100 K, inducing a transition from a (semi-)metal to an insulating state just below the ordering temperature. Our present work is aimed at the magnetism of newly synthesised A2Ir2O7 single crystals, which is discussed in the framework of antiferromagnetic domains and ferromagnetic domain interfaces.

[1] E. Lefrançois et al., Nat. Commun. 8, 209 (2017). [2] M. Kavai et al., Nat. Commun. 12, 1377 (2021). [3] Y. Otsuka et al., Sci. Rep. 11, 20270 (2021). [4] X. Wan et al., Phys. Rev. B 83, 205101 (2011). [5] X. Liu et al., Phys. Rev. Lett. 127, 277204 (2021).

MA 40.2 Thu 15:15 H20

Crystal growth and anisotropic magnetic properties of quasi-one-dimensional zigzag chain antiferromagnet: CaCoP2O7 — •Koushik Chakraborty[1], Aditi Agrawal[1], Isha Isha[1], M. Isobe[2], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Max-Planck-Institut f\"{u}r Festk\"{o}rperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We report crucible free optical floating zone crystal growth and anisotropic magnetic properties of quasi-one-dimensional zigzag chain antiferromagnetic compound CaCoP2O7. In this quasi one-dimensional zigzag chain compound, magnetic lattice is formed by the Co2+ ions. We have characterized the single-crystals and analyzed them by using x-ray and Laue diffraction which reveals single-phase nature and the as grown single-crystals were found of ultra high quality. Magnetic susceptibility and magnetization measurements reveal antiferromagnetic ordering, evidenced by a pronounced downturn in susceptibility below the Neel temperature (TN =6.6 K) and negative Curie-Weiss temperatures (Theta-CW = -39.4 K). Further, we found clear signature of field-induced phase

transition where on application of field AFM order is going to quantum paramagnetic state or maybe liquid phase (which needs further study to confirm).

MA 40.3 Thu 15:30 H20

Ultrasound Investigation of the Magnetic Phase Diagram of Rouaite $Cu_2(OH)_3NO_3$ — •Nikolai Pavlovskii[1], Anton Kulbakov[1], Aswathi M. Chakkingal[1], Justus Grumbach[1], Kaushick K. Parui[1], Ulrike Stockert[1], Maxim Avdeev[2,3], Ramender Kumar[4], Issei Niwata[4], Ellen Häussler[1], Roman Gumeniuk[5], Ross J. Stewart[6], Vladimir Pomjakushin[7], Sergey Granovsky[1], Mathias Doerr[1], Elena Hassinger[1], Sergei Zherlitsyn[8], Andreas Hauspurg[8], Yoshihiko Ihara[4], Darren C. Peets[1], and Dmytro Inosov[1] — [1]TU Dresden, Germany — [2]ANSTO, Sydney, Australia — [3]University of Sydney, Australia — [4]Hokkaido University, Japan — [5]TU Bergakademie Freiberg, Germany — [6]ISIS, United Kingdom — [7]PSI, Villigen, Switzerland — [8]HZDR, Dresden, Germany

Rouaite, $Cu_2(OH)_3NO_3$, is a low-dimensional quantum magnet with alternating ferromagnetic and antiferromagnetic spin chains. Its magnetic phase diagram has been studied using techniques such as magnetization and specific heat, revealing field-induced transitions. This work focuses on ultrasonic investigations, which uncover the coupling between magnetic and elastic properties. New results under hydrostatic pressure further demonstrate the tunability of the magnetic phases, highlighting the material's sensitivity to lattice modifications.

MA 40.4 Thu 15:45 H20

Emergent degeneracies in weakly coupled sawtooth chains: the case of bobkingite — •P. Peter Stavropoulos[1], Aleksandar Razpopov[1], Harrison LaBollita[2], Antia S. Botana[3], Michael R. Norman[4], and Roser Valentí[1] — [1]Goethe University, Frankfurt, Germany — [2]Flatiron Institute, New York, USA — [3]Arizona State University, Tempe, USA — [4]Argonne National Laboratory, Lemont, USA

The sawtooth chain, otherwise known as the Δ chain, has a long history as a minimal model of frustrated magnetism, serving as a realization of Shastry-Sutherland type solitons. While many material candidates, like delafossite, euchroit, atacamite, as well as fluorides, have been investigated, they leave much to be desired in the way of the ideal sawtooth chain. Here we present a proposal for revisiting a copper hydrate, bobkingite. Using ab initio methods we estimate the magnetic exchanges between copper sites, and find a spin model consisting of nearly ideal sawtooth chains, weakly coupled to its neighbors. We analyze the classical model of the coupled sawtooth chains, revealing emergent system size scaling degeneracies.

MA 40.5 Thu 16:00 H20

Trigonal distortion in the Kitaev candidate honeycomb magnet BaCo2(AsO4)2 — •M.M. Ferreira Carvalho[1,2], S. Roessler[1], Z. Hu[1], C.F. Chang[1], S. M. Valvidares[3], P. Gargiani[3], M. W. Haverkort[4], P. K. Mukharjee[5], P. Gegenwart[5], A. A. Tsirlin[6], and L.H. Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids,Dresden — [2]Institute of Physics II, University of Cologne — [3]ALBA Synchrotron Light Source, Barcelona, Spain — [4]Institute for theoretical physics, Heidelberg University — [5]Lehrstuhl für Experimentalphysik VI, Universität Augsburg — [6]Felix Bloch Institute for Solid-State Physics, University of Leipzig

We conducted X-ray linear dichroism (XLD) and magnetic circular dichroism (XMCD) measurements on single crystals of the Kitaev candidate honeycomb lattice compound BaCo2(AsO4)2. The measurements employed the bulk sensitive inverse partial fluorescence yield technique, which is ideal for acquiring reliable X-ray absorption spectra from highly insulating samples , enabling precise quantitative analysis. Our experimental results revealed a significant LD signal, indicating strong trigonal distortion in the CoO6 octahedra in BaCo2(AsO4)2. We performed a detailed analysis of the experimental XAS and XMCD spectra using a full-multiplet cluster model within the configuration interaction approach. This analysis indicated that the hole density is predominantly localized in the a1g orbital. Through XMCD sum rules and theoretical calculations, we quantified both the spin and orbital magnetic moments.

MA 40.6 Thu 16:15 H20

Single crystal growth and anisotropic magnetic properties of honeycomb quantum antiferromagnets: Ba2A(PO4)2 (A = Ni, Co, Mn) — •Aditi Agrawal[1], Koushik Chakraborty[1], Isha Isha[1], M. Isobe[2], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Max-Planck-Institut f\"{u}r Festk\"{o}rperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The magnetic framework (monoclinic-lattice) of the title compounds are composed of the honeycomb-lattice. We present a study of high-quality Ba2A(PO4)2 (A = Ni, Co, Mn) optically floating zone grown single crystals. Sharp anomalies were found in the thermodynamic measurements. The anomalies corresponding to the long-range-ordering (LRO) for all three single-crystals of honeycomb family were evident just below 5 K, reveals a long-range antiferromagnetic order in these single-crystalline samples. The dc-susceptibilities for in-plane and out-of-plane magnetic fields are strongly anisotropic. Our Curie-Weiss analysis for Ni, Co, and Mn suggest strong orbital magnetism but it was found significant for Co2+ case, as it is known due to its Kramers' degeneracy nature. Further, on application of external magnetic field, all compound shows spin-flop transition at moderate field. However, Ba2Co(PO4)2 is interestingly driven to another ordered phase due to the field-induced transition via a field tuned quantum critical point which is expected close to the critical field of Bc ~ 6.5 T, as evident from our phase boundaries analysis on in B-T plane.

15 min. break

MA 40.7 Thu 16:45 H20

Modelling thermal transport in spiral magnets — •Margherita Parodi[1,2] and Sergey Artyukhin[1] — [1]Italian Institute of Technology, Genova — [2]University of Genova, Italy

Magnetic memory and logic devices, including prospective ones based on skyrmions, inevitably produce heat. Thus, controlling heat flow is essential for their performance. Here we study magnon contribution to thermal conductivity in the most basic non-collinear magnet with a spin spiral ground state. Non-collinearity leads to anharmonic terms, resulting in magnon fusion and decay processes. These processes determine the magnon lifetime which can be used to estimate thermal conductivity in single mode approximation. However, by solving the full Boltzmann equation numerically, we find much higher thermal conductivity. This signifies that heat is carried not by individual magnons but by their linear combinations, called relaxons [1]. The thermal conductivity is found to be increasing with the diminishing twist angle, consistent with recent experiments [2]. The results pave the path to understanding magnetic thermal transport in other non-collinear magnets.

References: [1] A. Cepellotti and N. Marzari, Phys. Rev. X 6, 041013 (2016) [2] F. Sekiguchi et al., Nat. Commun. 13, 3212 (2022)

MA 40.8 Thu 17:00 H20

Pressure-tuning $Na_3Co_2SbO_6$ in the Kitaev Quantum Spin Liquid state — •Steven Gebel[1], Swarnamayee Mishra[1], Martin Sundermann[2], Marein Rahn[3], and Jochen Geck[1] — [1]Institute of Solid State and Materials Physics, Technische Universität Dresden, Haeckelstr. 3, 01069 Dresden, Germany — [2]PETRA III, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [3]Center for Electronic Correlations and Magnetism, University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

Honeycomb cobaltates with Co^{2+} ($3d^7$) ions have been proposed as materials that can host Kitaev's quantum spin liquid state (QSL). Specifically, $Na_3Co_2SbO_6$ has been predicted to exhibit a Kitaev QSL upon reduction of the trigonal ligand and crystal field splitting, which in turn might be possible via the elastic tuning of the lattice structure. This compound hosts edge-sharing CoO_6 octahedra and exhibits antiferromagnetic (AFM) zig-zag ordering below 7 K, reminiscent of other well-known QSL-candidate, α-$RuCl_3$. In this study, a combination of x-ray diffraction (XRD) and spectroscopy (NIXS) in diamond anvil cells (DACs) is used to establish the pressure dependence of the lattice structure and its effect on the electronic 3d-shell. The pressure dependent Co L-edge spectra are compared to multiplet calculations based on the structural data obtained from refinements of the XRD data. Combining elastic tuning of the lattice structure with XRD, Co L-edge spectra and core-level-spectroscopy simulations, is a very promising approach to confirm whether honeycomb cobaltates can be driven into the Kitaev QSL state.

MA 40.9 Thu 17:15 H20

Easy-axis Heisenberg model on the triangular lattice: from supersolid to gapped solid — •Martin Ulaga[1], Jure Kokalj[2,3], Takami Tohyama[4], and Peter Prelovšek[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Faculty of Civil and Geodetic Engineering, University of Ljubljana, Ljubljana, Slovenia — [3]Department of Applied Physics, Tokyo University of Science, Tokyo, Japan — [4]Jožef Stefan Institute, Ljubljana, Slovenia

We investigate the easy-axis Heisenberg model on the triangular lattice by numerically studying excitations and the dynamical spin structure factor $S^{\mu\mu}(\mathbf{q},\omega)$. Results are analyzed within the supersolid scenario, characterized by the translation-symmetry-breaking parameter m_z and the supersolid off-diagonal order parameter $m_\perp$. We find very robust $m_z > 0$ in the whole easy-axis anisotropy regime $\alpha = J_\perp/J_z > 0$, even enhanced by the magnetic field $h > 0$. Results also support $m_\perp > 0$ for intermediate $\alpha < 1$ and $h > 0$. Still, at small $\alpha \lesssim 0.2$, relevant for recent experiments on the magnetic material $K_2Co(SeO_3)_2$, we find at $h = 0$ rather vanishing $m_\perp \sim 0$, consistent with numerical evidence of a finite magnon excitation gap

MA 40.10 Thu 17:30 H20

Localized Magnons in the Generalized Model of the Sawtooth Chain with Dzyaloshinskii-Moriya Interactions — •Vadim Ohanyan[1,2], Johannes Richter[3,4], Michael Sekania[5,6], Marcus Kollar[7], and Lucas Giambattista[7] — [1]Laboratory of Theoretical Physics, Yerevan State University, 1 Alex Manoogian, 0025 Yerevan, Armenia — [2]CANDLE, Synchrotron Re-

search Institute, 31 Acharyan Str., 0040 Yerevan, Armenia — [3]Institut für Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany — [4]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany — [5]Reichenzentrum, University of Augsburg, 86135 Augsburg, Germany — [6]Center for Condensed Matter Theory and Quantum Computations, Ilia State University, 0162, Tbilisi, Georgia — [7]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We consider a generalized model of a spin-S sawtooth chain with three distinct exchange couplings and Dzyaloshinskii-Moriya (DM) interactions. The primary focus of our research is on various scenarios for magnonic flat-band formation and the corresponding properties of localized magnons. A general flat-band constraint is derived, which, due to the large number of parameters in the model, allows for a broad diversity of flat-band scenarios. We provide a detailed analysis of different solutions to the flat-band constraint, construct the associated localized magnon states, and study the properties of the one-magnon spectrum.

MA 41: Poster III

Time: Thursday 15:00–17:30 Location: P3

MA 41.1 Thu 15:00 P3

Electrical coupling of superparamagnetic tunnel junctions mediated by spin-transfer-torques — •Sinan Shu[1], Leo Schnitzspan[1,2], Mathias Kläui[1,2], and Gerhard Jakob[1,2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, 55122 Mainz, Germany — [2]Max Planck Graduate Center Mainz, 55122 Mainz, Germany

Superparamagnetic tunnel junctions (SMTJs) have garnered significant interest as potential building blocks for neuromorphic computing due to their unique stochastic switching behavior, driven by thermal excitations. This work investigates the impact of electrical coupling on the stochastic dynamics of two in-plane magnetized SMTJs, combining experimental measurements with simulation studies. The coupling mechanism, enabled by spin-transfer torque, modulates the state probability of each SMTJ and influences their cross-correlation. By analyzing time-lagged cross-correlation, we determine the strength and direction of the coupling, revealing that high positive voltages induce the strongest coupling effect. Furthermore, we demonstrate voltage-tunable state probabilities and coupling control. Our findings highlight the emergence of similarity and dissimilarity effects in the state probability transfer curves of coupled SMTJs [1]. These results not only provide new insights into the interplay between spin-transfer torque and stochastic behavior but also underline the potential of SMTJs for applications in energy-efficient neuromorphic computing.

[1] L. Schnitzspan, M. Kläui, G. Jakob, Appl. Phys. Lett. 123, 232403 (2023).

MA 41.2 Thu 15:00 P3

Self-ordered colloid of surfactant-free hard ferromagnetic hexaferrite nanoplatelets: SAXS study — •Andrei Chumakov[1], Matthias Schwartzkopf[1], and Dirk Menzel[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Technische Universität Braunschweig, Braunschweig

A novel type of stable magnetic colloids based on hard magnetic SrFe12O19 particles stabilized by electrical charge and dispersed in water was studied as an object of investigation. The colloidal single crystalline nanoparticles possess a plate-like shape with a mean lateral size of about 50 nm and thickness of 5 nm. Each particle carries a large permanent magnetic moment M and exhibits the highest intrinsic coercivity field HC values of about 0.4 T. The magnetic properties of a ferromagnetic colloid exhibit a minimal magnitude of the coercive force of the order of several Oe., which allows the change of particle's orientation easily under the action of an external magnetic field. Depending on the concentration, the nanoparticle can exist in the water media in the free 'gas', concentrated liquid crystal, and super concentrated 'solid' phases. Structural ordering in the concentrated magnetic colloids of nanoparticles was investigated by SAXS, SEM, and SQUID techniques. It was revealed that the self and externally-induced liquid crystal phase consists of stacks of magnetic nanoplatelets, which can be ordered to nematic or similar phases by the external magnetic field. Various methods for creating a concentrated liquid crystalline phase are considered. The features of interaction within alternating and constant magnetic fields were studied.

MA 41.3 Thu 15:00 P3

Current Induced Markov State Modeling with Skyrmions in Geometrical Confinements — Thomas Brian Winkler[1], Grischa Beneke[2], •Yuean Zhou[2], Johan Mentink[1], and Mathias Kläui[2] — [1]Radboud University, Institute for Molecules and Materials, Netherlands — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

Magnetic skyrmion in geometrical confinements have recently gained attention as a platform for neuromorphic computing for instance for Brownian Reservoir Computing [1, 2]. Despite significant progress with coarse-grained particle-based modeling of the stochastic dynamics of skyrmion [3], the interplay between stochasticity and device defects remains underexplored. Here, we extract the stochastic transitions of skyrmion between pinning sites using a simple Markov state framework. The resulting Markov state model enables system behavior prediction based on the effective energy landscape of the device. The time step for Markov state evolution is significantly faster than traditional simulations, which makes the system well-suited for leveraging the digital twin for predicting experimental outcomes and evaluating reservoir metrics. We also aim to implement energy-efficient Markov chain Monte Carlo algorithms in-materio.

[1] K. Raab et al., Nat. Commun. 13 (1), 6982 (2022)
[2] G. Beneke et al., Nat. Commun. 15 (1), 8103 (2024)
[3] T. B. Winkler et al., Appl. Phys. Lett. 124 (2), 022403 (2024)

MA 41.4 Thu 15:00 P3

Statistical Tests for True-Random-Number Generation with Superparamagnetic Tunnel Junctions — •Robin Tietgen[1], Leo Schnitzspan[1], Mathias Kläui[1,2], and Gerhard Jakob[1] — [1]Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany — [2]Max Planck Graduate Center Mainz, Mainz 55122, Germany

Superparamagnetic tunnel junctions (SMTJs) change their magnetoresistance due to switching of the ferromagnetic free layer by thermal excitations. This property of the SMTJ can be utilized to design a random number generator (RNG). Evaluating RNG output signals with statistical tests such as the NIST Statistical Test Suite (NIST STS) [1] provides a measure for the randomness quality and therefore the quality of the RNG itself. This quality assessment is crucial when deciding whether a (pseudo) RNG is suitable for a specific application.

We show nanosecond timescale random telegraph noise (RTN) generated by SMTJs with encryption-quality randomness [2].

Fast and high quality RNGs facilitate upcoming unconventional computing techniques such as probabilistic computing and machine learning with noise-based learning algorithms. For these applications SMTJs are promising true RNGs, offering very fast RTN, ultra-low power consumption and excellent scalability.

[1] L. Bassham et al., NIST SP 800-22 Rev 1a (2010)
[2] L. Schnitzspan et al., Phys. Rev. Appl. **20**, 024002 (2023)

MA 41.5 Thu 15:00 P3

Local spin textures stabilised by geometrically-induced strain in 2D magnet Fe3GeTe2 — •Yuhan Sun[1], Max Birch[2], Simone Finizio[3,5], Lukas Powalla[1], Sayooj Satheesh[1], Eberhard Goering[1], Bettina Lotsch[1], Klaus Kern[1], Alexander Holleitner[4], Markus Weigand[5], Sebastian Wintz[5], and Marko Burghard[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]RIKEN Center for Emergent Matter Science, Wako 351-0198, Japan — [3]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]Walter Schottky Institute and Physics Department, Technical University of Munich, 85748 Garching, Germany — [5]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut Nanospektroskopie, 12489 Berlin, Germany

Two-dimensional (2D) van der Waals ferromagnets have emerged as promising platforms for next-generation electronic and spintronic devices. However, achieving precise local control over magnetic domains and spin textures in these materials remains a significant challenge. Here, we demonstrate nanoscale manipulation of magnetism in the 2D ferromagnet Fe3GeTe2 (FGT) using geometrically-induced strain fields. Employing high-resolution scanning transmission X-ray microscopy, we directly visualize the impact of spatially varying uniaxial and shear strain profiles on the magnetic order of FGT sheets stamped onto nanopillar arrays. We observe that a strain of less than 0.5% locally elevates the Curie temperature of FGT by 10 K and stabilizes magnetic textures near the pillar corners.

MA 41.6 Thu 15:00 P3

Harnessing Van der Waals $CrPS_4$ and Surface Oxides for Nonmonotonic Exchange Bias in Fe_3GeTe_2 heterostructures — Aravind Puthirath Balan[1], Aditya Kumar[1], •Sadeed Hameed[1], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Centre for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Due to their atomically flat interfaces, two-dimensional van der Waals (vdW) heterostructures serve as the ideal platform to study interfacial effects like exchange bias. In this study, exchange bias in a vdW heterostructure composed of the antiferromagnetic material $CrPS_4$ and the ferromagnetic material Fe_3GeTe_2 (FGT) with a naturally oxidized surface layer (O-FGT) is investigated by per-

forming Anomalous Hall measurements. The observed exchange bias in this heterostructure exhibits a distinct and non-monotonic trend as a function of temperature below 140 K, which is attributed to the presence of ferrimagnetic Fe_3O_4 in the surface oxide layer whose induced exchange bias is modulated by the presence of the antiferromagnetic $CrPS_4$ layer. These findings highlight the multifaceted nature of exchange bias in van der Waals heterostructures and their potential for tailored manipulation and control of material properties.

[1] Puthirath Balan, A. et al., *ACS Nano* **18**, 8383-8391 (2024).

MA 41.7 Thu 15:00 P3

Exploring spin-lattice coupling in the Van-der-Waals Antiferromagnet FePS3 — •David Gutnikov, Fabian Mertens, David Mönkebüscher, Richard Leven, Sophie Bork, Umut Parlak, and Mirko Cinchetti — Department of Physics, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Femtosecond laser pulses drive coherent ultrafast lattice dynamics and hybridized phonon-magnon interactions in the antiferromagnetic van der Waals semiconductor $FePS_3$. This study investigates the coupling between lattice vibrations and the magnetic system by examining the effects of excitation photon energy, sample temperature, and applied magnetic field on their dynamic interplay. Building on our previous findings [1], we conducted additional femtosecond white-light transient absorption measurements. In addition to the previously reported 3.2 THz coherent phonon mode — whose amplitude diminishes near the Néel temperature and vanishes in the paramagnetic phase — we confirmed its strong hybridization with a magnon under an external magnetic field, resulting in a coupled phonon-magnon mode that underscores the rich magneto-elastic interactions in this material. Beyond this, we identified a previously hidden phonon mode at 7.5 THz and shear oscillations around 20 GHz. These findings provide deeper insights into the spin-lattice coupling in $FePS_3$ and open new avenues for controlling THz magnonic dynamics in van der Waals antiferromagnets, with significant implications for advancing two-dimensional spintronic technologies.

[1] F. Mertens et al, Adv. Mater. 35, 2208355 (2023).

MA 41.8 Thu 15:00 P3

Pauli-Equation on Riemannian Manifolds — •Johann Posanski, Benjamin Schwager, and Jamal Berakdar — Marthin-Luther-Universität Halle-Wittenberg Institut für Physik

Describing the behavior of quantum systems under geometric constraints is of relevance both for research in the foundations of physics and in applied fields, such as the development of designer materials. Implementing the restriction of a quantum particle to a Riemannian manifold with an explicit confining potential provides an effective description of the reduced quantum dynamics and implies a potential-like term dependent on the geometric invariants of the space. Expanding this formalism to spin-1/2 particles, such as electrons, is an active area of research. In this work, the dynamics of non-relativistic spin-1/2 particles on a two-dimensional Riemannian manifold embedded in three-dimensional Euclidean space are derived. We find that the spin degree of freedom is unaffected by real-space constraints and the tangent Pauli equation fully describes the spinor dynamics when the whole structure is exposed to an electromagnetic field. The Zeeman energy is found to be unaffected by the confinement and remains gauge-invariant.

MA 41.9 Thu 15:00 P3

Interplay of valley and spin at the interface of $MnPS_3|WS_2$ heterostructure — •Purba Dutta and Nirmal Ganguli — Indian Institute of Science Education and Research Bhopal, MP, India

This work is focused on the proximity-induced effects of the $MnPS_3|WS_2$ heterostructure, particularly on the change of valley and spin splitting in some high symmetry points under the effect of SOC, exhibits a unique interplay of electronic, spintronic, and valleytronic properties due to its type-II band alignment and strong spin-orbit coupling. This heterostructure facilitates efficient charge separation, driven by the staggered band alignment, making it ideal for optoelectronic applications such as spin-polarized photodetectors. The magnetic proximity effect from MnPS* induces a tunable U-dependent Rashba spin-splitting at the interface, where the magnitude of the Rashba effect can be controlled by the on-site Coulomb interaction parameter (U). This coupling enables robust control over spin texture and spin-dependent transport. Moreover, circularly polarized light selectively excites carriers in the distinct valleys of WS_2, leading to enhanced valley polarization, further modulated by the magnetic exchange interaction from $MnPS_3$. This synergy between Rashba like effect-induced spin textures and valley polarization creates a platform for multifunctional optospintronic devices, offering avenues for tunable spin and valley-selective photodetection, spin filters. The Interplay of valley and spin at the interface of $MnPS_3|WS_2$ heterostructure heterostructure thus provides a versatile framework for advancing spintronic and valleytronic technologies.

MA 41.10 Thu 15:00 P3

Manipulating the sign of the interlayer exchange coupling — Nathan Walker[1] and •George Browne[2] — [1]The Open University, Milton Keynes, UK — [2]The Open University, Milton Keynes, UK

We demonstrate, using computer simulations and a non-equilibrium Greens function approach, that the sign of the out-of-equilibrium interlayer exchange coupling (ooeIEC) changes in the presence of an external bias. The system consists of a double barrier connected to an exchange coupled ferromagnetic trilayer. We find a strongly non-linear dependence of the spin current on voltage which results in the exchange coupled tri-layer switching between parallel and antiparallel configurations. Our results are in excellent agreement with earlier theoretical calculations, which predict an approximately 2π topological phase change of the (equilibrium) IEC. We believe that this could act as an energy efficient mechanism for magnetic switching which does not rely on spin-transfer torque (STT). There are potential applications to magnetoresistive random-access memory (MRAM), one of the principal contenders for a universal memory.

MA 41.11 Thu 15:00 P3

Enhancing the ultrafast THz emission in spintronic emitters via interface engineering — •Krishna Rani Sahoo[1], David Stein[2], Jannis Bensmann[1], Alexander Heise[2], Robert Schmidt[1], Steffen Michaelis de Vasconcellos[1], Manfred Albrecht[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Physics, University of Augsburg, Universitätsstr. 1 Nord, 86159 Augsburg, Germany

Ultrafast THz spintronic emitters are based on the generation of THz radiation due to spin-to-charge conversion in magnetic (M) and nonmagnetic (NM) bilayer stacks. The development of THz spintronic emitters focuses on enhancing their intensity, manipulating the THz signal, and exploring potential applications. To improve the performance of THz spintronic emitters, it is important to choose suitable material combinations (M/NM) and tailor the interface between the M and NM layers. In this study, we focus on engineering the interface of archetypical Fe/Pt THz spintronic emitters via irradiation with foreign atoms. Indeed, we find that the THz emission can be substantially increased by the implantation of ions at the Fe/Pt interface. Our result paves the way for efficient low-cost ultrafast THz spintronic emitters based on thin metal films.

MA 41.12 Thu 15:00 P3

Exploring the Coupling of Broadband Terahertz Dipoles to Metasurfaces — •Daniel Geyer[1], Rieke von Seggern[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Terahertz (THz) spectroscopy has emerged as a powerful tool for accessing low-energy excitations in matter, offering direct insights into fundamental material properties that govern electronic, thermal, and magnetic behaviors. In addition to large-area THz emission spectroscopy, a strongly confined THz source can be employed to locally map a material's response.

In this work, we explore the implementations of ultrathin THz sources coupled to plasmonic structures. Firstly, we demonstrate the microscale mapping of the coupling strength between resonator structures and localized terahertz dipoles on a patterned spintronic emitter [1]. In addition, we investigate the THz response of near-field-coupled topological metasurfaces based on the Su-Schrieffer-Heeger (SSH) model [2]. Lastly, we discuss the application of novel THz sources based on two-dimensional van-der-Waals materials.

[1] Rathje et al., ACS Photonics 10, 3435 (2023)
[2] Moritake et al., Nanophotonics 11, 2183 (2022)

MA 41.13 Thu 15:00 P3

Enhancement of spintronic terahertz frequency conversion efficiency via grating structures — •Hatice Nur Koyun[1], Ruslan Salikhov[1], Ciaran Fowley[1], Jürgen Lindner[1], Stephan Winnerl[1], Artur Erbe[1,2], Manfred Helm[1,2], Jürgen Fassbender[1,2], and Sergey Kovalev[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062, Dresden, Germany — [3]Technische Universität Dortmund, 44227, Dortmund, Germany

Spintronic terahertz (THz) frequency conversion in ferromagnet/heavy-metal heterostructures has the potential to develop spintronic THz emitters for the high-speed communication and data processing units. Applying the ultrafast demagnetization gives rise to spintronic THz frequency conversion with the appearance of THz second harmonic generation (TSHG). In the case of optimizing the potential for the spintronic THz frequency conversion, the limitations of low power efficiency can be overcome by using subwavelength structures such as an arrays of slits. In this study, we explore a pathway for efficiency enhancement by utilizing periodic gold arrays with a grating period smaller than the THz wavelength, which results in increased local THz fields. By varying the gap and width of the gold arrays, we find that the TSHG power efficiency increases with decreasing gap size of the grating. Furthermore, we demonstrate the potential for cavity enhancement, which can improve and control THz emission from spin-

tronic THz emitters by placing a gold periodic array on the backside of a quartz glass substrate.

MA 41.14 Thu 15:00 P3

Terahertz field induced spin wave excitation in thin ferromagnetic metals — •Sergei Ovcharenko, Hoppe Wolfgang, Alexey Melnikov, and Georg Woltersdorf — Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, Halle 06120, Germany

In the novel concepts of charge-less data processing technologies spin waves are proposed as a carriers of data. One of the ways to excite and study the properties of spin waves on the picosecond time scale is to use the laser pulsed excitation and magneto optical probe. Optical excitation of spin waves in ferromagnetic metals has now been demonstrated using a short pulse of spin current leading to spin torque localized at the interfaces of a ferromagnetic and nonmagnetic metal, both with optical [1] and Terahertz (THz) excitation [2]. The use of short optical pulses in the THz spectral range to induce spin currents and generate spin-orbit torque (SOT) offers undeniable advantages: the SOT is linearly proportional to the THz field amplitude, the excitation and spin-wave frequencies can be well-matched, and minimal heating occurs due to the low excitation energy.

In our work, we demonstrate the optical excitation of spin waves in thin layers of ferromagnetic metals using the THz pump-optical probe technique, with a spintronic emitter as the source of THz radiation. We investigate the dependence of the excited modes on the thickness of the ferromagnetic metal. [1] Brandt Liane et al. Physical Review B 104.9 (2021): 094415. [2] Salikhov Ruslan et al. Nature Physics 19.4 (2023): 529-535.

MA 41.15 Thu 15:00 P3

Wide-field magnetic microscopy of two-dimensional magnetic materials with chiral overlayers — •Buddhika Hondamuni[1], Nir Bar-Gill[3], Angela Wittmann[2], and Dmitry Budker[1] — [1]Helmholtz Institute Mainz, Staudingerweg 18, 55128 Mainz, Germany — [2]Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany — [3]Hebrew University, Jerusellem, Israel

The objective is to investigate the interplay between magnetic domain structures (or skyrmions) in samples with Perpendicular Magnetic Anisotropy (PMA) and chiral polypeptides. Using Nitrogen Vacancy (NV) center-based continuous wave Optically Detected Magnetic Resonance (cw-ODMR) for stray magnetic field imaging in wide-field with a spatial resolution of $\sim$ 0.8 μm and magnetometric sensitivity up to sub-μT/$\sqrt{\text{Hz}}$ range within a field of view (FOV) of approximately 60×60 μm^2, we study how chiral molecules influence magnetic textures including magnetic domain pinning and coercive force changes. The Chirality Induced Spin Selectivity (CISS) effect provides a unique mechanism for manipulating spin orientations through molecular symmetry, offering the potential to control and enhance magnetic domain behavior. This NV-based imaging technique paves the way for advanced magnetic materials and spintronic devices by enabling precise nanoscale analysis of magnetic textures. This work is supported by the Carl Zeiss Stiftung and conducted in collaboration with the Hebrew University of Jerusalem, Israel.

MA 41.16 Thu 15:00 P3

Investigating Magnetic Material Parameters Using Latent Measures — •Kübra Kalkan, Omer Fetai, Ross Knapman, Janine Graser, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Magnetic materials are vital in shaping modern technology [1]. Inhomogeneities, however, influence material properties and potentially degrade their performance.

In this study, we focus on quantifying how the local and global dynamic behaviour of the magnetic material is influenced by local material parameters. We apply latent inference methods [2,3] on simulated micromagnetic data to unveil the memory and stochastic properties of the magnetic material. A deep understanding of inhomogeneities is key to enhancing the properties of magnetic materials.

[1] O. Gutfleisch et al., Adv. Mater., 23, 821 (2011).
[2] D. R. Rodriges et al., iScience, 24, 3 (2021).
[3] I. Horenko et al., Comm. App. Math. and Comp. Sci., 16, 2 (2021)

MA 41.17 Thu 15:00 P3

Modeling the magneto-optical Kerr effect in three-dimensional magnetic microstructures — •Florian Ott, Christian Janzen, Bhavadip Rakholiya, Rico Huhnstock, and Arno Ehresmann — Institute of Physics, University of Kassel, Germany

Topographically-elevated magnetic microstructures with complex three-dimensional geometries are promising for the discovery and study of novel magnetic effects [1]. These microstructures can in principle be magnetically characterized using MOKE-based measurement devices intended for conventional planar material systems, like for instance a Kerr microscope [2]. However, the interpretation of data is not trivial, because the MOKE depends on the local reflection geometry [3]. Theortical calculations have been performed to characterize MOKE in magnetic multilayer systems with arbitrary surface normals. Further, simulations of simple optical setups have been performed to investigate the effects of the associated surface tilt on the optical path of light in the system. It has been found that additional contributions to the change in polarization of light are obtained by considering the image forming optics of the measurement device.

[1] Streubel, R., Tsymbal, E. Y., et. al. *J. Appl. Phys*, 129, 210902. (2021); [2] Janzen, C., Rakholiya, B. B., et. al. "Advancing Kerr-Microscopy Imaging of Three-Dimensional Magnetic Structures", *INTERMAG Short papers*, Rio de Janeiro, Brazil, pp. 1-2. (2024); [3] Soldatov, I., Kolesnikova, V., et. al. *IEEE Magnetics Letters*, 12, pp. 1-4 (2021)

MA 41.18 Thu 15:00 P3

Estimation of the exchange stiffness constant via domain wall widths using magnetic bilayers — •Florian Gossing, Michael Vogel, Dennis Seidler, and Jeffrey McCord — Nanoscale Magnetic Materials, Department of Materials Science, Kiel University, Kaiserstraße 2, 24143 Kiel, Germany

The exchange stiffness constant is a key parameter influencing the energy of (micro)magnetic systems. Magnetooptical measurements on compensating Néel walls of a FeCoSiB double layer structure are performed to determine the exchange stiffness constant. Parasitic magnetooptical effects such as the unavoidable magnetooptical gradient effect are removed by evaluating neighboring domain wall pairs of equal chirality. Corresponding modeled domain wall widths are compared with the experimentally determined widths, taking into account also the thickness dependent magnetooptical sensitivity function. Thus, the integral domain wall widths allow for an estimation of the exchange stiffness constant. The methodology is readily applicable to various thin film magnetic materials. The estimated exchange stiffness constants are compared with those obtained from ferromagnetic resonance measurements.

MA 41.19 Thu 15:00 P3

Observing static and dynamic magnetic textures with nanoscale resolution using NV magnetometry — •Ephraim Spindler[1], Philipp Schwenke[1], Duc Tran[2], Vitaliy Vasyuchka[1], Mathias Kläui[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany

Magnetization and stray field imaging is an essential tool for the characterisation of various magnetic materials and phenomena. Techniques such as Kerr microscopy, magnetic force microscopy or Lorentz transmission electron microscopy are well established and ideal for certain applications. However, their sensitivity, spatial resolution or invasiveness make them unsuitable for other applications. Scanning nitrogen vacancy (NV) magnetometry offers a solution with an excellent combination of high sensitivity and spatial resolution, without distorting the magnetic system of interest. The quantitative nature of the measurement principle allows the determination of the magnetic stray field at the sample surface, allowing the visualisation of magnetic textures even in materials with a very low saturation magnetization, such as canted antiferromagnets like hematite at room temperature. We employ NV magnetometry to study static magnetic textures in bulk hematite samples, and metallic multilayer stacks with perpendicular magnetic anisotropy. An outlook on NV center based spin wave spectroscopy is given.

MA 41.20 Thu 15:00 P3

Magneto-Optical Kerr microscopy of 3D non-planar non-curved magnetic thin films: simulation and experiment — •Christian Janzen, Florian Ott, Bhavadip Bharatbhai Rakholiya, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology,, University of Kassel, Germany

Extending magnetic thin film systems to the third dimension by deposition of magnetic materials onto defined templating structures results in a further degree of freedom to tailor magnetic properties by shape, topology, and chirality [1]. In this work, we present advances in characterizing such 3D systems utilizing conventional magneto-optical Kerr microscopy [2]. By investigating non-planar and non-curved 3D geometries experimentally as well as theoretically, geometric parameters can be manipulated in a systematic way. With this, the magnetic and non-magnetic contributions to the MOKE can be deconvolved. By studying the influence of geometrical parameters that effectively change the initial polarization of the incident light as well as the angle of incidence, we deepen the understanding of Kerr-microscopic signals measured on 3D curved nanomagnetic systems.

[1] G. Gubbiotti et al, "2025 Roadmap on 3D Nano-magnetism" J.Phys.: Condens. Matter in press, 2024

[2] C. Janzen, et al, "Advancing Kerr-Microscopy Imaging of Three-Dimensional Magnetic Structures", INTERMAG Short papers, Rio de Janeiro, Brazil, pp. 1-2, 2024

MA 41.21 Thu 15:00 P3

Exact exchange kernel for spin waves in the spin-polarized homogeneous electron gas — •Michael Neugum, Alexandre Borrameo Alcaïde, and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Spin waves represent an important class of elementary excitations in magnetically ordered materials. *Ab initio* spin-wave calculations for real materials are often based on time-dependent density-functional theory. The crucial ingredient is the so-called exchange-correlation kernel, which incorporates the effects of the Coulomb interaction between the electrons. In general, the kernel is wavevector and frequency dependent, although its exact mathematical form is unknown. Practical implementations typically employ the adiabatic local-density approximation (ALDA), where the kernel is replaced by a simple constant. The results are generally in good qualitative agreement with experimental measurements but sometimes exhibit significant quantitative deviations. In this work, we implement the exact exchange kernel, which is based on a diagrammatic expansion to first order in the Coulomb interaction. We show results for the fully spin-polarized homogeneous electron gas in two and three dimensions. Overall, we observe a substantial discrepancy from the ALDA. In particular, the parabolic component of the dispersion, the spin-wave stiffness, is systematically lower for the exact exchange kernel. While the exact exchange kernel depends both on wavevector and frequency, the most significant effects are due to the wavevector dependence, whereas the frequency dependence may be neglected for practical purposes.

MA 41.22 Thu 15:00 P3

3D Trajectory Tracking of Remote-Controlled Superparamagnetic Particles in Liquid — •Nikolai Weidt, Rico Huhnstock, Yahya Shubbak, and Arno Ehresmann — Department of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

To develop Lab-on-a-chip systems, superparamagnetic particles (SPPs) can be surface-functionalized to specifically bind targeted analytes. A promising strategy for achieving analyte binding and transfer involves the directed transport of SPPs over magnetically stripe-patterned exchange bias layer systems. By precisely analyzing the three-dimensional trajectories of SPPs in this setup, we can detect events of analyte binding. To capture movement in the third dimension, we measure the defocusing of particles that exit the microscope's focal plane during transport steps. In this study, we quantify defocusing by calculating the Tenenbaum gradient (TG) for individual particles. This makes it possible to use a conventional light microscope combined with a piezo-controlled sample holder for 3D Trajectory tracking. Through a calibration process, we derive the z-coordinate of SPPs from the measured TG. The resulting 3D trajectories are validated through numerical simulations of SPP motion.

MA 41.23 Thu 15:00 P3

Experimental system of clinostat and Helmholtz cage for microgravity experiments in zero-value Earth magnetic field — Maciej Malczyk[1], Tomasz Blachowicz[1], and •Andrea Ehrmann[2] — [1]Institute of Physics - Center for Science and Education, Silesian University of Technology, 44-100 Gliwice, Poland — [2]Institute for Technical Energy Systems (ITES), Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences and Arts, 33619 Bielefeld, Germany

Plant cultivation under special conditions, in particular under different magnetic and gravitational conditions, is a relatively new research trend in connection with the development of space technologies. In addition to experiments in space, many studies are carried out under simulated microgravity with the help of a clinostat. Here, a self-designed and built system of coupled devices, a two-axis clinostat and a Helmholtz cage, is presented. The clinostat can, on average, cancel the effective gravitational field, while the correctly mounted Helmholtz cage can cancel the Earth's natural magnetic field [1]. Biological samples, such as plants or microalgae, can be placed in the central part of the system, in the special cultivation sphere. The system makes it possible to control the basic physical parameters and directly observe the growth process visually. The first experimental results of growth tests will be presented.

[1] M. Malczyk, T. Blachowicz, A. Ehrmann, Coupled system of dual-axis clinostat and Helmholtz cage for simulated microgravity experiments, Applied Sciences 14, 9517 (2024)

MA 41.24 Thu 15:00 P3

Finite-temperature DMRG calculations for big spin systems using matrix product states — •Lukas Horstmann and Jürgen Schnack — University of Bielefeld, Bielefeld, Germany

Doing finite-temperature calculations on bigger spin systems is often limited by the size of the Hilbert spaces being too large for algorithms such as exact diagonalisation or finite-temperature Lanczos. In order to work around this problem White proposed a method based on the Density Matrix Renormalization Group (DMRG) in the late 90th which allows the calculation of bigger systems by applying multiple local optimisation steps while truncating the size of the Hilbert space by a large amount without loosing too much information about the system. This method works, but it is slow. Therefore, the whole method was translated into a tensor representation using matrix product states where the full system and its operators are described by a tensor network which allows faster linear algebra calculations [1]. In this contribution we will expand this method to finite-temperature calculations using imaginity-time evolution with TenPy [2] to calculate thermodynamic properties for larger spin systems.

[1] Ulrich Schollwöck, doi: 10.1016/j.aop.2010.09.012

[2] Johannes Hauschild, Frank Pollmann, doi: 10.21468/SciPostPhysLectNotes.5

MA 41.25 Thu 15:00 P3

Probing the magnetic anisotropy in mononuclear $4f$- and $5f$-complexes by high-field/high-frequency EPR — •J. Arneth, B. Beier, and R. Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Germany

The quantitative experimental investigation of magnetic anisotropy in $4f$- and $5f$-compounds remains a challenging task as strong spin-orbit coupling and ligand field effects lead to complex electronic structures while magnetisation measurements often provide only scarce information. Here, we report high-frequency/high-field electron paramagnetic resonance spectroscopy (HF-EPR) studies on mononuclear Er(III) [1,2], U(IV) and U(V) [3] molecular complexes, the former in various ligand coordinations. Our experimental data allow for the direct determination of zero field splittings (ZFS) and effective g-factors of the magnetic ground state and the low-energy excited states. The effect of the ligand fields as well as its relevance for the static and dynamic magnetic properties are discussed.

[1] Arneth et al., submitted

[2] Bazhenova et al., Molecules 26, 6908 (2021)

[3] Lichtenberger et al., J. Am. Chem. Soc. 138, 9033 (2016)

MA 41.26 Thu 15:00 P3

Tunable π-magnetism in carbon-based materials — •Nan Cao[1] and Adam Foster[1,2] — [1]Department of Applied Physics, Aalto University, Helsinki, Finland — [2]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

Carbon-based π-magnetic structures have gained increasing interest for their promising role in spintronics, quantum computing, and advanced magnetic materials. Tailored functionalities in these structures are desired for their diverse applications. This study presents a systematic investigation of the tunability of these structures by incorporating different chemical linkages and doping with diverse heteroatoms. Using density functional theory (DFT) calculations, we explore how different linkage types - such as single, double bonds and aromatic, antiaromatic rings - and the introduction of dopants like nitrogen, boron, and sulfur affect the magnetic properties and electronic configurations of the π-conjugated carbon frameworks. Our results show that specific linkages can enhance magnetic coupling and stability, while heteroatom doping allows for precise control over magnetic moments and bandgap modulation. Furthermore, we identify optimal combinations of linkages and dopants that maximize tunability, offering pathways for designing customized π-magnetic materials with desired properties. These analyses deepen our understanding of structure-property relationships in carbon-based π-magnetic systems and provide a practical strategy for engineering next-generation magnetic materials with customized properties.

MA 41.27 Thu 15:00 P3

Exploring Data Representation Techniques in Deep Learning Models for Determining Ligand Field Parameters of Single-Molecule Magnets — •Preeti Tewatia, Zayan Ahsan Ali, Julius Mutschler, and Oliver Waldmann — Physikalisches Institut, Universitat Freiburg, D-79104 Freiburg, Germany

Single-Molecule Magnets (SMMs) present an exciting frontier in molecular electronics and quantum computing. According to ligand field theory, the single-ion magnetic anisotropies have in general to be characterized by 27 ligand field parameters. However, typical experimental data such as magnetic susceptibility as function of temperature measured on powder samples is pretty featureless, leading to an inverse problem where multiple parameter sets can equally describe the data. To address this challenge, a deep learning approach based on a Variational Autoencoder and an Invertible Neural Network hybrid architecture was employed. The model has been demonstrated before to be capable of handling the above inverse problem. This work focuses on improving the results of the model using data representation and augmentation techniques. For instance, augmenting the input data with simulated susceptibility curves which include experimental errors were found to enhance the robustness of the model with respect to these errors. This approach leads to better performance than conventional fitting techniques.

MA 41.28 Thu 15:00 P3

Inelastic Neutron Scattering on a Family of 3*d*-4*f* Mn_2Ln_2 Single Molecule Magnets — •Vishali Vishali[1], Julius Mutschler[1], Amal Bouraoui[1], Christopher E. Anson[2], Oliver Waldmann[1], and Annie K. Powell[2] — [1]Physikalisches Institut, Universitat Freiburg, D-79104 Freiburg, Germany — [2]Institut of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany

Recent studies in the Single Molecule Magnet (SMM) research area have increasingly focused on 4*f* ions, which offer enhanced magnetic anisotropy and angular momentum, offering new avenues for SMM research. However, the analysis of experimental data remains a challenge for 4*f* based SMMs due to overparametrization, and in the case of Inelastic Neutron Scattering (INS) due to low scattering intensities in pure 4*f* SMMs. A promising approach to overcome these challenges involves expanding the study to heterometallic SMMs incorporating both 3*d* and 4*f* ions. The inclusion of 3*d* ions can enhance INS intensities and improve the quality of INS data. This increases the amount of information on the 4*f* ion properties which can be drawn from the experiment. In this work, high quality INS data of Mn_2Ln_2-square complexes with Ln = Y, Tb, Ho, and Dy are presented. A comprehensive analysis and interpretation of the INS data as well as magnetic data is presented, providing deeper insights into the magnetic behavior of these systems.

MA 41.29 Thu 15:00 P3

Magnetic behavior of cuprate 1/2 spin quantum molecular magnet — •Jakub Šebesta and Dominik Legut — IT4Innovations, VŠB-TU Ostrava, 17.listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

Magnetic materials have long been the subject of scientific inquiry. Nevertheless, the research started to expand its focus beyond aiming at low-dimensional systems. Exploring beyond the traditional bulk magnets could bring innovations thanks to different confinements and the resulting unique physical properties. Apart from layer materials, molecular magnets are significant representatives. In this work, we are discussing an organometallic cuprate 1/2 spin quantum magnet bearing a 2D layered magnetic structure. Combining DFt calculation, an evaluation of magnetic exchange interactions with experimental results, we discuss the complex magnetic structures and the interplay of particular constituent elements in relation to the experimental observation.

MA 41.30 Thu 15:00 P3

Spin Seebeck effect in post-annealed $NiFe_2O_4$ thin films with varying lattice constants — •Fabian Meier, Julian Strassburger, Jan Biedinger, Tapas Samanta, Luana Caron, and Timo Kuschel — Bielefeld University, Germany

The longitudinal spin Seebeck effect (LSSE) in nickel ferrite (NFO) is a widely studied subject in the field of spin caloritronics [1]. Here, the dependence of the LSSE on the lattice constant is investigated in the ferrimagnetic insulator NFO. Two sample series have been fabricated by reactive DC magnetron sputter deposition [2], consisting of 45 nm thick NFO layers grown on $MgAl_2O_4$ substrates and post-annealed in an oxygen atmosphere at different temperatures ranging from 400 °C to 800 °C. Subsequently, the samples are capped by 3 nm of Pt for the spin current detection via the inverse spin Hall effect. The varying lattice constants of NFO, induced by the post-annealing, are analyzed with x-ray diffraction. The LSSE saturation voltage is determined by comparing the LSSE curves with magnetization measurements. Therewith, a linear contribution due to the ordinary Nernst effect in Pt is removed by adjusting the slope of the LSSE curve to match the magnetization curve in the saturation region. Afterwards, the averaged saturation values are determined as a function of the heat flux flowing through the sample. The spin Seebeck coefficient is calculated for each sample and the dependence on the post-annealing temperature, the lattice constants and the unit cell volume is examined.

[1] D. Meier et al., Nat. Commun. 6, 8211 (2015)
[2] C. Klewe et al., J. Appl. Phys. 115, 123903 (2014)

MA 41.31 Thu 15:00 P3

Sliding Through Topology: Unlocking the Tunable Hopf Index — Maria Azhar, •Sandra Chulliparambil Shaju, Ross Knapman, Alessandro Pignedoli, and Karin Everschor-Sitte — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

Recently, there has been growing interest in three-dimensional magnetic structures [1-3], especially regarding their intriguing topological properties and the calculation of their topological index [4]. In this study, we introduce a new approach to determine the Hopf index of magnetic textures, focusing on contributions from both the self-linking and cross-linking of flux tubes [5]. This alternative perspective provides deeper insight into the topological nature of magnetic textures, particularly those exhibiting non-integer topological indices, which we interpret as states of "mixed topology". We emphasize the critical role of the background magnetization in these three-dimensional textures, which influences whether the Hopf index is an integer or not. To illustrate these concepts, we present examples of three-dimensional magnetic textures within various backgrounds, including ferromagnetic, helical, and screw-dislocation configurations.

References:

[1] P. Sutcliffe, Phys. Rev. Lett. 118 (2017).
[2] F. Zheng, et al., Nature 623 (2023).
[3] M. Azhar, et al., Phys. Rev. Lett. 128 (2022).
[4] R. Knapman, et al., arXiv:2410.22058 (2024).
[5] M. Azhar, Sandra. C. Shaju, et al., arXiv:2411.06929 (2024).

MA 41.32 Thu 15:00 P3

Effective Geometric Model for a Magnetic Skyrmionium — •Finn Feldkamp, Alessandro Pignedoli, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

A Skyrmionium consists of a Skyrmion nested within another Skyrmion of opposite topological charge, rendering it a non-topological magnetic soliton. We use an effective geometric model to describe a Skyrmionium as a closed-loop domain wall in a thin magnetic film, extending approaches previously used for Skyrmions [1]. Our model not only provides insights into the stability of a Skyrmionium but also facilitates the analytical investigation of its excitation modes.

[1] D. R. Rodrigues, et al., PRB 97, 134414 (2018)

MA 41.33 Thu 15:00 P3

Inelastic neutron scattering in multi-Q structures in centrosymmetric systems — •Artem Nosenko and Dmitri Efremov — Leibniz Institute for Solid State and Materials Research, Dresden, Germany

In the current study we investigate centrosymmetric spin systems on a square lattice with spin frustration. We show that spin frustration leads to several single-Q helical structures and a double-Q structure.

We study the magnon spectra and calculate the dynamical structure factor for these magnetic structures. The results obtained show that inelastic neutron scattering can be a perfect tool for the identification of double-Q structures.

MA 41.34 Thu 15:00 P3

Gesture recognition with Brownian reservoir computing using geometrically confined skyrmion dynamics — •Grischa Beneke[1], Thomas Brian Winkler[1], Klaus Raab[1], Maarten A. Brems[1], Fabian Kammerbauer[1], Pascal Gerhards[2], Klaus Knobloch[2], Sachin Krishnia[1], Johan Mentink[3], and Mathias Kläui[1,4] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Infineon Technologies Dresden, Germany — [3]Radboud University, Institute for Molecules and Materials, the Netherlands — [4]Center for Quantum Spintronics, Norwegian University of Science and Technology, Norway

Physical reservoir computing utilizes complex physical systems' dynamics for efficient information processing, minimizing training and energy requirements. Magnetic skyrmions, topologically stabilized spin textures, offer promising reservoir computing capabilities through their stability, strong non-linear behaviour, and energy-efficient manipulation. We demonstrate a time-multiplexed skyrmion reservoir computing approach to overcome traditional limitations in temporal pattern recognition [1]. By aligning the reservoir's timescales with real-world data, our approach processes hand gestures captured by Range-Doppler radar. This method scales to the nanometer regime and demonstrates competitive or superior performance compared to energy-intensive software-based neural networks. Our hardware approach's key advantage is its ability to integrate sensor data in real-time without temporal rescaling, enabling numerous applications. [1] G. Beneke et al., Nat. Commun. 15, 8103 (2024).

MA 41.35 Thu 15:00 P3

Direct Manipulation of Topological Spin Textures with Magnetic Force Microscopy — •Minh Duc Tran[1], Elizabeth Martin Jefremovas[1], Mona Bhukta[1], Thomas Brian Winkler[1], Robert Frömter[1], Dennis Meier[2], and Mathias Kläui[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), 7034 Trondheim, Norway — [3]Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

We present a method to manipulate skyrmions in CoFeB-based multilayer stacks using magnetic force microscopy (MFM). By employing single-pass MFM scans, we eliminate disturbances from the initial topography mapping, allowing for direct control over the interaction with the complex spin textures [1]. Through precise tuning of the scan parameters such as lift height and write speed, we achieve localized transformations of the metastable skyrmion state into the energetically favored stripe domains [2]. Our findings offer a potential approach for generating more exotic spin textures by selectively creating/annihilating magnetic domains in a confined region [3].

[1] A. V. Ognev et al., ACS Nano 14, 11, 14960-14970 (2020).
[2] A. Casiraghi et al., Commun. Phys. 2, 145 (2019).
[3] E. M. Jefremovas et al., Appl. Phys. Lett. 125, 192402 (2024).

MA 41.36 Thu 15:00 P3

Minimizing pinning of magnetic skyrmions in multilayer thin films — •Alen John[1,2], Maria Andromachi Syskaki[1,2], Jürgen Langer[2], Gerhard Jakob[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Singulus Technologies AG, Kahl am Main, Germany

Topological solitons, such as skyrmions, have attracted widespread attention due to their potential applications in unconventional computing and sensing. In this work, we present an optimization process for creating and stabilizing magnetic skyrmions with low pinning in multilayer thin films, using magnetron sputtering. We investigate Ta/CoFeB/MgO stacks with perpendicular magnetic anisotropy, systematically varying deposition parameters like sputter power and pressure to optimize skyrmion formation. Additionally, we introduce a Ta dusting layer between the ferromagnetic and MgO layers to fine-tune the magnetic anisotropy. This approach enables the fabrication of ultra-low pinning skyrmion samples that host room-temperature, thermally diffusing skyrmions[1], which are particularly promising for a range of emerging unconventional computing applications, including reservoir computing [2].

[1] J. Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019) [2] G. Beneke et al., Nat. Commun. 15, 8103 (2024).

MA 41.37 Thu 15:00 P3

Exploring Topological Magnetism in Magnet-Superconductor Hybrid Systems — •Sayan Banik[1] and Ashis Nandy[2] — [1]National Institute of Science Education and Research, Jatni 752050, India — [2]National Institute of Science Education and Research, Jatni 752050, India

In this study, we engineer magnet-superconductor hybrids (MSHs) by placing 3d transition metals (TM) on the surface of the s-wave superconductor (SC), Nb. By employing a systematic search approach, we select a few members within this MSH family that exhibit magnetism according to Hund's first rule, depending on two different superconducting surfaces. Interestingly, the weak spin-orbit coupling at these interfaces causes the magnetic behavior to differ from what Hund's rule predicts.

By employing detailed ab initio electronic structure calculations followed by spin-lattice simulations, we further explored these materials, discovering many complex and unusual spin textures. For example, Cr/Nb(110) and Mn/Nb(110) are found to exhibit antiferromagnetic spin spiral (AFM-SS) ground states. In contrast, Fe/Nb(001) exhibits antiferromagnetic (AFM) order, while Cr/Nb(001) displays a magnetic state with an AFM chain along the x-direction and a spin spiral modulation along the y-direction. The strain affects these magnetic ground states, finding that the AFM-SS of Mn/Nb(110) changes to AFM order when in-plane strain is applied.

We find a hexagonal skyrmion lattice by covering the top surface of the TM-SC with two layers of heavy metal.

MA 41.38 Thu 15:00 P3

Resonant X-ray Elastic Scattering of Chiral Magnets — Sina Mehboodi[1,3], •Mathew James[4], Victor Ukleev[2], Chen Luo[2], Florin Radu[2], Christian H Back[1,3], and Aisha Aqeel[1,3,4] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [4]University of Augsburg, Augsburg, Germany

Resonant Elastic X-ray Scattering (REXS) is an element specific synchrotron X-ray technique that combines diffraction and spectroscopy. It can be used to study complex magnetic materials and provides a sensitive probe for the spatial modulation of spin configuration. This technique has been used to explore a chiral magnet Cu_2OSeO_3. Cu_2OSeO_3 is a unique magnetic insulator that exhibits a complex spin configuration, including helices, conical spirals, and skyrmions. We studied the skyrmion phase and the tilted cone phase of the high-quality single crystal Cu_2OSeO_3 at low temperature [1] using the REXS technique, which occurs when the energy of the incident X-ray photon is matched near the absorption edge of a magnetic element, in this case Cu. We carried out all the experiments by tuning the photon energy to the L_3 edge of Cu. We can directly observe the magnetic diffraction pattern caused by the magnetic arrangement of Cu^{2+} ions in different phases of Cu_2OSeO_3.

[1] A. Aqeel et al., Physical Review Letters 126, 017202 (2021)

MA 41.39 Thu 15:00 P3

Topological Phase Transition and Topological Protection in Van Der Waals Ferromagnet Fe3GeTe2 Thin Flake — •Sourav Chowdhury[1], Michael Schneider[2], Soumyaranjan Dash[3], Christopher Klose[2], Chithra Sharma[4,5], Lisa-Marie Kern[2], Tim Butcher[2], Josefin Fuchs[2], Santanu Pakhira[6], Amir-Abbas Haghighirad[6], Sujit Das[7], Sanjeev Kumar[3], Bastian Pfau[2], and Moritz Hoesch[1] — [1]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]Max-Born-Institut, Berlin, Germany — [3]Indian Institute of Science Education and Research, Mohali, India — [4]University of Hamburg, Hamburg, Germany — [5]Christian-Albrechts-University Kiel, Kiel, Germany — [6]Karlsruhe Institute of Technology, Karlsruhe, Germany — [7]Indian Institute of Science, Bengaluru, India

Topological spin textures in 2D van der Waals (vdW) magnets are increasingly sought for high-performance spintronic devices, presenting transformative potential for ultra-dense data storage, energy-efficient operation, and advanced data processing capabilities [1]. We image various topological spin textures within a vdW ferromagnet Fe3GeTe2 thin flake. We observed topological protection versus non-protection behavior at close-to versus well-below the ferromagnetic transition temperature. Monte-Carlo calculation suggests that the switching among distinct topological spin textures can be achieved with the interplay between the Rashba spin-orbit coupling and the uniaxial-magnetic-anisotropy.

[1] K. Chang et al. Science 2016, 353, 274.

MA 41.40 Thu 15:00 P3

Thiele model computer simulations of magnetic skyrmions — •Anna Endres, Simon M. Fröhlich, Jan Rothörl, Maarten A. Brems, Raphael Gruber, Leonie-C. Dany, Tobias Sparmann, Mathias Kläui, and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz, Germany

Magnetic skyrmions can be approximated as rigid particles in 2D in the framework of the Thiele model [1]. This coarse-grained approach in principle enables simulations of hundreds or even thousands of skyrmions on experimentally relevant time and length scales [2]. Skyrmion interactions and pinning landscapes can be inferred directly from corresponding experiments [3][4]. Recently, we have also developed methods to match time and force scales of simulations with experiments, enabling quantitative and predictive simulations. In this poster we summarize our results and provide details on our modelling approach [5].

[1] A. A. Thiele, Phys. Rev. Lett. 30, 230 (1973)
[2] J. Zázvorka et al., Adv. Funct. Mater. 30, 2004037 (2020)
[3] Y. Ge et al., Commun. Phys. 6, 30 (2023)
[4] R. Gruber et al., Nat. Commun. 13, 3144 (2022)
[5] M. A. Brems et al., in preparation

MA 41.41 Thu 15:00 P3

Effective field theory of the Quantum Skyrmion Hall Effect — •Vinay Patil[1,2], Rafael Flores-Calderòn[1,2], and Ashley M. Cook[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 38, 01187, Dresden, Germany

Motivated by phenomenology of myriad recently-identified topologically non-trivial phases of matter, we introduce effective field theories (EFTs) for the quantum skyrmion Hall effect (QSkHE). We employ a single, unifying generalisation for this purpose: in essence, a lowest Landau level projection defining a non-commutative, fuzzy sphere with position coordinates proportional to SU(2) generators of matrix representation size N, may host an intrinsically 2+1 dimensional, topologically non-trivial many-body state for small N as well as large N . That is, isospin degrees of freedom associated with a matrix Lie algebra with N * N generators potentially encode some finite number of spatial dimensions for N > 1, where isospin has previously been treated as a label. This statement extends to more general p-branes subjected to severe fuzzification as well as membranes. As a consequence of this generalisation, systems with d cartesian spatial coordinates and isospin degrees of freedom encoding an additional δ fuzzy coset space coordinates can realise topologically non-trivial states of intrinsic dimensionality up to d+δ+1. We furthermore generalise these EFTs to space manifolds with local product structure exploiting the dimensional hierarchy of (fuzzy) spheres.

MA 41.42 Thu 15:00 P3

A C*-algebraic approach to orbital magnetization in skyrmion crystals and finite magnetic fields — •Pascal Prass[1], Duco van Straten[2], and Yuriy Mokrousov[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Institute of Mathematics, Johannes Gutenberg University Mainz, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

Skyrmion crystals can induce orbital magnetization even in the absence of spin-orbit coupling [1]. This depends on the skyrmion density determining the strength of the emergent magnetic field. As the length scale of a skyrmion crystal approaches the lattice constant of its host material, topological gaps may open in the associated electronic system similar to the formation of Landau levels. However, the smooth texture approximation for the emergent magnetic field is no longer satisfied [2]. Therefore, we utilize a fully algebraic framework to describe a tight-binding system coupled to a skyrmion crystal, that allows us to numerically evaluate topological gap invariants [3] and orbital magnetization even in the presence of finite magnetic flux. This way, we can describe the dependence of the orbital magnetization on the magnetic field for different skyrmion densities. In the appropriate limit, this approach coincides with the expression from the modern theory of orbital magnetization [4]. [1] Göbel et al. Phys. Rev. B **99**, 060406(R) (2019). [2] Lux et al. Phys. Rev. Res. **6**, 013102 (2024). [3] Prass et al. SciPost Phys. Core, *in press* (2024). [4] Schulz-Baldes et al. Commun. Math. Phys. **319**, 649-681 (2013)

MA 41.43 Thu 15:00 P3

Stoichiometry-control of topological ground states in the Kondo lattice CeAlGe — •Soohyeon Shin[1,2], Igor Plokhikh[2], Jonathan White[2], Vladimir Pomjakushin[2], Pascal Puphal[3], and Ekaterina Pomjakushina[2] — [1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich, Lichtenbergstrasse 1, D-85747 Garching, Germany — [2]PSI Center for Neutron and Muon Sciences, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

CeAlGe crystalises in tetragonal structure I41md, where the spatial-inversion symmetry is broken, and is expected to exhibit Weyl fermions near a Fermi surface that becomes more stable by broken time-reversal symmetry. CeAlGe grown by the flux method, off-stoichiometric case, exhibits a commensurate antiferromagnetic order below T = 5.1 K, whereas the crystal grown by floating-zone methods with 30 bar of Ar gas (p=30 bar), stoichiometric case, exhibits an incommensurate order below T = 4.4 K in which topological Hall effects are induced by external magnetic fields applied in the c-axis. In this presentation, we show the newly synthesised CeAlGe using the same floating-zone method but with lower Ar pressure of p=5 bar. Our neutron diffraction and electrical Hall transport experiments revealed that the topological magnetism remains with shorter periodicity. Given all experimental results of flux-grown and two floating-zone-grown CeAlGe, we will discuss the mechanism of topological magnetism with respect to the Kondo coupling strength.

MA 41.44 Thu 15:00 P3

Quasiparticle interference in an altermagnetic tight-binding model — •Eric Petermann, Kristian Maeland, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

Altermagnets constitute novel magnetic systems characterized by compensated magnetic ordering and momentum-dependent spin splitting without net magnetization. We employ tight-binding models to analyze quasiparticle interference (QPI) patterns in altermagnetic lattices. In the presence of impurities, scattering processes give rise to spatial modulations of charge and spin densities emerging from the interference of quasiparticles. This interference results in QPI patterns near those impurities. We relate the QPI patterns with the type of altermagnetic order.

MA 41.45 Thu 15:00 P3

Spin-Orbit Torque in RuO_2|Py multilayer systems — •Niklas Schmolka, Maik Gaerner, Jan Schmalhorst, and Günter Reiss — Bielefeld University, Germany

Spin torques like the Spin-Orbit torque (SOT) offer fast and energy efficient data writing techniques in magnetic memory devices (MRAM). As a new class of materials, Altermagnets, like RuO_2, are able to generate a current induced SOT while possessing zero net magnetization. As such, Altermagnets offer multiple advantages compared to existing MRAM devices based on Ferromagnets like higher stability against external magnetic fields and THz Switching [1][2].
Here, we use the harmonic Hall measurement technique to determine the Spin Hall Angle (SHA) in RuO_2|Py multilayer system via the Harmonic Response Modell [3]. To accurately determine the SHA we first characterize our samples using X-ray diffraction, X-ray reflection, Alternating Gradient Magnetometry and measure the magnetization and the Anomalous Hall Effect. We compare our experimental results to the existing literature and reflect on the influence of the crystal structure on the generated spin current [4].

[1] A. Bose et al., Nat. Electron. 5 267 (2022)
[2] S. Schlauderer et al., Nature 569 383 (2019)
[3] M. Meinert et al., Phys. Rev. Applied 14 064011 (2020)
[4] H.Bai et al., Phys. Rev. Lett. 128 197202 (2022)

MA 41.46 Thu 15:00 P3

Growth of altermagnetic MnTe thin films — •Lena Hirnet, Marco Dittmar, Hannes Haberkamm, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Recently, altermagnets have attracted great attention combining antiferromagnetic spin alignment in real space with a momentum-dependent spin polarization of the electronic states in the band structure. One of the proposed altermagnet work horse materials is MnTe [1,2]. Here, we investigate the epitaxial growth of MnTe on different substrates ranging from trivial band insulators to topological van der Waals metals with spin-momentum-locked surface states. The atomic and electronic structure of these films is studied employing low-energy electron- and x-ray diffraction as well as soft x-ray angle-resolved photoemission spectroscopy, respectively.

[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 031042 (2022)
[2] J. Krempaský *et al.*, *Nature* **626**, 517-522 (2024)

MA 41.47 Thu 15:00 P3

Interplay and Robustness of Dual-sublattice Altermagnetic Ordering in $Er_2Ru_2O_7$ — •Michele Reticcioli[1], Paolo Radaelli[2], and Alessandro Stroppa[1] — [1]CNR-SPIN L'Aquila, Italy — [2]University of Oxford, United Kingdom

Altermagnets, a novel class of magnetic materials, bridge the gap between conventional antiferromagnets and ferromagnets by hosting spin-split electronic structures without net magnetization. These materials hold promise for spintronic applications due to their unique symmetry-driven properties. In this work, we explore altermagnetism in the oxide semiconductor $Er_2Ru_2O_7$, which exhibits a rare double altermagnetic ordering arising from the Er and Ru magnetic sublattices. Using density functional theory, we investigate the interplay between the two sublattices, giving rise to two Neel vector order parameters, revealing a complex interplay that shapes the material's magnetic behavior. Furthermore, we analyze the impact of doping on the magnetic properties. Our findings show that while the Er sublattice demonstrates remarkable robustness against p-doping, the Ru sublattice undergoes significant changes. Notably, local substitution of oxygen atoms with nitrogen dopants leads to a drastic alteration in the Ru-sublattice magnetic ordering. These results shed light on altermagnetism in oxides, particularly on the interplay between sublattices and the sensitivity to doping, opening new avenues for tailoring magnetic properties in altermagnets for technological applications.

MA 42: Members' Assembly

Time: Thursday 18:00–19:00 Location: H20

All members of the Magnetism Division are invited to participate.

MA 43: Skyrmions III / Non-Skyrmionic Magnetic Textures II

Time: Friday 9:30–13:15 Location: H16

MA 43.1 Fri 9:30 H16

All-Optical Control of Bubble and Skyrmion Breathing — •Tim Titze[1], Sabri Koraltan[2], Timo Schmidt[3], Dieter Suess[2], Manfred Albrecht[3], Stefan Mathias[1], and Daniel Steil[1] — [1]I. Physikalisches Insitut, University of Göttingen — [2]Physics of Functional Materials, Faculty of Physics, University of Vienna — [3]Institute of Physics, University of Augsburg

Topologically protected magnetic skyrmions promise tremendous potential for innovative applications, such as unconventional computing schemes. Deterministic control of the dynamics of such spin objects is one key ingredient for future data processing devices. Using ultrafast Kerr spectroscopy, we investigate the spin dynamics of ferrimagnetic $[Fe(0.35\,nm)/Gd(0.40\,nm)]_{160}$ multilayers hosting a dense bubble/skyrmion (BSK) lattice at ambient temperature [1, 2]. Ultrafast laser excitation of the BSK lattice leads to coherent spin dynamics in the form of BSK breathing [3]. By tuning the time delay between excitations in a dual pulse excitation scheme we demonstrate optical control of the breathing dynamics of the BSK lattice in amplitude and phase [4]. This fast and reversible technique presents a promising pathway towards future BSK-based spintronic and magnonic devices.

[1] S. A. Montoya *et al.*, Phys. Rev. B **95**, 2024415 (2017)
[2] M. Heigl *et al.*, Nat. Commun. **12**, 261 (2021)
[3] T. Titze *et al.*, Adv. Funct. Mater. **34**, 2313619 (2024)
[4] T. Titze *et al.*, Phys. Rev. Lett. **133**, 156701 (2024)

MA 43.2 Fri 9:45 H16

Spiral multiferroics as a natural skyrmion racetrack — •Luca Maranzana[1,2], Maxim Mostovoy[3], Naoto Nagaosa[4], and Sergey Artyukhin[1] — [1]Quantum Materials Theory, Italian Institute of Technology, Via Morego 30, Genoa, Italy — [2]Department of Physics, University of Genoa, Via Dodecaneso 33, Genoa, Italy — [3]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 3, 9747 AG Groningen, Netherlands — [4]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan

Magnetic skyrmions are localized spin textures with a nontrivial topology. This property ensures excellent stability even at nanometer length scales, establishing skyrmions as promising information carriers in magnetic storage and processing devices. Still, their fate in a wide variety of magnetic backgrounds is poorly understood. Here, we show that spiral multiferroics, some of the most basic noncollinear magnets, host bimerons, a particular type of skyrmion. Multiferroic properties of a spin spiral endow the bimeron with magnetic and ferroelectric dipole moments that, surprisingly, depend on its position relative to the spiral. This enables precise positioning of the bimeron by a rotating magnetic field (e.g. of a circularly polarized electromagnetic wave). At low frequencies, the bimeron magnetic moment rotates in sync with the field, and this topological spin texture is pumped in the Archimedean screw fashion. The results establish spiral multiferroics as a natural racetrack, where one full rotation of the field moves the bimeron by one spiral period.

MA 43.3 Fri 10:00 H16

Pathways to Bubble and Skyrmion Lattice Formation in Fe/Gd Multilayers — Tim Titze[1], Sabri Koraltan[2], Timo Schmidt[3], Dieter Suess[2], Manfred Albrecht[3], Stefan Mathias[1], and •Daniel Steil[1] — [1]University of Goettingen — [2]University of Vienna — [3]University of Augsburg

Fe/Gd multilayers host a rich variety of magnetic textures, including topologically trivial bubbles and topologically protected skyrmions [1-4]. Using time-resolved Kerr spectroscopy, we highlight how different control strategies including temperature T, out-of-plane magnetic fields H and femtosecond light excitation can be used to create such textures via different pathways. We find that varying the magnetic field at constant temperature leads to a different (H,T) phase diagram of magnetic textures than moving along a temperature trajectory at constant magnetic field, which is corroborated by micromagnetic simulations. We furthermore show that bubble and skyrmion (BSK) creation by impulsive light excitation is at least partially a non-adiabatic process, as the creation occurs in parts of the (H,T) phase diagram, where neither the constant T nor the constant H trajectory predict their existence. We discuss a possible scenario for the creation of BSKs in this material system involving the inhomogeneity of the excitation process.

[1] S. A. Montoya *et al.*, Phys. Rev. B **95**, 2024415 (2017)
[2] M. Heigl *et al.*, Nat. Commun. **12**, 261 (2021)
[3] T. Titze *et al.*, Adv. Funct. Mater. **34**, 2313619 (2024)
[4] T. Titze *et al.*, Phys. Rev. Lett. **133**, 156701 (2024)

MA 43.4 Fri 10:15 H16

Nitrogen-vacancy scanning imaging of a room-temperature skyrmion lattice in a van der Waals ferromagnet Fe3-xGaTe2 — •Young-Gwan Choi[1], Hayden Binger[1], Luke Turnbull[1], Yejin Lee[1], Lotte Boer[1], Chenhui Zhang[2], Haneul Kim[3], Claire Donnelly[1], Hyunsoo Yang[2], and Uri Vool[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Electrical and Computer Engineering, National University of Singapore, 117583 Singapore, Singapore — [3]Department of Physics, University of Ulsan, 44610 Ulsan, Korea

We report the visualization of the magnetic stray field from a room-temperature skyrmion lattice in the van der Waals ferromagnet Fe3-xGaTe2(FGaT) by nitrogen-vacancy (NV) scanning. By employing a field-cooled process, we observed the transition from labyrinth domain structures to a stable skyrmion lattice state, demonstrating the formation of a stable skyrmion lattice phase. The experiments were conducted on FGaT flakes with an approximate thickness of 100 nm, revealing detailed insights into the stable formation of the skyrmion phase even at room temperature. These results highlight the capability of NV scanning for direct and quantitative imaging of room-temperature skyrmions, offering valuable insights into their properties and advancing the understanding of skyrmion lattices. This study provides a basis for further exploration of skyrmion-based spintronic applications.

MA 43.5 Fri 10:30 H16

Controlling topolopogical spin textures in Heusler magnetic nanowires — •Rikako Yamamoto[1,2], Luke Turnbull[1,2], Marisel Di Petro Martinez[1,2], Jeffrey Neethirajan[1], José Claudio Corsaletti Filho[1], Simone Finizio[3], Tim Butcher[3,4], Igor Beinik[5], Claas Abert[6], Dieter Suess[6], Praveen Vir[1], Chandra Shekar[1], Claudia Felser[1], and Claire Donnelly[1,2] — [1]MPI-CPfS, Dresden, Germany — [2]WPI-SKCM2, Higashi-Hiroshima, Japan — [3]PSI, Villigen, Switzerland — [4]MBI, Berlin, Germany — [5]MAX-IV, Lund, Sweden — [6]University of Vienna, Vienna, Austria

Nontrivial topological spin textures, such as magnetic skyrmions and antiskyrmions, have been attracting considerable interest due to their fundamental properties and potential applications. Antiskyrmions, commonly found in materials with anisotropic Dzyaloshinskii-Moriya interactions, are of particular interest due to their complex winding, and prospect for unidirectional motion. However, such textures are energetically degenerate, and their formation remains open to exploration. Here we gain control over the formation and stability of antiskyrmions by nanopatterning anti-skyrmion-hosting Heusler magnets. By patterning nanowires oriented at different angles to the crystallographic unit cell, we combine intrinsic and geometrical anisotropies. Using x-ray dichroic ptychography to image the magnetic configuration of these nanowires, we observe that the competition between geometrical and intrinsic anisotropy can lead to preferential formation of topological objects in the nanostructure. This approach provides new opportunities for enhanced control of topological spin textures.

MA 43.6 Fri 10:45 H16

Confinement-Induced Magnetoresistances in Skyrmion-based Magnetic Tunnel Junctions — •Moritz Winterott[1,2] and Samir Lounis[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Innovations are essential to address the rapidly growing demand for data. One of the most promising solution are magnetic tunnel junctions [1] (MTJs) which utilize spin-dependent tunnelling between two ferromagnetic layers separated by an insulating barrier and present a high-speed, non-volatile, and energy-efficient memory solution. Combining MTJs with skyrmions offers great potential [2] due to the nanoscale size and topological protection of the later ones. However creation and efficient electrical detection of skyrmions in MTJs remains challenging. We demonstrate that a strong splitting of spin-channels leads to confined states inside the skyrmion, complementary to Friedel oscillations reaching far outside the skyrmion. These non-trivial signatures in the electronic structure induce new magnetoresistances augmenting the efficiency of those enabled by spin-orbit coupling and magnetic non-collinearity [3], which could facilitate electrical detection of skyrmions in MTJs. We employ a tight-binding scheme to explore the impact of the skyrmion size, Fermi energy and splitting of the spin-channels.

– [1] Parkin et al., Nat. Mater. 3, 862 (2004); [2] Chen et al., Nature 627, 522-527 (2024); [4] Fernandes et al., Nat. Com. 13, 1576 (2022).

MA 43.7 Fri 11:00 H16

Field-induced Reversal of Magnetic Anisotropy in Skyrmion Hosts — •Hans-Albrecht Krug von Nidda, Bertalan Szigeti, Mamoun Hemmida, Dieter Ehlers, and István Kézsmárki — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany

Skyrmions show up in non-centrosymmetric magnets due to the complex interplay of anisotropic Dzyaloshinskii-Moriya interaction, uniaxial magnetic anisotropy, and magnetic dipolar interactions. A magnet is commonly classified as either easy-axis or easy-plane, when the magnetic anisotropy forces the magnetization to align parallel or perpendicular to the high-symmetry axis, respectively. We show that this simple classification fails for systems with competing anisotropy terms. Our multi-frequency electron spin resonance spectroscopy study on the skyrmion hosts GaMo4S8 and GaV4Se8 reveals counteracting exchange and g-factor anisotropies. Consequently, the total aniotropy changes sign in moderate magnetic fields: GaMo4S8 turns from an easy- to a hard-axis magnet, while GaV4Se8 does the opposite. These findings underscore the significance of precisely quantifying all anisotropy components, because a single effective value, when encompassing conflicting terms, proves to be insufficient for an accurate description of magnetic states.

MA 43.8 Fri 11:15 H16

Short-pitch skyrmions in layered rare-earth frustrated magnets — •Vladislav Borisov[1], Rohit Pathak[1], Sagar Sarkar[1], Anna Delin[2,3,4], and Olle Eriksson[1,3] — [1]Uppsala University, Sweden — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]Wallenberg Initiative Materials Science for Sustainability (WISE) — [4]SeRC (Swedish e-Science Research Center), KTH Stockholm, Sweden

While most skyrmionic systems rely on the presence of Dzyaloshinskii-Moriya interaction (DMI), there are a few known compounds, such as $GdRu_2Si_2$ with 122-type structure, where extremely compact skyrmions around 2 nm are stabilized without DMI, as discovered in recent experiments [1]. Several theory studies, including our recent work [2], suggest the importance of magnetic frustration and local anisotropy for the skyrmion stability. The present work explores further the variety of magnetic phases in other compounds with the 122-type crystal structure using density functional theory and atomistic spin dynamics at finite temperature and applied magnetic field. Various chemical compositions, included those from [3], are considered here and interesting trends for RKKY-like Heisenberg interactions between the rare-earth moments, calculated using magnetic force theorem, and real-space textures are analyzed.

1. N. D. Khanh et al., Nature Nanotech. 15, 444-449 (2020).
2. S. Sarkar et al., arXiv:2409.06736.
3. T. Nomoto, R. Arita, J. Appl. Phys. 133, 150901 (2023).

This work was financially supported by the Knut and Alice Wallenberg (KAW), Göran Gustafsson, and Carl Tryggers Foundations.

15 min. break

MA 43.9 Fri 11:45 H16

Tunable magnetic skyrmion bubbles in centrosymmetric magnets — Dola Chakrabartty[1], István Kézsmárki[1], and •Ajaya Kumar Nayak[2] — [1]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany — [2]School of Physical Sciences, National Institute of Science Education and Research, HBNI, Jatni, 752050, Bhubaneswar, India

Magnetic skyrmions are topologically protected spin textures that can avoid defects and be mobilized by low current densities, making them potential candidates for high-density and low-power consuming logic and memory devices. Skyrmion-like spin textures with different helicities and vorticities have recently been found also in centrosymmetric magnets, stabilized by competing dipolar interaction and out-of-plane magnetic anisotropy. The primary motivation of this study is to explore the extensive tunability of magnetic skyrmion bubbles in centrosymmetric magnets with internal and external parameters. We have demonstrated that in the centrosymmetric system by applying external magnetic field and tuning magnetic anisotropy one can transform skyrmions (topological number -1) to type-II bubble (topological number 0) through Bloch line formation. We found that the skyrmions are stable when there is only out-of-plane uniaxial anisotropy, whereas the introduction of small in-plane anisotropy turns them to type-II bubbles. Presently, we are in the process of exploring the tunability of skyrmions in such systems with other external stimuli, such as uniaxial strain and laser irradiation.

MA 43.10 Fri 12:00 H16

Gate-Voltage-Induced Changes of the Magnetic Properties of Skyrmion-Hosting Gd/Fe Multilayers — •Sebastian Hofmann[1], Steffen Wittrock[2], Tamer Karaman[1], Sascha Petz[2], Daniel Metternich[2], Krishnanjana Puzhekadavil Joy[2], Kai Litzius[1], and Felix Büttner[1,2] — [1]Universität Augsburg Institut für Physik, Universitätsstraße 1, 86159 Augsburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Ionic gating has recently emerged as a versatile method to induce large and controllable changes of the local magnetic properties of thin films. This allows, for example, to manipulate the existence [1] and chirality [2] of magnetic skyrmions. However, existing gating experiments have focused on ultrathin films, where skyrmions are usually micron sized. Here, we show that ionic gating with oxygen and hydrogen can be used to control ferrimagnetic Gd/Fe multilayer materials with thicknesses of more than 40 nm, in which sub-100 nm skyrmion can be observed. We find that ionic gating can shift the compensation temperature by more than 100 K, i.e., by a similar magnitude as in sub-10 nm thick films [3]. However, unlike ultrathin films, our thicker materials exhibit vertical variation of magnetic properties, suggesting a pathway toward gate-control of spin textures in 3D. [1] Yang, S. et al. Adv. Mat. 2208881 (2022). [2] Fillion, C.-E. et al. Nat. Comm. 13, 5257 (2022). [3] Huang, M. et al. Nat. Nanotechnol. 16, 981 (2021).

MA 43.11 Fri 12:15 H16

Shape anisotropy in helimagnets — •Jan Masell[1], Maurice Colling[2], Mariia Stepanova[2], Mario Hentschel[3], and Dennis Meier[2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [3]University of Stuttgart, Stuttgart, Germany

In chiral magnets, the competition between ferromagnetic exchange and Dzyaloshinskii-Moriya interaction (DMI) stabilizes a long-ranged helical state as the ground state. The orientation and pitch of the helix is described by the q-vector. For isotropic model systems, the q-vector can point in any direction while in real materials its orientation is pinned by anisotropies, such as exchange or single ion anisotropy.

In this talk, I will discuss the impact of the shape of the magnet on the orientation of the helical phase. While shape anisotropy is a well-established phenomenon in ferromagnets, its role in chiral magnets remains less explored. I will present our theoretical results for a new type of DMI-shape-anisotropy for non-trivial magnetic textures, caused by the competition between standard shape anisotropy and the chiral surface twist inherent to systems with DMI. Our experimental data on FeGe confirm the existence of such non-trivial anisotropy, challenging present models for magnetic textures in nanostructures with DMI.

MA 43.12 Fri 12:30 H16

Extraordinary return point memory of Pt/Co/Dy ferrimagnetic multilayers — •Tamer Karaman[1], Kai Litzius[1], Sebastain Wintz[2], Aladin Ullrich[1], Daniel Metternich[1,2], Steffen Wittrock[2], Krishnanjana Joy[1,2], Sebastian Hoffman[1], Timo Schmidt[1], Manfred Albrecht[1], and Felix Büttner[1,2] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Chiral magnetic spin textures are promising candidates for various spintronics applications [1]. These applications rely fundamentally on the controlled motion of spin textures under external stimuli. In this study, we report on the contrary and unique behaviour of Pt/Co/Dy rare-earth transition metal (RE-TM) ferrimagnetic multilayers, particularly their demonstration of full return-point memory. By studying the domain and domain wall response with field cycling using real-space imaging techniques, we observe deterministic behaviour where domains completely return to their original positions, even after exposure to high applied fields. Such observation is rarely documented in the literature and invites a variety of interpretations [2, 3]. This study emphasizes the significance of unexplored aspects of RE-TM ferrimagnets, advancing deeper exploration and broader utilization of these materials.

1. Fert, A. et al. Nat. Rev. Mater. 2, 17031 (2017). 2. Kappenberger, P. et al. Phys. Rev. Lett. 91, 267202 (2003). 3. Seu, K. A. et al. New J. Phys. 12, 035009 (2010).

MA 43.13 Fri 12:45 H16

Fascinating mesoscale magnetic textures in the topological Kagome system $TbMn_6Sn_6$ — •Ralph Rajamathi[1], Manuel Zahn[1,2], Kai Litzius[1], István Kézsmárki[1], and Sándor Bordács[3] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology — [3]Department of Physics, Budapest University of Technology and Economics

In recent years, the Kagome ferrimagnet $TbMn_6Sn_6$ has garnered significant interest due to its unconventional band topology, which realizes exotic quantum states like a Chern insulating phase. It exhibits a spin-reorientation transition (SRT) from easy-axis to easy-plane at 310 K, where skyrmion bubbles have been observed in lamellae. However, magnetic textures in bulk crystals have been unexplored so far. Here, we used magnetic force microscopy (MFM) to image the magnetic pattern on the surface of bulk crystals, and magnetometry to study the role of second order magnetic anisotropy. Two types of textures were observed, namely long-ranged stripes that invert contrast on reversing the tip's magnetization, decorated by star-shaped structures whose contrast is independent from the the tip's magnetization. Reorientation of the stripes and creation/elimination of the "stars" in an external magnetic field indicate low magnetic pinning. Analyzing the in-plane magnetometry data, a metastable magnetization state was observed below the SRT temperature, indicating the possibility of an intermediate in-plane state, which was observed by MFM in the vicinity of SRT.

MA 43.14 Fri 13:00 H16

Domain walls with 90° magnetization rotation in the topological kagome magnet $TbMn_6Sn_6$ — •Manuel Zahn[1,2], Ralph Rajamathi[1], Kai Litzius[1], Dennis Meier[2], Sándor Bordács[3], and István Kézsmárki[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU) — [3]Department of Physics, Budapest University of Technology and Economics

The layered Kagome ferrimagnet, $TbMn_6Sn_6$, attracts much attention due to its topologically non-trivial features. The bulk electronic band structure realizes a Chern insulating state and in the real space, skyrmion bubbles have been observed in thin lamellae of this compound. $TbMn_6Sn_6$ exhibits a zero-field first-order spin reorientation transition at T_{SR} = 315 K, below/above which the magnetic moment points perpendicular/parallel to the Kagome plane. Here, using magnetic force microscopy, we reveal peculiar domain textures in the vicinity of T_{SR} on the surface of bulk $TbMn_6Sn_6$ crystals. Upon approaching T_{SR} from lower temperatures, we observed a broadening of the domain walls separating regions oppositely magnetized perpendicular to the Kagome plane, and the emergence of a strictly in-plane magnetized region at the center of the walls. We compared these results with analytical calculations based on a continuum magnetic model and found that the $\pi/2$ stepwise rotation of the magnetization is a universal effect at the spin reorientation transition.

MA 44: Focus Session: Physics of the van der Waals Magnetic Semiconductor CrSBr II (joint session HL/MA)

The joint focus session of the divisions HL and MA presents the latest developments of the rapidly growing community working with the van der Waals magnetic semiconductor CrSBr with distinct excitonic and magnetic properties, and it is organized by Shengqiang Zhou (HZ Dresden-Rossendorf), Farsane Tabata-Vakili (TU Braunschweig), and Florian Dirnberger (TU Munich).

Time: Friday 9:30–13:00 Location: H17

See HL 60 for details of this session.

MA 45: Computational Magnetism

Time: Friday 9:30–12:30 Location: H18

MA 45.1 Fri 9:30 H18

Magnetic Interactions and Spin Coupling in Endohedral Fullerene Nanostructures — •Arkamita Bandyopadhyay and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3 06120 Halle/Saale

Our work investigates the spin-spin interactions in endohedral fullerene clusters, with a particular focus on the effects of different cluster geometries (linear, triangular, and more complex arrangements). By examining various configurations, we aim to provide a deeper understanding of how the interactions between spins in these clusters are governed by both the unique structural features of the fullerene molecules and their molecular levels. Our compuational study explores the role of spin exchange interactions, the potential for spin frustration, and how these phenomena can be manipulated to achieve desired magnetic behaviors, thus it can guide the design of new materials for spintronic devices, quantum information processing, and other applications where precise control over spin-spin interactions is key.

MA 45.2 Fri 9:45 H18

Intrinsic Spin Nernst Effect and Chiral Edge Modes in vdW Ferromagnetic Insulators: Dzyaloshinskii-Moriya vs. Kitaev Interactions — •Verena Brehm and Alireza Qaiumzadeh — NTNU Trondheim, Norway

The thermomagnetic Nernst effect and chiral edge states are key signatures of nontrivial topology and emerging Berry curvature in magnonic systems. Implementing atomistic spin simulations, we theoretically demonstrate the emergence of chiral magnon edge states at the boundaries of a ferromagnetic hexagonal lattice in the presence of Dzyaloshinskii-Moriya and Kitaev interactions, which are robust against nonlinear magnon interactions. In our simulations, we consider the spin parameters of CrI3 as a prototype of van der Waals magnetic layers. We show that the spin accumulation is reduced in the presence of Kitaev spin interactions compared to systems governed by Dzyaloshinskii-Moriya interactions. This reduction stems from the breaking of the U(1) symmetry, which leads to a shorter spin coherence length imposed by the Kitaev interaction. We propose that measuring the angular dependence of the Nernst signal in a magnetic field provides an effective indirect method for identifying the microscopic origin of topological magnons. Our findings hold promising potential for advancing next-generation energy-harvesting Nernst materials and facilitating the integration of topological magnetic materials with spintronic-based quantum technologies.

MA 45.3 Fri 10:00 H18

Origin of MAE and second order MAE due to the magnetostriction in tetragonal systems - FePt study — •Dominik Legut[1] and Pablo Nieves[2] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia — [2]University of Oviedo, Oviedo, Spain

The origin of magnetocrystalline anisotropic energy (MAE) guided by spin-orbit coupling in the $L1_0$-FePt alloy was analyzed and the correlations among MAE and magnetoelastic (magnetostriction) constants $b's(\lambda's)$ by means of the electronic structure eigenvalues (orbital energies) and eigenfunctions (orbital occupancies) were established[1]. Our numerical analysis includes the convolution of the projected wave-function (density of states) of each orbital of the Fe and Pt sub-lattices into their orbital energies and its contribution to the MAE,$b's$, and $\lambda's$. However, this corresponds to the zero strain situation. For a zero stress (realistic conditions used in experiments) situtation a very small correction is found for the first anisotropy constant $\Delta K_1/K_1 = 0.07\%$, while a much more significant contribution is obtained for the second one $\Delta K_2/K_2 = 21.86\%$. General analysis of this effect for tetragonal crystals is provided, finding that ΔK_1 will be always positive for any stable phase with this symmetry[2].

References:
1. T. Das, P. Nieves, D. Legut, J. Phys. D: Appl. Phys. **58**, 035004 (2025)
2. D. Legut, P. Nieves, Solid State Sciences (accepted)

MA 45.4 Fri 10:15 H18

High-throughput workflow for predicting magnetic ground states — •Hao Wang and Hongbin Zhang — Technical University of Darmstadt, 64287 Darmstadt, Germany

Obtaining the correct magnetic ground state is crucial for understanding the nature of magnetism and serves as a foundation for engineering functional magnetic materials for interesting applications. In this work, we present a high-throughput computational workflow designed to accurately determine the exchange interaction J_{ij} matrices and other relevant parameters for a wide range of magnetic systems. Combining the four-state energy mapping method with the Green's function approach, we construct symmetrized Heisenberg Hamiltonians to model magnetic interactions. Furthermore, by integrating atomistic spin dynamics Vampire package, our framework enables the efficient prediction of magnetic ground states. This scalable workflow not only improves computational efficiency for complex magnetic materials but also provides a robust platform for exploring the fundamental properties of magnetic systems.

MA 45.5 Fri 10:30 H18

Semiclassical approach to the exchange interactions and spin waves in double-layered antiferromagnets — Seo-Jin Kim[1], Zdeněk Jirák[2], Jiří Hejtmánek[2], Karel Knížek[2], Helge Rosner[1], and •Kyo-Hoon Ahn[2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czechia

We investigate the stability and magnonic properties of double-layered antiferromagnets using two model systems—the linear chain (LC) and a more complex railroad trestle (RT) geometry—as well as the real solid antiferromagnetic (AFM) CrN in its rock-salt structure. In the LC model, the spin-paired order $(\cdots{+}{+}{-}{-}\cdots)$ requires alternating ferromagnetic (FM) and AFM interactions. In contrast, the RT geometry allows some frustration, and the spin-paired order can be stable even for all magnetic exchange interactions being AFM. In the hypothetical cubic phase of CrN, magnetic Cr ions form a face-centered cubic lattice with equivalent AFM links to twelve nearest neighbors. However, the magnetostructural transition to an orthorhombically distorted phase below the Néel temperature (T_N = 287 K) diversifies the Cr-Cr nearest-neighbor distances, suppressing frustration. Using *ab initio* exchange parameters, we calculate the magnon dispersion relation and the temperature-dependent evolution of ordered magnetic moments. Our findings demonstrate that the stability of the double-layered AFM structure in CrN is attained, even when intra-sublattice interactions remain all AFM, consistent with the RT model.

MA 45.6 Fri 10:45 H18

Tuning Magnetic Anisotropy in Fe3Y Through Transition Metal Doping: An Ab-Initio High-Throughput Study — •Md Nur Hasan and Heike Herper — Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden

The advancement of permanent magnet systems is essential for various applications, including energy generation and information technology. This research focuses on developing and optimizing new permanent magnetic materials using an ab initio based first-principles approach. The Fe3Y system was initially selected for its in-plane magnetic anisotropy with a Curie temperature of 550 K, which, although advantageous, constrains its use in scenarios that require uniaxial (out-of-plane) anisotropy. The main goal of this study is to transition the magnetic anisotropy from the in-plane to a uniaxial configuration. Various transition metals were systematically introduced into both the Y and Fe sites of the Fe3Y structure to facilitate this shift. This doping approach enabled the tuning of the magnetic properties and provided insight into the mechanisms governing magnetic anisotropy. As a result, we identified several promising compositions with significant alterations in magnetic behavior, including systems that exhibit uniaxial anisotropy with Curie temperatures of ~ 550K, making them

suitable for high-performance magnetic applications. Initial findings suggest that certain transition metal dopants can significantly modify spin-orbit coupling and crystal field effects, achieving the desired anisotropy realignment with the potential to discover a new category of high-performance permanent magnets.

15 min. break

MA 45.7 Fri 11:15 H18

Programmable Magnetophononics: Selective Damping of Surface Acoustic Waves — •Michael Karl Steinbauer[1], Peter Flauger[1], Bernhard Emhofer[1], Matthias Küss[2], Stephan Glamsch[2], Manfred Albrecht[2], and Claas Abert[1] — [1]University of Vienna — [2]University of Augsburg

Surface acoustic wave (SAW) bandpass filters are an indispensable part of modern telecommunications infrastructure [1]. Spin waves (SWs) can be excited by SAWs in radio-frequency bands, making their coupling a topic of current scientific interest [2].

In this work, we utilize this magnon-phonon interaction to demonstrate the theoretical viability of a novel device composed of exchange-decoupled magnetic islets on a piezoelectric substrate. Depending on the magnetic orientation of neighboring islets, a shift in the dispersion relation of the SW is predicted to occur due to their stray field interaction. This shift increases or decreases the efficiency with which the SAW can excite the SWs, leading to a difference in the amount of energy the magnetic system absorbs. For certain geometries, a gap in the SAW power after traversing the device of 10 dB/mm or more is predicted to occur.

For this study, a new algorithm for efficiently calculating SAW attenuation under the assumption of a continuous signal was developed for the micromagnetic simulation library magnum.np [3].

[1] P. Delsing et al., J. Phys. D: Appl. Phys. 52, 353001 (2019).
[2] M. Küß et al., Phys. Rev. Appl. 15, 034046 (2021).
[3] F. Bruckner et al., Sci. Rep. 13, 12054 (2023).

MA 45.8 Fri 11:30 H18

Mean-Field Approximation and ab-initio calculations in Tetragonal Mn_2-based Heusler compounds. — •Jorge Cardenas-Gamboa[1,5], Arthur Ernst[2], Maia G Vergniory[3,4], Edouard Lesne[1], Claudia Felser[1], and Paul McClarty[6] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Johannes Kepler University of Linz, Linz, Austria. — [3]Donostia International Physics Center, Donostia-San Sebastian,Spain — [4]Université de Sherbrooke, Sherbrooke J1K 2R1 QC, Canada. — [5]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [6]Universite Paris-Saclay, Gif-sur-Yvette, France.

Achieving flexible control over magnetic properties is possible in multicomponent systems consisting of several magnetic sublattices with competing interactions.In 2014, Meshcheriakova et al. demonstrated that the Heusler compound Mn_2RhSn exhibits substantial strong noncollinearity and its magnetic structure undergoes a spin-reorientation transition, driven by the competition between its magnetic sublattices. In this work, we use a mean-field approximation to analyze the exchange interactions between the sublattices and investigate how different magnetic regimes develop as a function of temperature. Additionally, we perform first-principles calculations to derive the exchange interactions and assess their influence on the magnetic properties, extending our analysis to other tetragonal Heusler magnets. We then explore the topological properties that arise from the magnetism, focusing on the Weyl nodes and surface states.

MA 45.9 Fri 11:45 H18

First-Principles Study of Non-Collinear Magnets: Spin Models and Cluster Multipole Theory — •Juba Bouaziz[1,2], Takuya Nomoto[3], and Ryotaro Arita[1,2,4] — [1]RCAST, University of Tokyo, Japan — [2]CEMS, RIKEN (Wako), Japan — [3]Tokyo Metropolitan University, Japan — [4]Department of Physics, University of Tokyo, Japan

We present a computational approach for modeling complex non-collinear magnets using the cluster multipole (CMP) method [1] to determine symmetry-allowed magnetic configurations. The magnetic ground state is obtained by comparing the energies of candidate CMP solutions within a spin model Hamiltonian that includes isotropic exchange interactions, relativistic anisotropic terms, and higher-order biquadratic interactions. The parameters of the spin model are systematically calculated using the magnetic force theorem from the paramagnetic reference state [2]. This method is successfully applied to the TM3X Kagome magnet family (TM = Mn, Fe; X = Ga, Ge, Sn), demonstrating its computational efficiency and potential for high-throughput studies of unconventional non-collinear magnetic systems.

[1] M. T. Suzuki et al., Phys. Rev. B 95, 094406 (2017); [2] B. L. Gyorffy et al., J. Phys. F: Met. Phys. 15 1337 (1985).

MA 45.10 Fri 12:00 H18

Memory-Efficient Inverse Design for Advanced Magnonic Devices Using Level-Set Optimization — •Andrey Voronov[1,2], Marcos Cuervo Santos[2,3], Florian Bruckner[1,4], Dieter Suess[1,4], Andrii Chumak[1], and Claas Abert[1,4] — [1]Faculty of Physics, University of Vienna, Vienna, Austria — [2]Vienna Doctoral School in Physics, University of Vienna, Vienna, Austria — [3]Faculty of Sciences, University of Oviedo, Oviedo, Spain — [4]Research Platform MMM Mathematics - Magnetism - Materials, University of Vienna, Vienna, Austria

Inverse design in magnonics utilizes the wave nature of magnons and machine learning to develop logic devices with unique functionalities. However, existing methods face memory constraints, limiting the exploration of complex systems.

To address this, we integrate a level-set parameterization approach with an adjoint state method for memory-efficient simulations of magnetization dynamics. Implemented in neuralmag, a GPU-accelerated micromagnetic software, this framework enables efficient optimization of device topologies.

We validate the approach through two tasks: optimizing the shape of a magnetic nanoparticle to control hysteresis behavior and designing a 300-nm-wide yttrium iron garnet demultiplexer for frequency-selective spin-wave separation. These results showcase the algorithm's robustness and versatility in enabling the design of advanced magnonic devices for computational logic technologies.

MA 45.11 Fri 12:15 H18

Magnetoelectric coupling in type-I multiferroics via domain walls — •Aditya Putatunda and Sergey Artyukhin — Istituto Italiano di Tecnologia, Genova, Italy 16123

Type-I multiferroics, where ferroelectricity (FE) and magnetism arise independently with a large FE polarization but often tend to have a much weaker coupling to spins, e.g.: prototypical BiFeO3. Electric polarization, arising from inversion breaking, causes structural modifications across polarization domains in such materials. Here we demonstrate an effective coupling mechanism caused due to such structural modifications which in turn modifies the magnetic exchanges between the ions using first-principles density functional calculations. Magnetic domain walls, generally more mobile than polarization walls, depending on the nature of the materials, experience an effectively attractive or repulsive potential due to these modified exchanges. Such a potential can be taken advantage of in driving magnetic domain walls by sweeping polarization domains using electric field, thus giving rise to a cross-coupling mechanism, a highly sought phenomenon for novel low-power device applications.

MA 46: Surface Magnetism

Time: Friday 9:30–12:30 Location: H19

MA 46.1 Fri 9:30 H19

Investigation of the magnetic structure of Eu on W(110) — •Patrick Härtl[1], Vijayalaxmi Sankeshwar[1,2], Markus Leisegang[1], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Indian Institute of Science Education and Research(IISER), Pune, Maharashtra 411008, India

Rare earth metal (REM) films are renowned for their complex magnetic properties, primarily governed by the element-specific sign and wavelength of the RKKY interaction. Due to the complexity of their cleaning procedures, the magnetic domain structure of REM surfaces has remained largely unknown until today and is an ongoing topic of debate. In this study, we investigate the structural, electronic, as well as the complex magnetic structure of Europium (Eu) films on W(110) using spin-polarized scanning tunneling microscopy (SP-STM).

In the bulk, Eu has a half-filled $4f$- and an empty $5d$-shell and adopts a body-centered crystal structure. In thin epitaxial films, however, a metastable hexagonal close-packed structure is expected, accompanied by helical spin ordering below $T_{\text{Néel}} = 91$ K. With optimal preparation conditions, we successfully grew clean, smooth films. In the tunneling spectra of these Eu films we observed two intense peaks at positive bias voltages which we interpret as the unoccupied and exchange-split $5d_{z^2}$-like surface state. Beyond a critical film thickness, striped regions with a periodicity of $\approx$ 3 nm were identified. Experiments with differently magnetized STM tips and the application of an external magnetic field up to ± 2.5 T revealed the magnetic nature of the stripes.

MA 46.2 Fri 9:45 H19

The magnetic domain structure of Ho(0001)/W(110) — •Vijayalaxmi Sankeshwar[1,2], Patrick Haertl[2], and Matthias Bode[2] — [1]Indian Institute of Science Education and Research (IISER), Pune, Maharashtra 411008, India — [2]Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Rare-earth metal (REM) films exhibit diverse magnetic phenomena driven by the indirect RKKY coupling of localized $4f$ orbital moments, which promotes the formation of helical spin structures. Holmium (Ho), notable for its exceptionally high magnetic moment ($\approx 10\,\mu_B$), develops stable helical configurations across a wide temperature range [1]. In its bulk form, Ho crystallizes in a hexagonal close-packed structure, transitioning from a helical spin spiral state below $T_N = 131$ K to a conical magnetic state below $T_C = 20$ K. At reduced thicknesses, theoretical studies predict the emergence of intricate magnetic textures, including block spin structures [2].

We present an investigation of epitaxial Ho films grown on W(110) using spin-polarized scanning tunneling microscopy (SP-STM). Through a detailed, thickness-dependent analysis of the structural, electronic, and magnetic properties, we observed large in-plane magnetic domains spanning several hundred nanometers, interspersed with worm-like striped patterns exhibiting periodicities of $\approx$ 20 nm in the magnetic signal. Our findings provide valuable insights into the relationship between dimensionality and magnetic order in REM films.

[1] D. L. Strandburg *et al.*, Phys. Rev. **127**, 2046 (1962)
[2] E. Weschke *et al.*, Phys. Rev. Lett. **93**, 157204 (2004)

MA 46.3 Fri 10:00 H19

Influence of higher order interactions on the thermal behaviour of magnetic order in Mn/Re(0001) — •Leo Kollwitz[1], Moritz Alexander Goerzen[2,1], Hendrik Schrautzer[3,1], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [2]CEMES, Université de Toulouse, CNRS, France — [3]Science Institute and Faculty of Physical Sciences, University of Iceland, 107 Reykjavík, Iceland

Non-trivial multi-Q states, which consist of the superposition of periodically modulated spin textures, are known to arise in Mn monolayers on the Re(0001) substrate due to higher-order exchange interactions (HOI) [1]. However, to date little is known about the thermodynamic properties of these highly ordered phases. Here, we perform Monte Carlo simulations based on an atomistic spin model parametrized by density functional theory, in order to investigate thermal phase transitions in this material. It is found that the explicit consideration of HOI in the simulations leads to a significant decrease of the Néel temperature and to an introduction of a new transition between single-Q and multi-Q states at low temperatures. Recent experiments show that a similar transition occurs in $Co_{1/3}TaS_2$ [2]. By modelling the free energy landscape of the system in terms of thermal excitations, which are expressed in the eigenbasis of the Hamiltonian, we further identify the important degrees of freedom responsible for this additional entropy mediated transition.

[1] J. Spethmann *et al*, Phys. Rev. Lett. **124**, 227203 (2020)
[2] P. Park *et al*, Nat. Comm. **14**, 8346 (2023)

MA 46.4 Fri 10:15 H19

Anisotropic magnetic exchange in a metal-organic interface with $4f$ electrons: the case of Cu Phthalocyanine on $HoAu_2$ and $GdAu_2$ — •María Blanco-Rey[1,2,3], Rodrigo Castrillo[3], Frederik M. Schiller[3,2], and Laura Fernández[3] — [1]Universidad del País Vasco UPV/EHU, Spain — [2]Donostia International Physics Center DIPC, Spain — [3]Centro de Física de Materiales MPC-CSIC-UPV/EHU, Spain

Heterostructures formed by organic molecules on ferromagnetic substrates merge optoelectronic and spintronic functionalities. We have studied CuPc molecules deposited on monolayer-thick $REAu_2$ (RE=Ho, Gd) alloys, which exhibit long-range commensurability and vacuum level pinning of the LUMO. Many-body electron interactions renormalize the molecular levels. Here trivalent Ho and Gd species favour a downward shift of the HOMO, approaching ambipolarity [1]. The Curie temperatures are reduced from $\sim$ 20 K to $\sim$ 15 K due to CuPc, as the hybrid interfacial electronic structure affects the RKKY-mediated RE-RE exchange. The spin-orbit coupling of the RE leads to a dependence of the CuPc-RE antiferromagnetic exchange coupling constant $\mathscr{J}_{ex}$ on the field orientation, following the orbitally-dependent exchange (ODE) mechanism. ODE is enhanced by the large $L = 6$ value of trivalent Ho, yielding a ratio $\mathscr{J}_{ex}^{\parallel}/\mathscr{J}_{ex}^{\perp} = 4.2$, while the anisotropy is weak in the presence of Gd, with a half-field $4f$ shell [2].

[1] R. Castrillo et al, Nanoscale, 15, 4090 (2023).
[2] M. Blanco-Rey et al, Small, 20, 2402328 (2024).

MA 46.5 Fri 10:30 H19

Excitons design via topological spin-textures — •Karim Rezouali[1,2] and Samir Lounis[2,1] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Excitons are at the heart of many photonic and optoelectronic phenomena, including luminescence, lasing, and the operation of solar cells. Their study is essential for developing next-generation technologies, such as light-harvesting systems and quantum information devices. Here, we explore the impact of topological magnetism [1] on excitons by unveiling signatures of topology on the magnetic properties of excitons, their stability and manipulation. We address in particular skyrmions emerging in Pd/Fe/Ir(111) [2] surface, which affect the singlet and triplet exciton states hosted by a monolayer MoS_2 [3]. Our work promotes the use of skyrmions for the control and manipulation of excitons, which provides unprecedented opportunities for exciton-based devices.

[1] M. V. Berry, Proc. R. Soc. Lond. A 392, 45 (1984).
[2] N. Romming, A. Kubetzka, C. Hanneken, K. von Bergmann, and R. Wiesendanger, Phys. Rev. Lett. 114, 177203 (2015)
[3] M. Palummo, M. Bernardi, and J. C. Grossman, Nano Letters 15, 2794 (2015).
Project funded by DFG (SPP 2137: LO 1659/8-1).

MA 46.6 Fri 10:45 H19

Observation of the sliding phason mode of the incommensurate magnetic texture in Fe/Ir(111) — •Wulf Wulfhekel[1], Hung-Hsiang Yang[1], Louise Desplat[2], Volodymyr Kravchuk[1], Marie Hervé[1], Timofey Balashov[1], Simon Gerber[1], Markus Garst[1], and Bertrand Dupé[2] — [1]Karlsruhe Institute of Technology — [2]Université de Liège

The nanoscopic magnetic texture forming in a monolayer Fe/Ir(111) is uniaxially incommensurate with respect to the Ir(111) substrate. As a consequence, a low-energy magnetic excitation is expected that corresponds to the sliding of the texture along the incommensurate direction, i.e., a phason mode, that we confirm with atomistic spin simulations. Using Sp-STM, we observed this phason mode experimentally. It can be excited by the STM tip leading to a random telegraph noise in the tunneling current that we attribute to the presence of two minima in the phason potential due to the presence of disorder in the sample. This provides the prospect of a floating phase in cleaner samples and, potentially, a commensurate-incommensurate transition as a function of external control parameters.

15 min. break

MA 46.7 Fri 11:15 H19

Quantifying the interplay between local order and dynamics in a self-induced spin glass — •Lorena Niggli[1], Julian H. Strik[1], Anders Bergman[2], Mikhail I. Katsnelson[1], Daniel Wegner[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Nether- lands — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Spin glasses are a puzzling form of magnetic matter characterized by an amorphous spin texture in space. They exhibit ongoing magneti- zation dynamics that are often referred to as aging. However, direct experimental access to the spatially dependent magnetization and its link to aging, has been limited. Here, we study the spatiotemporal dy- namics of the self-induced spin glass state of Nd(0001) [1, 2]. To this end, we induce magnetization dynamics through magnetic field cycles and resolve the local order using spin-polarized scanning tunneling microscopy. We develop a new method to access the spatiotemporal dynamics based on a wavelet transformation. Using this, we quantify the Q-dependent local order in space and follow its evolution over time. Together this provides insight into the complex energy landscape of a (self-induced) spin glass. [1] Kamber et al., Science 368 (2020). [2] Verlhac et al., Nature Physics 18 (2022).

MA 46.8 Fri 11:30 H19

Bilayer triple-Q state driven by interlayer higher-order exchange interactions — •Bjarne Beyer, Mara Gutzeit, Tim Drevelow, Isabel Schwermer, Soumyajyoti Haldar, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

Superpositions of spin spirals – so-called multi-Q states – are complex spin structures which are of fundamental interest and promising for future spintronic applications. A prominent example is the triple-Q state predicted more than 20 years ago [1] and only recently observed in Mn monolayers on the Re(0001) surface [2,3]. Here, we predict a triple-Q state as the magnetic ground state of a Mn bilayer on the Ir(111) surface using first-principles calculations based on density functional theory (DFT). In a bilayer two types of the triple-Q state can occur which differ by the spin alignment between the layers. Based on an atomistic spin model, we demonstrate that the triple-Q state favored by DFT is stabilized by the interplay of antiferromagnetic interlayer exchange and interlayer higher-order exchange interactions. In this bilayer triple-Q state nearest-neighbor spins within a layer and between layers exhibit tetrahedron angles and the topological orbital moments of the two Mn layers are aligned in parallel [4].

[1] P. Kurz *et al.*, PRL **86**, 1106 (2001).
[2] J. Spethmann *et al.*, PRL **124**, 227203 (2020).
[3] F. Nickel *et al.*, PRB **108**, L180411 (2023).
[4] V. Saxena *et al.*, arXiv:2408.12580 (2024).

MA 46.9 Fri 11:45 H19

Antiferromagnetic merons in a Mn monolayer on Ta(110) — •Tim Drevelow[1], Felix Zahner[2], André Kubetzka[2], Roland Wiesendanger[2], Stefan Heinze[1], and Kirsten von Bergmann[2] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstraße 15, 24098 Kiel, Germany — [2]Department of Physics, University of Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany

Non-collinear topological spin structures in ultrathin transition-metal films are interesting for spintronic applications. When hosted in antiferromagnets, they are robust to external perturbations, possess vanishing demagnetization fields, and the Skyrmion-Hall effect does not occur. Ultrathin Mn-layers are intrinsically antiferromagnetic and exhibit non-collinear spin structures, such as the conical spin structure in Mn on W(110) [1]. Here, using spin-polarized scanning tunneling microscopy and density functional theory, we discover a cycloidal spin spiral and a c(2 × 2) antiferromagnet in Mn mono- and double-layers on the Ta(110) surface, respectively. Micromagnetic simulations on the sublattice reveal a transition of spin spirals into antiferromagnetic, meronic spin structures of non-trivial topology near the interface to the collinear antiferromagnet of the film due to competing anisotropies of the Mn mono- and double-layer.

[1] Yoshida *et al.* Phys. Rev. Lett. **108**, 087205 (2012)

MA 46.10 Fri 12:00 H19

Magnetic bi-stability of columnar Transition-metal-oxide molecules on MgO films — •SUFYAN SHEHADA[1,2], Manuel dos Santos Dias[3], Muayad Abusaa[2], and Samir Lounis[1,4] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, Arab American University, Jenin, Palestine — [3]Scientific Computing Department, STFC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom — [4]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

At the heart of quantum information technology is the realization of stable atomic magnetic bits, which partly hinges on large out-of-plane magnetic anisotropy energy (MAE). Although the seminal work of Rau et al.[1] reported the maximum MAE for a 3d element by positioning a Co atom on MgO(100) [1], the system did not exhibit magnetic bi-stability. Motivated by that work, we explore via density functional theory (DFT) simulations columnar oxide molecules made of transition metals (TM-O), which might show large MAE while reducing the hybridization of the adatoms' electronic states with those of the substrate, increasing the chances of magnetic bi-stability. Following our initial investigations based on 3d elements [2], we address here the case of 4d atoms and focus on the scenario where the TM atoms are decoupled from the surface via an Oxygen atom.

–Work funded by (BMBF–01DH16027).

[1] Rau *et al.*, Science **344**, 988 (2014). [2] Shehada *et al.*, ArXiv:2403.05432, accepted in PRB (2024).

MA 46.11 Fri 12:15 H19

Tailoring magnetism in a 2D Van der Waals material with a chemical approach for magnonic applications — •Sourav Dey, Gonzalo Rivero, and José Baldoví — ICMol, University of Valencia, Valencia, Spain

The discovery of two-dimensional (2D) magnets offers an ideal platform for magnonics and spintronics at the limit of miniaturization given their high flexibility and tunability.The magnetic properties of this family of materials have been tuned by several approaches such as strain engineering, atomic layer substitution, or molecular deposition, among others. In the latter case, the effect of organometallic/inorganic complexes on the magnetic properties of 2D magnetic materials is still unexplored. To investigate this, we have selected two molecular qubits (quantum bits) with long coherence time such as CpTiCOT (Cp = η5-cyclopentadienyl, COT = η8-cyclooctatetraene) and VOPc (Pc = phthalocyanine) which are proved to be stable after the deposition on metallic substrate. Here, we analyze and interpret the magnetic properties of single-layer CrSBr after deposition of CpTiCOT and VOPc, via first-principles calculations. Our results predict a significant modulation of magnetic exchange in CrSBr after deposition due to the significant charge transfer from the molecules to 2D material, allowing us to corroborate both properties. Furthermore, a significant change in the magnon frequencies and group velocities was observed, which opened new avenues in designing smart molecular/2D materials where magnons can be fine-tuned by a chemical approach.

MA 47: Altermagnets III

Time: Friday 9:30–11:00 Location: H20

MA 47.1 Fri 9:30 H20

Growth and spectroscopy of altermagnetic MnTe — •Marco Dittmar, Lena Hirnet, Hannes Haberkamm, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

As a new type of fundamental magnetic order next to ferro- and antiferromagnetism, altermagnetism has recently attracted great attention [1]. It is characterized by antiferromagnetic spin alignment combined with rotational lattice symmetry, which results in a momentum-dependent spin-split band structure with spin polarized electronic states. One of the "workhorse" materials potentially exhibiting this type of magnetic order is MnTe in its hexagonal NiAs-type crystal structure [1,2]. Here, we investigate MnTe thin films grown by molecular beam epitaxy. The high film quality is confirmed by structural characterization methods, while we assess the three-dimensional bulk band structure using soft X-ray angle-resolved photoemission spectroscopy. The experimentally observed spectral features agree well with band structure calculations and — based on that — the possible occurance of the characteristic momentum-dependent spin splitting will be discussed.

[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 031042 (2022)
[2] J. Krempaský *et al.*, *Nature* **626**, 517-522 (2024)

MA 47.2 Fri 9:45 H20

Phonon-mediated unconventional superconductivity in altermagnets: A solid-state analog of the A_1 phase of superfluid Helium 3 — •Kristoffer Leraand[1], Kristian Maeland[2], and Asle Sudbø[1] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We have considered the possibility of phonon-mediated unconventional superconductivity in a recently discovered new class of antiferromagnets, dubbed altermagnets. Within a weak-coupling approach, and using a minimal band model for altermagnets [1], we have found a dominant superconducting instability odd in momentum and even in spin with fully spin-polarized Cooper pairs, a 2D solid-state analog of the A_1-phase of superfluid Helium 3 [2]. We discuss the origin of this unusual result in terms of phonon-modes and electron form factors. [1] B. Brekke, A. Brataas, and A. Sudbø, PRB 108, 224421 (2023). [2] G. Volovik, The Universe in a Helium Droplet, Oxford Science Publications (2003).

Work supported by Norwegian Research Council, through Grant No. 262633, "Center of Excellence on Quantum Spintronics", as well as Grant No. 323766.

MA 47.3 Fri 10:00 H20

Non-linear anomalous Edelstein response at altermagnetic interfaces — •Mattia Trama[1,2], Irene Gaiardoni[3], Claudio Guarcello[3,4], Jorge I. Facio[5], Alfonso Maiellaro[3,6], Francesco Romeo[3,4], Roberta Citro[3,4,6], and Jeroen van den Brink[1,2] — [1]IFW Dresden — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Università degli studi di Salerno — [4]INFN - Sezione collegata di Salerno — [5]Centro Atomico Bariloche, Instituto de Nanociencia y Nanotecnologia (CNEA-CONICET) and Instituto Balseiro — [6]CNR-SPIN

In altermagnets, time-reversal symmetry breaking spin-polarizes electronic states, while total magnetization remains zero. In addition, at altermagnetic surfaces Rashba-spin orbit coupling is activated due to broken inversion symmetry, introducing a competing spin-momentum locking interaction. Here we show that their interplay leads to the formation of complex, chiral spin textures that offer novel, non-linear spin-to-charge conversion properties. Whereas altermagnetic order suppresses the canonical linear in-plane Rashba-Edelstein response, we establish the presence of an anomalous transversal Edelstein effect for planar applied electric and magnetic field, or alternatively, an in-plane magnetization. Moreover the non-linear Edelstein response resulting purely from electric fields also triggers the anomalous out-of-plane magnetization. We determine the anomalous response with a model based on the ab-initio electronic structure of RuO2 bilayers, ultimately opening experimental avenues to explore spin-charge conversion phenomena at altermagnetic interfaces.

MA 47.4 Fri 10:15 H20

A Heisenberg model for g-wave altermagnets: the comparative analysis of CrSb and MnTe — •Volodymyr Kravchuk[1,2], Kostiantyn Yershov[1,2], Oleg Janson[1], and Jeroen van den Brink[1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine

Here we construct a discrete Hamiltonian of the magnetic subsystem of altermagnets belonging to the crystallographic group 6/*mmm*. The altermagnetic properties are captured through the additional Heisenberg exchange interactions whose symmetry respects the positions of the nonmagnetic atoms. We derive the dispersion relation for magnons for two opposite cases of magnetocrystalline

anisotropy: easy-axis (as for CrSb) and easy-plane (as for MnTe). Due to the different magnetic ground states of CrSb and MnTe, their magnon spectra are drastically different. While the splitting of the magnon bands of CrSb possesses the g-wave symmetry, the splitting of the magnon bands of MnTe does not alternate sign within the Brillouin zone and does not possess g-wave symmetry. We formulate the continuous approximation of the model and derive the expression for magnetization of the noncollinear magnetization structures. We find that the amplitude of the magnetization of a domain wall in CrSb depends on the domain wall orientation relative to crystallographic axes, and determine twelve orientations that correspond to the maximal magnetization.

MA 47.5 Fri 10:30 H20

P-wave magnetism and spin symmetries — •Anna Birk Hellenes[1], Tomáš Jungwirth[2,3], Rodrigo Jaeschke-Ubiergo[1], Atasi Chakraborty[1], Jairo Sinova[1,4], and Libor Smejkal[1,2,5,6] — [1]JGU Mainz — [2]Czech Academy of Sciences — [3]University of Nottingham — [4]Texas A&M University — [5]MPI-PKS — [6]MPI-CPfS

The recent discovery of altermagnets was enabled by an unorthodox symmetry toolbox, crystallographic spin groups, allowing for the rigorous delineation of all collinear spontaneous exchange symmetry breakings. This raises a question: are further magnets with hitherto unknown symmetries and electronic structures hiding in plain sight? Our contribution will start with a brief history of a century-long debate on whether p-wave magnetic orders can exist. We will resolve this debate by demonstrating p-wave magnetism using the spin group formalism. We show that a collinear p-wave order arises in coplanar magnets for a subclass of noncentrosymmetric, noncollinear magnets with a combined translation and time-reversal symmetry. Contrary to common assumptions, we establish that such magnets can display non-relativistic spin-split electronic band structures. We demonstrate that these splittings preserve time-reversal symmetry, starkly contrasting splittings in ferromagnets and altermagnets, which break it. With first-principles calculations and symmetry analysis, we predict large, non-relativistic spin-splittings of several hundred meV and identify more than 40 realistic material candidates. Our work opens a wide range of possibilities for studying p-wave magnetism and using it for spintronics and topological physics. arXiv:2309.01607v3

MA 47.6 Fri 10:45 H20

Spin polarons in Altermagnets — •Maria Daghofer[1], Krzysztof Wohlfeld[2], and Jeroen van den Brink[3] — [1]FMQ, Universität Stuttgart, Stuttgart, Germany — [2]University of Warsaw, Warsaw, Poland — [3]IFW Dresden, Dresden, Germany

We numerically investigate hole motion in altermagnetic Mott insulators, beyond the weakly interacting case, where a mean-field description is applicable. In this strongly correlated regime, hole motion is strongly affected by coupling to quantum fluctuations of the magnetic background. We find that the underlying altermagnetic symmetries manifest themselves in spin-momentum locking of the coherent quasi-particle: At certain momenta, it has a spin-polarized character, while states corresponding to the opposite spin are considerably more incoherent. We also address the impact of quantum fluctuations.

MA 48: Ultrafast Magnetization Effects II

Time: Friday 11:15–13:00 Location: H20

MA 48.1 Fri 11:15 H20

Measurement of time resolved magneto-optic Kerr effect on ruthenium dioxide — •Holger Grisk[1], Maik Gaerner[2], Jakob Walowski[1], Timo Kuschel[2], and Markus Münzenberg[1] — [1]Institute of Physics, Greifswald University, Germany — [2]Faculty of Physics, Bielefeld University, Germany

Altermagnetism is a novel fundamental phase of magnetism with exciting properties such as spin split bands.Ruthenium dioxide is one of the mostly investigated altermagnetic candidates. The antiparallel alignment of the Ru spins along with the anisotropic distribution of oxygen atoms leads to time reversal symmetry breaking and non-relativistic, anisotropic spin-splitting in the band structure. We used the time-resolved magneto-optic Kerr effect to measure the transient Kerr angle and reflectivity change after excitation with a femtosecond laser pulse to access the potential magnetic properties of ruthenium dioxide. The setup for the measurement exploits the pump-probe technique. A femtosecond laser pulse is split into a powerful pump and a low-power probe beam. The pump beam is used to photoexcite the electrons in the ruthenium dioxide. The probe beam is used to measure the shift in the Kerr rotation. Delaying the pump temporally and probing the evolution of the Kerr signal we can measure the ultrafast spin dynamics of ruthenium dioxide. The measurement shows Terahertz dynamics in the Kerr signal that is an order of magnitude faster than conventional ferromagnets. The studies were performed at room temperature and with small in plane magnetic field.

MA 48.2 Fri 11:30 H20

Dynamical renormalization of the magnetic excitation spectrum via high-momentum nonlinear magnonics — •Julian Bär[1], Lennart Feuerer[1], Alfred Leitenstorfer[1], Dominik Juraschek[2], and Davide Bossini[1] — [1]Department of Physics and Center for Applied Photonics, University of Konstanz, D-78464 Konstanz, Germany — [2]Department of Applied Physics and Science Education, Eindhoven University of Technology, Eindhoven, Netherlands

Manipulating the macroscopic properties of solids with light is a key challenge in condensed matter physics. While resonantly driving low-momentum collective excitations has led to nonlinear lattice and spin dynamics [1,2], controlling magnon spectra in terms of amplitude and frequency remains unexplored. In my talk I will discuss the resonant excitation of pairs of high-momentum magnons in Hematite (α-Fe2O3). By exciting hematite in its weak-ferromagnetic phase, our approach results in a direct coupling between high- and low-momentum magnons. In particular, the spectrum of the latter is modified. This astonishing effect is explained with a resonant light-scattering mechanism that couples high- and low-momentum eigenmodes across momentum space [3]. As hematite undergoes a phase transition at 260 K to a collinear antiferromagnetic state, we have developed a cryogenic pump-probe setup. Preliminary results reveal behaviour distinct from that observed in the weak ferromagnetic phase. [1] A. S. Disa et al., Nat Phys 17, 1087-1092 (2021). [2] Z. Zhang et al., Nat Phys., 1-6 (2024). [3] C. Schoenfeld et al., arXiv:2310.19667 (2024)

MA 48.3 Fri 11:45 H20

Bias field studies of all-optical helicity-dependent switching. — •Kevin Jäckel[1], Marcel Kohlmann[1], Jakob Walowski[1], Markus Münzenberg[1], Yuta Sasaki[2], and Karel Carva[3] — [1]University of Greifswald, Germany — [2]Research Center for Magnetic and Spintronic Materials, Japan — [3]Charles University, Czech Republic

The mechanisms underlying all-optical helicity-dependent switching AOHDS need a better understanding to improve the process towards single pulse switching. We apply external magnetic fields (anti-) parallel of up to $H_{\mathrm{ext}} = 72\,\mathrm{mT}$, (opposing) supporting the desired magnetization direction in FePt granular media to disentangle the contribution of the inverse Faraday effect IFE within the switching process. Those measurements, performed on samples with varying average grain size diameters of $d = 10\,\mathrm{nm}$, $d = 6\,\mathrm{nm}$ nm, and $d = 4\,\mathrm{nm}$, reveal a grain size dependent impact of the applied field strength. Using the helicity-dependent refractive index calculated from density functional theory (DFT) calculations, we calculate the absorbed laser fluence for each grain size using the transfer matrix method. The absorption data, combined with the inverse Faraday constant, allows us to quantify the optically induced magnetization ΔM by the IFE. From this data, we can estimate the contribution of the IFE to the switching process. The research is funded by DFG, Fundamental aspects of all-optical pulse switching in nanometer-sized magnetic storage media Project number: 439225584.

MA 48.4 Fri 12:00 H20

Terahertz study of antiferromagnetic resonance in α MnTe — •Michal Šindler[1], Roman Tesař[1], Karel Výborný[1], Stáňa Tazlerů[1], Christelle Kadlec[1], Peter Kubaščík[2], Lukáš Nádvorník[2], Marcin Bialek[3], Jan Dzian[2,4], and Milan Orlita[4] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]Institute of High Pressure Physics Polish Academy of Sciences, Warszawa, Poland — [4]Laboratoire National des Champs Magnétiques Intenses, Université Grenoble Alpes, CNRS-UPS-INSA-EMFL, Grenoble, France

Antiferromagnetic resonance in bulk α-MnTe crystal was studied in the terahertz (THz) range. First, we will describe the three experimental methods used: (i) infrared Fourier transform spectroscopy,(ii) time-domain THz spectroscopy, and (iii) frequency-domain terahertz spectroscopy with linearly and circularly polarized THz beams. Second, we will present experimental results featuring a magnon mode ($k = 0$) with the low-temperature energy of 3.5 meV and its temperature and magnetic field evolution. Finally, we will show how to extract the out-of-plane component of the single-ion magnetic anisotropy $D \approx 40\,\mu$eV using a simple spin model of antiferromagnetic resonance in an easy-plane antiferromagnet.

MA 48.5 Fri 12:15 H20

Indications of terahertz spin transport in the altermagnet candidate RuO2 — •Oliver Gueckstock[1], Clara Simons[1], Maik Gaerner[2], Zdenek Kaspar[3], Jiri Jechumtal[3], Tom S. Seifert[1], Lukas Nadvornik[3], Günter Reiss[2], and Tobias Kampfrath[1] — [1]FU Berlin — [2]U Bielefeld — [3]Charles University Prague

The recently emerging material class of altermagnets has large potential to offer properties like strong spin splitting, which are so far rather typical for classical ferromagnets [1]. RuO2 appears to be a promising metallic altermagnet candidate with huge spin splitting in the electronic band structure and for photoinduced spin and orbital transport with a Néel temperature above room temperature [1,2]. Here, we apply femtosecond laser pulses to RuO2(110)|HM stacks consisting of a twinned RuO2 layer and a heavy-metal layer HM of Pt or W. We observe THz emission signals with distinct pump-polarization dependence. The signals change sign when HM=Pt is replaced by W and exhibit a marked temperature dependence, thereby suggesting a magnetism-related signal origin. We discuss possible mechanisms of THz-signal generation, including an ultrafast photoinduced spin current from RuO2 to HM and its conversion into in-plane charge in HM, which gives rise to the emission of a THz electromagnetic pulse.

[1] Smejkal et al., Phys Rev. X 12, 040501 (2022)
[2] Adamantopoulos et al., npj spintronics 2, 46 (2024)

MA 48.6 Fri 12:30 H20

THz emission control in exchange-coupled spintronic emitters. — •Roman Adam[1], Derang Cao[1,2], Daniel Bürgler[1], Sarah Heidtfeld[1], Christian Greb[1], Fangzhou Wang[1], Debamitra Chakraborty[3], Jing Cheng[3], Ivan Komissarov[3], Markus Büscher[1], Martin Mikulics[4], Hilde Hardtdegen[4], Roman Sobolewski[3], and Claus Schneider[1] — [1]Research Centre Jülich, Peter Grünberg Institute (PGI-6), 52425 Jülich, Germany — [2]College of Physics, Qingdao University, 266071 Qingdao, China — [3]University of Rochester, Rochester, New York 14627-0231, USA — [4]Research Centre Jülich, Ernst Ruska Centre (ERC-2), 52425 Jülich, Germany

Optical laser pulses impinging at the ferromagnet/metal thin film stacks can generate a pico-second electro-magnetic transients with frequency content extending into THz frequency range. We fabricated Si/SiO2//Ta/Fe/Ru/Ni/Al2O3 and Si/SiO2//Pt/Fe/Cr/Fe/Pt spintronic THz emitters in which we varied interlayer exchange coupling between the ferromagnetic thin films by varying the thicknesses of either the Ru or Cr spacer layer. As a result, THz emission shows a dramatic variation of amplitude in weak external magnetic fields due to an interference of THz transiens generated at the individual Fe/Ru, Ru/Ni or Fe/Pt emitters. We explore the effect of the ambient temperature and the spacer layer thickness variations on the THz amplitude.

MA 48.7 Fri 12:45 H20

On-Chip Multilayer Spintronic THz Emitters — •Wolfgang Hoppe[1], Amine Wahada[2], Stuart Parkin[3], and Georg Woltersdorf[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany — [2]Department of Physical Chemistry, Fritz Haber Institute, Faradayweg 4-6, 14195 Berlin, Germany — [3]Max Planck Institute for Microstructured Physics, Weinberg 2, 06120 Halle, Germany

Nanometer thin ferromagnet/heavy metal bilayers illuminated by intense short laser pulses have proven to be a realiable source for THz emission [1]. When integrated into a gold waveguide structure, the bilayer can be used as an on-chip source for ultrafast current pulses from the GHz to the THz regime [2]. Stacking severeral bilayers, each separated by a thin MgO interlayer enhances the charge current amplitude, as the MgO suppresses spin-currents in between the individual bilayers [3]. In this way we construct multilayers where all charge currents add up constructively, enhancing the signal up to a factor of three. As one possible application these ultrafast currents could be used to switch the magnetization of an adjacent ferromagnet, similar to previous experiments [4]. Electro-optic sampling is employed to characterize the charge current with sub-ps time resolution.

[1] Seifert et al., Nat. Photonics 10 (2016) 438-488
[2] W. Hoppe et al., ACS. Appl. Nano Mater. 4,7 (2021) 7454-7460
[3] A. Wahada et al., ACS Nano Lett. 22, 9 (2022) 3539-3544
[4] Y. Yang et al., Sci. Adv. 3, 11 (2017) e1603117

Metal and Material Physics Division
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Overview of Invited Talks and Sessions

(Lecture halls H10, H22, and H23; Poster P2)

Invited and Topical Talks

MM 2.1	Mon	9:30–10:00	H10	**Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations** — •Roger De Souza
MM 5.1	Mon	15:00–15:30	H10	**Room-temperature dislocations in oxide ceramics: from understanding to active engineering** — •Xufei Fang
MM 10.1	Tue	9:30–10:00	H10	**Understanding the impact of disconnection flow on microstructure evolution** — •Marco Salvalaglio
MM 11.1	Tue	10:15–10:45	H10	**The role of disconnections in the shear-migration coupling of grain boundaries** — •Marc Legros, Armin Rajabzadeh, Romain Gautier, Nicolas Combe, Frédéric Mompiou
MM 11.4	Tue	11:30–12:00	H10	**Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics** — •Fadi Abdeljawad
MM 11.7	Tue	12:30–13:00	H10	**Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling** — •Helene Zapolsky, Gilles Demange, Yuri Borges Gomes Lima, Anastasiai Titova, Renaud Patte
MM 13.1	Tue	14:00–14:30	H10	**Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles** — •Eugen Rabkin, Jonathan Zimmerman
MM 15.1	Wed	9:30–10:00	H10	**Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties** — •Christina Scheu, Ruben Bueno Villoro, Siyuan Zhang, Baptiste Gault, Duncan Zavanelli, Gerald Jeffrey Snyder
MM 16.1	Wed	10:15–10:45	H10	**Microstructure and transport in model isotropic amorphous solids** — •Peter Derlet
MM 16.5	Wed	11:45–12:15	H10	**Structural relaxation and deformation of bulk metallic glasses** — •Gerhard Wilde
MM 19.1	Wed	15:00–15:30	H10	**Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys** — •Laure Bourgeois, Nikhil Medhekar, Matthew Weyland
MM 20.1	Wed	15:45–16:15	H10	**Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting** — •Paola Tiberto
MM 20.5	Wed	17:15–17:45	H10	**Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations** — Johannes Sandberg, Leon F. Granz, •Thomas Voigtmann
MM 20.7	Wed	18:00–18:30	H10	**The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys** — •Ralf Busch
MM 25.1	Thu	9:30–10:00	H10	**Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments** — •David Rodney
MM 33.1	Fri	9:30–10:00	H10	**Fatigue in steels: Micromechanical modelling of cyclic damage** — •Petra Sonnweber-Ribic, Alexandra Stark, Christian Elsässer

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli

SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

MM 1.1–1.1	Sun	16:00–18:15	H15	**Tutorial: Automated Worksflows (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	H10	**Invited Talk: R. de Souza**
MM 3.1–3.10	Mon	10:15–13:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 4.1–4.11	Mon	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**
MM 5.1–5.1	Mon	15:00–15:30	H10	**Invited Talk: X. Fang (joint session MM/KFM)**
MM 6.1–6.10	Mon	15:45–18:30	H10	**Phase Transformations**
MM 7.1–7.5	Mon	15:45–17:00	H22	**Materials for the Storage and Conversion of Energy**
MM 8.1–8.5	Mon	17:15–18:30	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 9.1–9.74	Mon	18:30–20:30	P1	**Poster**
MM 10.1–10.1	Tue	9:30–10:00	H10	**Topical Talk: M. Salvalagio**
MM 11.1–11.7	Tue	10:15–13:00	H10	**Topical Session: Defects of Defects**
MM 12.1–12.10	Tue	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**
MM 13.1–13.5	Tue	14:00–15:30	H10	**Topical Session: Defects of Defects**
MM 14.1–14.5	Tue	14:00–15:15	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 15.1–15.1	Wed	9:30–10:00	H10	**Invited Talk. C. Scheu**
MM 16.1–16.8	Wed	10:15–13:00	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 17.1–17.9	Wed	10:15–12:45	H22	**Development of Calculation Methods**
MM 18.1–18.11	Wed	10:15–13:15	H23	**SYMD contributed**
MM 19.1–19.1	Wed	15:00–15:30	H10	**Invited Talk: L. Bourgois**
MM 20.1–20.7	Wed	15:45–18:30	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 21.1–21.11	Wed	15:45–18:30	H22	**Interface Controlled Properties, Nanomaterials and Microstructure Design**
MM 22.1–22.4	Wed	15:45–16:45	H23	**Materials for the Storage and Conversion of Energy**

MM 23.1–23.5	Wed	17:15–18:30	H23	**Phase Transformations**
MM 24	Wed	18:45–20:45	H10	**Members' Assembly**
MM 25.1–25.1	Thu	9:30–10:00	H10	**Invited Talk: D. Rodney**
MM 26.1–26.6	Thu	10:15–11:45	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 27.1–27.10	Thu	10:15–13:00	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 28.1–28.5	Thu	10:15–11:30	H23	**Mechanical properties**
MM 29.1–29.3	Thu	12:00–12:45	H10	**Liquid and Amorphous Materials**
MM 30.1–30.5	Thu	11:45–13:00	H23	**Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)**
MM 31.1–31.11	Thu	15:00–18:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 32.1–32.10	Thu	15:00–17:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 33.1–33.1	Fri	9:30–10:00	H10	**Invited Talk: P. Sonnweber-Ribic**
MM 34.1–34.7	Fri	10:15–12:15	H10	**Development of Calculation Methods**
MM 35.1–35.6	Fri	10:15–11:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 36.1–36.10	Fri	10:15–13:00	H23	**Mechanical Properties**
MM 37.1–37.3	Fri	12:00–12:45	H22	**Functional and Complex Materials**

Members' Assembly of the Metal and Material Physics Division

Wednesday 18:45–20:45 H10

Room	Montag, 17.3. H10	H22	H23	H1	Dienstag, 18.3. H10	H22	H23	Mittwoch, 19.3. H10	H22	H23	Donnerstag, 20.3. H10	H22	H23	Freittag, 21.3. H10	H22	H23
08:30	Plenary Talk				Plenary Talk			Plenary Talk			Plenary Talk			Plenary Talk		
08:45																
09:00																
09:15																
09:30	Invited Talk R. de Souza MM2				Topical Talk M. Salvalaglio MM10			Invited Talk C. Scheu MM15			Invited Talk D. Rodney MM25			Invited Talk Sonnweber-Ribic MM33		
09:45																
10:00																
10:15	Big Data MM3	Energy Materials			Topical: Defects MM11	Energy Materials MM12		Topical: BMG MM16	Calc. Methods MM17	SYMD contr. MM18	Topical: BMG MM26	Transport MM27	Mechanical Properties MM28	Calc. Methods MM34	Transport MM35	Mechanical Properties MM36
10:30																
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11:45	Big Data MM3	Energy Materials MM4						Topical: BMG MM16	Calc. Methods MM17	SYMD contr. MM18	Liquid and Amorphous Met. MM29	Transport MM27	Functional & Complex Materials MM30	Calc. Methods MM34	Complex MM37	Mechanical Properties MM36
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14:00	Plenary Talk Jörg Neugebauer (MM) H2				Topical: Defects MM13	Energy Materials MM14		Plenary Talk			Plenary Talk					
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15:00	Invited Talk X. Fang MM5			SYMD AI-driven Materials Design AudiMax				Invited Talk L. Bourgeois MM19			Big Data MM31	Transport MM32				
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15:45	Phase Trafo MM6	Energy Materials MM7						Topical: BMG MM20	Nanomaterials MM21	Energy Materials MM22						
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17:15	Phase Trafo MM6	Energy Materials MM8						Topical: BMG MM20		Phase Trafo MM23						
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18:15																
18:30	MM Poster Session P2 MM9							Bier & Brezeln								
18:45																
19:00								Member's Assembly MM Devision (all contributors) MM24 H10 best MM poster awards								
19:15																
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19:45																
20:00																
20:30																

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

MM 1: Tutorial: Automated Worksflows (joint session MM/TUT)

Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: H15

Tutorial MM 1.1 Sun 16:00 H15

Hands-on Tutorial: Automated Workflows and Machine Learning for Materials Science Simulations — •Jörg Neugebauer[1], Tilmann Hickel[2], and Ralf Drautz[3] — [1]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [2]BAM, Berlin, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application.

In this hands-on tutorial, we provide an interactive, practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The tutorial gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, all steps of the workflow for the construction of ab initio phase diagrams will be performed interactively by all participants, e.g. the generation of DFT datasets, the training and validation of machine learning potentials as well as the construction of the phase diagram.

MM 2: Invited Talk: R. de Souza

Time: Monday 9:30–10:00 Location: H10

Invited Talk MM 2.1 Mon 9:30 H10

Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

Simulation studies play a central role, in interpreting and explaining experimental data on ion transport, in providing insights at the atomic scale, and in predicting data for new systems. Ion migration in ABX_3 perovskites has been examined with both molecular-static and molecular-dynamic calculations, employing classical pair potentials, reactive force-fields or quantum-mechanical calculations.

In this contribution, taking ion migration in $BaTiO_3$, $CaTiO_3$, and $MAPbI_3$ as examples, I draw attention to problems that may arise when using molecular-static calculations to obtain activation barriers for higher symmetry perovskite phases. In general, a far more critical consideration of simulation results in the literature is required.

MM 3: Data-driven Materials Science: Big Data and Worksflows

Machine Learning, Potential Development

Time: Monday 10:15–13:00 Location: H10

MM 3.1 Mon 10:15 H10

Benchmarking DFT Functionals at Finite Temperature with ASSYST and MLIPs — •Marvin Poul and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien

A key ingredient to the accuracy of Density Functional Theory (DFT) calculations is the chosen approximation to the exchange-correlation functional. Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) calculations often bracket experimental observations, but systematic exploration of the behavior of different density functionals is hindered by the high computational cost of DFT in realistic applications, especially concerning finite temperature properties. Using the ASSYST[1] method, we automatically generate unary, general purpose Atomic Cluster Expansion (ACE) Machine Learning Interatomic Potentials (MLIPs) for a range of metals using LDA, PBE and r2SCAN functionals. The key advantage of ASSYST lies in the small cells ($\leq$ 10 atoms per cell) that it generates as training data. This allows us to relabel the data using different functionals very efficiently. We then use these potentials to calculate melting curves, thermal expansion, and formation energies of various defects (grain boundaries, surfaces, point defects) to systematically assess strengths and weaknesses of the DFT functionals. In general, we find good agreement with corresponding DFT results, showing that ASSYST can reliably create transferable potentials for metals at DFT accuracy.

[1]: https://www.researchsquare.com/article/rs-4732459/v1

MM 3.2 Mon 10:30 H10

Assessing the role of physical constraints in machine learning potentials — •Marcel F. Langer, Sergey N. Pozdnyakov, Filippo Bigi, and Michele Ceriotti — Laboratory of Computational Science and Modeling (COSMO) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Machine learning potentials, which approximate the potential energy surface of atomistic systems to enable larger and longer simulations than first-principles methods, have advanced rapidly in recent decades. Much of this development has been driven by the increasingly sophisticated treatment of physical symmetries, in particular invariances, in the underlying machine learning models. However, the rise of so-called unconstrained models, which replace exact invariance with learned approximations, has sparked debate over this approach. Some models even choose to directly predict forces, rendering the resulting force fields non-conservative. We investigate the effectiveness of such models and evaluate the impact of disregarding physical constraints for practical simulations. In particular, we study the effects of breaking rotational symmetry in a machine-learning potential for water [1] and discuss the potential consequences of direct force predictions.

[1]: M.F. Langer, S.N. Pozdnyakov, and M. Ceriotti, Mach. Learn.: Sci. Technol. 5 04LT01 (2024)

MM 3.3 Mon 10:45 H10

Fast and flexible range-separated models for atomistic machine learning — •Philip Loche, Marcel F. Langer, and Michele Ceriotti — Laboratory of Computational Science and Modeling (COSMO), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Most machine learning (ML) interatomic potentials rely on a locality ansatz, decomposing energy into short-ranged, atom-centered contributions. This limits their ability to describe problems dominated by long-range physical effects, such as electrostatics. We present a framework integrating established algorithms for non-bonded interactions – including Ewald summation, PME, and P3M – into atomistic ML. Reference implementations are provided in PyTorch and JAX. Beyond Coulomb potentials, we introduce Exterior Potential Features for general long-range ML applications. Our modular libraries enable accurate physical force evaluations, seamless integration with local ML schemes via automatic

differentiation, and flexible architectures for advanced models. We benchmark these tools for molecular dynamics, range-separated ML potentials, and long-range atomic descriptors.

MM 3.4 Mon 11:00 H10

Beyond Numerical Hessians: Applications for Higher Order Derivatives in Machine Learning Interatomic Potentials — •Nils Gönnheimer[1,2], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]University of Bayreuth — [2]Fritz-Haber-Institut der MPG, Berlin

The development of machine learning interatomic potentials (MLIPs) has revolutionized computational chemistry by enhancing the accuracy of empirical force fields while retaining a large computational speed-up compared to first-principles calculations. Despite these advancements, calculating Hessian matrices remains challenging due to the lack of analytical second-order derivatives, necessitating the use of computationally expensive finite difference methods (which can lead to numerical instabilities because of rounding errors). Automatic differentiation (AD) offers a promising approach to reducing this computational effort and making the calculation of Hessian matrices more efficient and accurate. In this contribution, we discuss the implementation of AD Hessians in the equivariant MACE framework. This new methodology finds applications in screening the heat capacities of metal-organic frameworks (MOFs) and in the calculation of infrared (IR) spectra, which are an ubiquitous tool for molecular characterization.

MM 3.5 Mon 11:15 H10

Diversity-Driven Active Learning of Interatomic Potentials for Reaction Network Exploration — •Francesco Cannizzaro, King Chun Lai, Patricia Poths, Sebastian Matera, Vanessa J. Bukas, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

We present an automatic workflow for the simultaneous active learning of Machine-Learning Interatomic Potentials (MLIPs) and exploration of complex networks of activated events. This workflow consists of alternating periods of training and the generation of candidate structures for the enrichment of the training set using the recently developed Automatic Process Explorer (APE) [1]. This allows us to determine elementary processes and corresponding barriers without the need of human supervision. From the output of the APE explorations, we identify maximally diverse atomic structures utilizing the DECAF fuzzy classification algorithm [2] and add only these to the training set. We exemplify this strategy on carbon intercalation in Pd, using GAP and MACE as MLIP frameworks. We find that this diversity driven approach outperforms state-of-the-art training set designs based on molecular dynamics for finding activated events and corresponding barriers. Particularly, our workflow performs very well in reducing outliers, which is of utmost importance for activated event dynamics since this is often controlled by only a few barriers.

[1] Lai *et al.*, ChemRxiv, https://doi.org/10.26434/chemrxiv-2024-jbzr7 (2024).
[2] Lai *et al.*, J. Chem. Phys. **159**, 024129 (2023).

15 min. break

MM 3.6 Mon 11:45 H10

Accelerating Materials Exploration with Active Machine Learning: Integrating SISSO with FHI-aims — Yi Yao[1,2], Lucas Foppa[1], Akhil Sugathan Nair[1], Andrei Sobolev[1,2], •Konstantin Lion[1,2], Sebastian Kokott[1,2], and Matthias Scheffler[1] — [1]NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Molecular Simulations from First Principles e.V., Berlin, Germany

We present a user-friendly web application for active learning-based materials exploration with the goal of broadening the usability of AI tools. The platform integrates the SISSO (Sure Independence Screening and Sparsifying Operator) method [J. Chem. Phys. 159, 114110 (2023)] with FHI-aims software [Comp. Phys. Commun. 180, 2105 (2009)] to provide interpretable modeling and reliable property predictions. SISSO dynamically updates models during the exploration process, while FHI-aims ensures accurate all-electron density functional theory (DFT)-based calculations. The property prediction workflow is managed using the atomate2 library, providing many "standard" DFT workflows and efficient utilization of compute resources ranging from local machines to cloud infrastructures. By leveraging SISSO-based uncertainty prediction, the application implements active learning to efficiently identify materials with desirable target properties. Two case studies, the exploration of the bulk modulus in perovskites and the prediction of stable oxides under harsh conditions, demonstrate the platform's ability to accelerate materials discovery.

MM 3.7 Mon 12:00 H10

Data-driven design of mechanically hard soft magnetic high-entropy alloys — •Mian Dai[1], Yixuan Zhang[1], Xiaoqing Li[2], Stephan Schönecker[2], Liuliu Han[3], Ruiwen Xie[1], Chen Shen[1], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germnay — [2]Department of Materials Science and Engineering, KTH - Royal Institute of Technology, Stockholm, Sweden — [3]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The rational design of mechanically hard soft magnets, combining high hardness with magnetically soft properties, represents a critical frontier in materials science. Here, we introduce a comprehensive data-driven framework to navigate the vast compositional space of high-entropy alloys (HEAs) and identify candidates optimized for these dual functionalities. Utilizing a curated dataset of 1,842,628 density functional theory calculations, encompassing 45,886 quaternary and 414,771 quinary equimolar HEAs derived from 42 elements, we employ ensemble learning to synergistically integrate multiple predictive models. This methodology captures the relationships between composition, crystal structure, mechanical performance, and magnetic behavior, enabling the identification of alloys with a unique combination of high hardness and magnetic softness. Our framework establishes a robust pathway for the accelerated discovery of next-generation hard-soft magnetic materials, underscoring the transformative potential of data-driven strategies in materials design.

MM 3.8 Mon 12:15 H10

Autonomous optimization of coin-cell batteries and thin-film growth — •Edan Bainglass[1,6], Peter Kraus[2,5], Francisco Ramirez[3,6], Enea Svaluto-Ferro[2], Loris Ercole[3,6], Benjamin Kunz[2], Sebastiaan Huber[3,6], Nukorn Plainpan[2], Nikita Shepelin[1], Nicola Marzari[1,3,6], Corsin Battaglia[2,3,4], and Giovanni Pizzi[1,3,6] — [1]PSI, Villigen, Switzerland — [2]Empa, Dübendorf, Switzerland — [3]EPFL, Lausanne, Switzerland — [4]ETH Zurich, Zurich, Switzerland — [5]TUB, Berlin, Germany — [6]MARVEL, Switzerland

Advancements in materials science are increasingly driven by the integration of automation of both experiments and simulations, machine learning, and robust data management frameworks. In this talk, we discuss the integration of experimental systems with the AiiDA [1] workflow management system, both battery coin cell assembly and cycling [2], and for thin film growth by pulsed laser deposition (PLD). We discuss the ongoing integration of these platforms with the FINALES [3] fast intention-agnostic learning server towards fully autonomous optimization of battery end-of-life (EOL) performance. We also discuss preliminary results demonstrating the feasibility of autonomously optimizing the layer-by-layer thin-film growth with PLD. These case studies demonstrate the potential of automated workflows to accelerate the discovery and optimization of functional materials.

[1] S. P. Huber et al., Sci. data 7, 300 (2020)
[2] P. Kraus et al., J. Mat. Chem. A 12, 10773 (2024)
[3] M. Vogler et al. Adv. Ener. Mat. 2403263 (2024)

MM 3.9 Mon 12:30 H10

Learning Disorder in Generative Materials Discovery - Bridging Prediction and Experiment — •Konstantin Jakob[1], Aron Walsh[2], Karsten Reuter[1], and Johannes T. Margraf[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Imperial College London, London, UK — [3]University of Bayreuth, Bayreuth, Germany

In recent years, generative machine learning (ML) models have demonstrated tremendous potential for the design and discovery of new materials. This has led to extensive predictions of previously unknown, potentially stable inorganic materials. However, current models suffer from the fact that the underlying training data is purely based on density functional-calculations for small, ideal crystals. As a consequence, many of the supposedly new materials are in fact experimentally known as disordered crystals. In this work, we address this issue by performing a thorough analysis of crystal disorder in the experimental structures of the Inorganic Crystal Structure Database (ICSD). Based on this, we develop disorder classification models and representations that can predict the likelihood of disorder across chemical space. Eventually, these concepts will allow us to extend current generative models to realistic crystal systems and bridge the gap between prediction and experiment.

MM 3.10 Mon 12:45 H10

Materials-Discovery Workflows Guided by Symbolic Regression: Identifying Stable Oxides for Catalytic Applications — •Akhil S. Nair, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany

AI-driven workflows will accelerate materials discovery by efficiently guiding experiments or simulations towards materials with desired properties. However, probabilistic AI approaches commonly used in these workflows are limited by the relatively small size of high-quality datasets and they rely on typically unknown, low-dimensional representations. Herein, we discuss the recent advancements in applying symbolic regression based on the sure-independence screening and sparsifying operator (SISSO) approach within iterative frameworks for materials discovery. This involves an ensemble approach for the uncertainty quantification of SISSO models as well as the development of optimization strategies to efficiently explore promising regions of the materials space. These developments present an opportunity to integrate SISSO into sequential-learning workflows for materials discovery. Importantly, SISSO provides materials-property maps covering the entire materials space, further reducing the risk that the workflow misses promising materials that were overlooked in the initial dataset. We demonstrate the effectiveness of the SISSO-guided workflows by identifying stable oxides for catalytic applications.

MM 4: Materials for the Storage and Conversion of Energy

Metal Hydrides, Hydrogen Embrittlement

Time: Monday 10:15–13:00 Location: H22

MM 4.1 Mon 10:15 H22

Atomic cluster expansion potential for the palladium hydride system — •Minaam Qamar[1], Apinya Ngoipala[2], Matous Mrovec[1], and Matthias Vandichel[2] — [1]ICAMS, Ruhr-University Bochum, Germany — [2]Department of Chemical Sciences and Bernal Institute, University of Limerick, Ireland

Palladium (Pd) is extensively studied for metal-hydrogen interactions due to its remarkable ability to absorb large amounts of hydrogen under standard temperature and pressure conditions, forming stable palladium hydride structures. This property makes Pd a critical material for various hydrogen-related applications, including hydrogen storage and as a catalyst for hydrogen evolution reactions. We developed a highly accurate and computationally efficient Atomic Cluster Expansion (ACE) potential to unravel atomistic insights into the Pd-H interaction. This potential was utilized to perform molecular dynamics and Monte Carlo simulations, providing a detailed understanding of the formation mechanisms of palladium hydride nanoclusters and bulk structures.

MM 4.2 Mon 10:30 H22

Hydrogen kinetics in HPT-deformed bulk Mg and Mg-based alloys — •Giorgia Guardi[1], Sabine Schlabach[1,2,3], Julia Ivanisenko[2], Stefan Wagner[1], and Astrid Pundt[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WK), Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT), Karlsruhe, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe, Germany

Magnesium (Mg) is a light and abundant element that can store hydrogen with a gravimetric density of 7.6 wt. % and a volumetric density of 110 kgH/m^3. Therefore, it is a highly promising hydrogen storage material for a sustainable energy economy. However, its technical use is hindered by an inherent kinetic blockade in magnesium hydride. A high content of grain boundaries is expected to improve hydrogen kinetics in Magnesium samples, particularly in the magnesium hydride phase. This can be achieved in bulk samples through the use of severe plastic deformation techniques, such as High-Pressure Torsion (HPT).

High-pressure torsion is not fully effective in reducing the grain size in pure bulk magnesium due to dynamic recrystallization. To overcome this lower limit to bulk magnesium grain size, Mg- 2.3 at.% Zn- 0.17 at. % Zr alloys are used, reaching a final grain size of approximately 100 nm after HPT. This study examines the impact of the sample's microstructure on hydrogen kinetics. Hydrogen absorption is studied at room temperature by gas-phase and electrochemical hydrogen loading.

MM 4.3 Mon 10:45 H22

A first principles study on the free energy landscape of chemisorbed hydrogen atoms on a Pt (111) surface modified by transition metals — •Bingxin Li, Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

Platinum (Pt) is considered an excellent catalyst for the hydrogen evolution reaction (HER) due to its optimal hydrogen binding strength, as suggested by the Sabatier principle and the volcano plot of the HER. In surface-catalysed electrochemical reactions, the incorporation of adsorbates or dopants into a host surface can significantly enhance the catalytic selectivity, activity, and stability compared to the pristine surface while also introducing some novel properties not observed on the parent surfaces. Transition metals (TMs), such as Cu, Ag, Au, Pd, Ru, Rh, and Ir, form metal-hydrogen bonds with unique characteristics, resulting in varied H adsorption patterns and distinct hydrogen evolution behaviours. Consequently, doping these transition metals into a Pt (111) surface can significantly alter its catalytic properties for the HER, either by modifying H adsorption configurations or by impacting the reaction barrier of the fundamental steps for the hydrogen evolution, though the underlying mechanisms remain unclear. To this end, we employ ab initio molecular dynamics (AIMD) simulations to investigate H adsorption on TM-doped Pt (111) surfaces in the presence/absence of explicit water by constructing laterally resolved free energy maps of chemisorbed H atoms.

MM 4.4 Mon 11:00 H22

Local hydrogen concentration and distribution in Pd nanoparticles: An in-situ STEM-EELS approach — •Svetlana Korneychuk[1,2], Stefan Wagner[1], Darius Rohleder[3], Philipp Vana[3,4], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology — [2]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [3]Institute of Physical Chemistry, Georg-August-University Göttingen — [4]Wöhler Research Institute for Sustainable Chemistry (WISCh), Georg-August-University Göttingen

Local detection of hydrogen concentration in metals is of central importance for many areas of hydrogen technology, such as hydrogen storage, detection, catalysis, and hydrogen embrittlement. We demonstrate a novel approach to measure the hydrogen concentration in a model system consisting of cubic palladium nanoparticles, with a lateral resolution down to 4 nm. By measuring the shift of the Pd bulk plasmon peak with scanning transmission electron microscopy combined with energy electron loss spectroscopy during in-situ hydrogen gas loading and unloading, local detection of the hydrogen concentration is achieved in TEM [1]. With this method, concentration changes inside the NPs at various stages of hydrogenation/dehydrogenation are observed with nanometer resolution. The versatility of in-situ TEM allows to link together microstructure, hydrogen concentration and local strain, opening up a new chapter in hydrogen research. [1] S. Korneychuk, et al., 'Local hydrogen concentration and distribution in Pd nanoparticles: An in-situ STEM-EELS approach', Small, accepted

MM 4.5 Mon 11:15 H22

Hydride formation in open thin film metal hydrogen systems: Cahn-Hilliard-type phase-field simulations coupled to elasto-plastic deformations — •Stefan Wagner[1], Alexander Dyck[2], Johannes Gisy[2], Frederik Hille[2], Astrid Pundt[1], and Thomas Böhlke[2] — [1]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Engineering Mechanics (ITM), Karlsruhe Institute of Technology, Germany

Metal-hydrogen systems are versatile model systems to study alloy thermodynamics and structural phase transitions. Hydrogen absorption and hydride formation in metals induce a volume expansion of the metal, leading to incompatibility stresses at internal and external interfaces. Resulting changes of the thermodynamic stability of phases in response to the mechanical constraint conditions can be understood by investigating the chemo-mechanical coupling [1,2]. Utilizing niobium-hydrogen thin films, combining a Cahn-Hilliard type phase-field theory and Finite-Element-Modeling (FEM) we study the feedback-loop of the local stress state, elasto-plastic deformations and hydrogen diffusion, determining the driving force of precipitation and growth of the hydride phase under open-system conditions. The simulation results are informed by and compared to measurements of the concentration-dependent stress state, chemical potential and phase separation in epitaxial niobium-hydrogen thin films adhered to sapphire substrates [3]. [1] A. Dyck, T. Böhlke, A. Pundt, S. Wagner, Scr. Mat. 247 (2024) 116117. [2] A. Dyck et al., Scr. Mat. 251 (2024) 116209. [3] A. Dyck et al., accepted to Mech. of Mat.

MM 4.6 Mon 11:30 H22

Hydrogen: a catalyst for abnormal grain growth in inert-gas condensed nanocrystalline Pd-Au? — •Fabian Andorfer[1], Jules M. Dake[1], Markus Ziehmer[1], Johannes Wild[2], Torben Boll[2], Dorothée Vinga Szabó[2], Stefan Wagner[2], Astrid Pundt[2], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University — [2]Institute of Applied Materials - Materials Science and Engineering (IAM-WK), Karlsruhe Institute of Technology

Heat treatment causes some polycrystalline materials to manifest abnormal grain growth (AGG), during which a few grains acquire a significant growth advantage compared to the remaining matrix grains, resulting in a bimodal distribution of grain sizes. Inert-gas condensed nanocrystalline Pd-Au alloys undergo an extreme form of AGG. This system is known to absorb hydrogen. When Pd-Au alloys are exposed to hydrogen below a certain gas pressure, hydrogen atoms primarily occupy grain boundaries and interstitial sites. This segregation is expected to lower the excess energy of the grain boundaries, which should have a noticeable effect on subsequent grain growth. To test this, Pd-Au samples were heat treated in argon and hydrogen atmospheres, respectively. The average size of the abnormally grown grains was determined, and the grain shape was characterized by calculating the circularity. Hydrogen appeared to increase the rate of abnormal grain "nucleation" without affecting the resulting grain shape.

MM 4.7 Mon 11:45 H22

The liquid intermediate phase for a hydrogen storage material — •Anastasiia Thase[1], Oliver Alderman[2], Chiara Milanese[3,4], Alessandro Girella[4], Claudio Pistidda[5], Martin Müller[5,6], and Sebastian Busch[1] — [1]GEMS MLZ, Helmholtz-Zentrum Hereon WPN — [2]ISIS Neutron and Muon Source — [3]C.S.G.I. Department of Chemistry, Physical Chemistry Division, University of Pavia — [4]Pavia Hydrogen Lab — [5]Helmholtz-Zentrum Hereon WTN — [6]CAU zu Kiel, Leibnitzstr. 19, 24098 Kiel, Germany

Hydrogen storage in light hydrides for mobile applications is a widely discussed but a highly controversial topic because of its ability to form explosive mixtures with oxygen. However, this danger is eliminated, if hydrogen is stored in complex hydrides, which provide hydrogen only under significant heat impact.

The main issue for complex hydride mixtures is the kinetics of the reversible reaction with hydrogen. One of prospective candidates is $6Mg(NH_2)_2$:9LiH, which promptly interacts with hydrogen when doped with $LiBH_4$. Its catalytic impact is explained by the formation of low-melting intermediate phases with high Li-ion conductivity: a metastable $Li_2BH_4NH_2$ and a peritectically melting $Li_4BH_4(NH_2)_3$.

In the $LiNH_2 - LiBH_4$ phase diagram, the eutectic point is located at the 1:2 ratio and 90°C. This eutectic mixture was characterized by various techniques, including neutron total scattering, and its intrinsic structure under the reaction conditions was elucidated by EPSR, which gave a hint about its role as a liquid-phase catalyst in the corresponding hydrogen storage composition ($6Mg(NH_2)_2$:9LiH:6$LiBH_4$).

MM 4.8 Mon 12:00 H22

Machine Learning Interatomic Potentials for Studying Hydrogen Storage in TiCr2 Laves Phase Alloys — •Pranav Kumar, Blazej Grabowski, and Yuji Ikeda — Institut für Materialwissenschaft, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Efficient hydrogen storage is a crucial challenge for the widespread absorption of hydrogen as a clean energy carrier. TiCr2 Laves phase alloys, with their exceptional hydrogen absorption and diffusion properties, represent a promising class of materials for this purpose. This study employs a multiscale computational strategy, integrating density functional theory (DFT) and machine learning interatomic potentials (MLIPs), to investigate hydrogen behavior in TiCr2 Laves phases. Key areas of focus include hydrogen binding energies, diffusion pathways, and the complex effects of hydrogen clustering, which influence storage capacity and transport. Notably, our findings reveal possible equilibrium hydride structures consistent with experimental observations, offering valuable validation of the computational models. By leveraging large-scale DFT simulations within an active learning framework, we develop accurate MLIPs that enable efficient exploration of the phase space across diverse hydrogen concentrations. These MLIPs bridge atomic-scale simulations, facilitating precise calculations of hydrogen diffusion coefficients and shedding light on the mechanisms of hydrogen mobility. The insights derived from this work enhance our understanding of hydrogen-metal interactions and provide critical information for optimizing hydrogen storage materials.

MM 4.9 Mon 12:15 H22

The impact of Mn and Al on the trapping and diffusion of hydrogen in γ-Fe: An atomistic insight — •Bikram Kumar Das[1], Poulami Chakraborty[1], Mauricio Rincón Bonilla[1], and Elena Akhmatskaya[1,2] — [1]Basque Center for Applied Mathematics, Bilbao, Spain — [2]Ikerbasque - Basque Foundation for Science, Spain

We propose a first principles-based framework to systematically unlock the physical underpinnings of local distribution of the solute atoms on hydrogen trapping and diffusion in Mn/Al-alloyed γ-Fe. In our scheme, all thermodynamically stable substitutional solute sites were identified (<= 5.4 wt% Mn; <= 4 wt% Al) up to the third nearest neighbour (NN) shell of a single H atom. The impact of Mn/Al on H-binding was quantitatively evaluated, indicating a surprisingly strong correlation with the local Al distribution regardless Mn content, and indirect stabilization by Al when present in the 2nd NN shell. Nonetheless, Al strongly repels H bonding. The contradictory role of Al was explained in terms of bonding/antibonding orbitals occupancy in H-M interactions (M = Al, Mn, Fe). The barriers to H hopping between adjacent local environments and the corresponding jump frequencies were subsequently calculated, providing insights into the limits imposed by the presence of Al and Mn on H mobility in Mn/Al-alloyed γ-Fe. Most notably, presence of Al in the 2nd NN shell of H severely reduces the H jump frequency, leading to irreversible trapping at high Al contents. Such behaviour may critically contribute to mitigate H-induced delayed fracture in Al-rich austenite steel.

MM 4.10 Mon 12:30 H22

Hydrogen - Microstructure Interaction in Ferritic Steels: From Ab-initio Simulations to Experiments — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]IMPRS SusMet, Max Planck Institute for Sustainable Materials, Germany — [2]Institute for Materials, Chair of Materials Technology, Ruhr-University Bochum, Germany — [3]ICAMS, Ruhr-University Bochum, Germany

Hydrogen embrittlement (HE) is a phenomenon where hydrogen negatively impacts the mechanical properties of metallic materials. Mitigating HE requires minimizing hydrogen diffusion in microstructures and understanding how local heterogeneities influence this process across different length scales. While advanced experimental and computational methods exist, their application to varying systems complicates model validation. To address this, simplified ferritic Fe-based alloys were produced, and subjected to thermomechanical treatments, and their microstructures were characterized using EBSD. This approach aims to assess the hydrogen storage capacities of microstructural heterogeneities and their influence on the effective diffusion coefficient. Complementary ab initio density functional theory calculations were performed to evaluate hydrogen trapping energies and diffusion barriers under different chemical environments and CSL boundaries. These calculations inform predictions of hydrogen solubility and distribution within the experimental microstructures, to be validated experimentally. This work shows the importance of combining simulations and experiments to understand microstructural heterogeneities' role in HE.

MM 4.11 Mon 12:45 H22

Hydrogen Embrittlement in fatigue damage of ferritic steel: Theoretical investigation of failure mechanisms in varying hydrogen environments — •Alexandra Stark[1,2], Petra Sonnweber-Ribic[1], and Christian Elsässer[2] — [1]Robert Bosch GmbH, CR, 71272 Renningen — [2]Fraunhofer IWM, 79108 Freiburg

In this theoretical study, the influence of hydrogen on the fatigue behavior of a ferritic steel is examined by using a coupled hydrogen-diffusion and crystal-plasticity finite-element (CPFE) model. The damaging effect of hydrogen on structural materials, particularly ferritic and martensitic steels, poses a significant challenge for a wide range of technical applications. Despite being known for about 150 years, the underlying mechanisms of hydrogen embrittlement remain the subject of scientific debates. CPFE models are suitable for ensuring a microstructure-sensitive modelling and enabling the description of local plastic deformation, both essential factors in the complex process of metal fatigue. The presented study investigates the individual and combined effects of different damage models based on proposed hydrogen embrittlement failure mechanisms [1]. Furthermore, the work explores the impact of diverse environmental conditions on the cyclic material damage. The effects of varying local hydrogen concentration and distribution on the fatigue damage, as implemented in the CPFE model, are examined and discussed. [1] A. Stark, P. Sonnweber-Ribic, and C. Elsässer, Theoretical study of individual and combined effects of HELP- and HEDE-based damage models on the fatigue behavior of ferritic steel by hydrogen, submitted (2024).

MM 5: Invited Talk: X. Fang (joint session MM/KFM)

Time: Monday 15:00–15:30 Location: H10

Invited Talk MM 5.1 Mon 15:00 H10

Room-temperature dislocations in oxide ceramics: from understanding to active engineering — •Xufei Fang — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

In the conventional picture, dislocations are most relevant for metals while ceramics are considered brittle and exhibit little or no plasticity at room temperature. However, recent years' research on dislocations in ceramics suggests that dislocations may have been much under-appreciated in ceramics. Proofs-of-concept for dislocation-tuned functional properties suggest that dislocations may hold great technological potential in advanced ceramics. As the prerequisite to harvest dislocation-tuned properties, engineering dislocations into ceramics without brittle fracture has thus become a pressing bottleneck. To tackle this challenge, we have separately examined the dislocation behavior including dislocation nucleation, multiplication and motion, enabling us to tune dislocations into ceramic oxides at room temperature. We can now achieve a dislocation density up to ~10^15/m^2 with a plastic zone size of up to milli-/centimetres using a mechanical deformation toolbox. We further extend the material toolbox by discovering and reporting more oxide perovskites that can be plastically deformed at room temperature across the length scale. The combined deformation and material toolboxes offer a new platform for studying the dislocation-tuned functional properties (e.g., electrical and thermal conductivity) and the mechanical properties (such as plasticity, toughness, and damage tolerance) over a wide range of length scales.

MM 6: Phase Transformations

Time: Monday 15:45–18:30 Location: H10

MM 6.1 Mon 15:45 H10

Phase transitions in 2D halide perovskites using machine learned potentials — •Erik Fransson, Julia Wiktor, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

Hybrid halide perovskites are a promising class of materials for various applications, including high-efficiency solar cells, lasers, and light-emitting diodes. So-called two-dimensional (2D) halide perovskites, composed of a small number of perovskite layers stacked on top of each other and separated by organic cations that act as spacers, have much improved stability compared to their 3D counterparts. Here, we focus on the prototypical perovskite methylammonium lead halide (MAPI), and demonstrate that the dimensionality of these 2D materials and the choice of organic linker molecules can have a strong impact on phase transitions in these systems. This is investigated through large-scale molecular dynamics simulations using machine-learned potentials. We analyze the phase transition temperatures and characteristics with varying numbers of perovskite layers to understand how the transition properties change as a function of the system's dimensionality. For a larger number of perovskite layers, the 3D bulk phase transition temperature is recovered, whereas, for only a few perovskite layers, the phase transition temperature shifts up by about 100 K. Additionally, we observe surface effects, such as the surface layers (closest to the organic linker) exhibiting stronger octahedral tilting and undergoing phase transitions at higher temperatures (about 100 K) compared to the interior bulk layers.

MM 6.2 Mon 16:00 H10

Quantum phase diagram of sulfure hydride — •Marco Cherubini and Michele Casula — IMPMC, CNRS, Paris, France

In the recent rush towards room temperature superconductivity, hydrogen-based materials are the most prosiming candidates. Sulfulr hydride exhibits a maximum superconductive critical temperature of about 200K at 150 GPa. To our knowledge, a comprehensive theoretical characterization of the phase diagram of sulfur hydride in a wide temperature range is still missing in literature. To address this, we performed path integral molecular dynamics simulations (PIMD). The description of the low temperature regime has been made feasible by the use a machine learning potential trained on ab-initio data. We found three different regimes. At high pressure, the phase diagram is dominated by a paraelectric phase, with symmetric hydrogen bonds. Reducing the pressure, we observed first a regime characterized by finite local dipole moments and finally, at even lower pressures, the ferroelectric regime. Quantum simulations show that the formation of finite local moments is temperature-independent, unlike the transition to the ferroelectric regime. Classical simulations, by contrast, showed stronger temperature dependence for both the transitions and significantly higher critical pressures, highlighting the impact of quantum nuclear fluctuations.

MM 6.3 Mon 16:15 H10

Magnetic-field induced phase transition crossover in the triangular-lattice antiferromagnet: Ba_3CoSbO_9 — •Sanjay Kumar[1], Koushik Chakraborty[2], Aditi Agrawal[2], Shalini Mishra[3], M. P. Saravanan[2], Arvind Kumar Yogi[2], Satyapal S. Rathore[4], and Rashi Nathawat[1] — [1]Functional Ceramics and Smart Materials Lab, Department of Physics, Manipal University Jaipur, Jaipur - 303007, India — [2]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [3]Department of Physics, Govt. Holkar Science College, Indore (M.P.) 452001, India — [4]Department of Physics, Cluster University of Jammu, Jammu * 180001, India

We report magnetic and structural properties of triangular-lattice antiferromagnet Ba_3CoSbO_9 by means of x-ray diffraction (XRD), magnetic susceptibility, specific heat, x-ray photoelectron spectroscopy (XPS), and dielectric measurements. Thermodynamic measurements show a long-range ordered (LRO) state at Néel temperature T_N = 3 K which was found to be shift at higher temperatures at about T_N = 4.1 K under the higher magnetic fields. Moreover, we have found higher Curie-Weiss temperature θ_{CW} ~-133.2 K from the inverse susceptibility fit which reveals frustration parameter about 44, suggesting magnetic lattice is highly frustrated. Further, a spin-glass state signature was evident at around 6.5 K, which was found to be fully suppressed at a higher magnetic field (H ~16 T). Interestingly, Ba_3CoSbO_9 exhibits a broad maximum at around T_{max} ~5 K which becomes pronounced as the magnetic field is increased.

MM 6.4 Mon 16:30 H10

Anomalous spin-lattice coupling in the quasi-one-dimensional spin-1 corrugated skew-chain antiferromagnet: $Ni_2V_2O_7$ — •Arvind Kumar Yogi[1], Hemant Singh Kunwar[1], Koushik Chakraborty[1], Aditi Agrawal[1], Binoy Krishna De[1], Pragati Sharma[1], Shalini Mishra[2], D. T. Adroja[3], Mayanak Kumar Gupta[4], R. Mittal[4], R. Venkatesh[1], and V. G. Sathe[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Department of Physics, Govt. Holkar Science College, Indore (M.P.) 452001, India — [3]ISIS Neutron and Muon Facility, STFC, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, United Kingdom — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Trombey, Mumbai-400005, India

We report spin-lattice coupling through detailed structural, magnetic, and lattice-dynamics studies of the S = 1 quasi-one-dimension lattice $Ni_2V_2O_7$ compound. Our susceptibility χ (T) and heat capacity measurements (C_P/T) measurement conclusively show that the antiferromagnetic transition occurs at T_{N1} = ~6.7 K and T_{N2} = ~5.8 K. From detailed lattice dynamics, two Raman mode showed anomalous lattice softening below ~100 K due to Ni dimerization as supported by ordering of the J_1 exchange interaction. Importantly, the spin-lattice coupling has been established below ~100 K and the spin-lattice coupling constant (λ_{sp}) for various Raman modes has been deduced which shows multiferroic behaviour below T_{N1}. In addition, the detailed study of lattice dynamics by first principle calculation is presented.

MM 6.5 Mon 16:45 H10

Chirality in the Kagome Metal CsV_3Sb_5 — H.J. Elmers[1], O. Tkach[1], Y. Lytvynenko[1], P. Yogi[1], M. Schmitt[2,3], D. Biswas[2], J. Liu[2], S.V. Chernov[4], Q. Nguyen[5], M. Hoesch[4], D. Kutnyakhov[4], N. Wind[4,6], L. Wenthaus[4], M. Scholz[4], K. Rossnagel[4,6], A. Gloskovskii[4], C. Schlueter[4], A. Winkelmann[7], A.-A. Haghighirad[8], T.-L. Lee[2], M. Sing[3], R. Claessen[3], M. Le Tacon[8], J. Demsar[1], G. Schönhense[1], and •O. Fedchenko[1] — [1]JGU Mainz, Germany — [2]DIAMOND, Didcot, United Kingdom — [3]Physikalisches Institut Würzburg, Germany — [4]DESY, Germany — [5]SLAC, Menlo Park, USA — [6]CAU Kiel, Germany — [7]University of Krakow, Poland — [8]KIT, Karlsruhe, Germany

Using x-ray photoelectron diffraction (XPD) and angle-resolved photoemission spectroscopy, we study photoemission intensity associated with the changes in the geometric and electronic structure of the kagome metal CsV_3Sb_5 upon transition to an unconventional charge density wave (CDW) state. The XPD patterns reveal the presence of a chiral atomic structure in the CDW phase. Using circularly polarized x-rays, we have found a pronounced non-trivial circular dichroism in the angular distribution of the valence band photoemission in the CDW phase, indicating a chirality of the electronic structure. This observation is consistent with the proposed orbital loop current order. The results suggest an antiferromagnetic coupling of the orbital magnetic moments along the c-axis.

[1] H.J. Elmers et al., e-print on arXiv, 2408.03750 (2024).

15 min. break

MM 6.6 Mon 17:15 H10

Pressure-temperature phase diagram of calcium using quantum-accurate finite-temperature free energies — •Raynol Dsouza[1], Marvin Poul[1], Liam Huber[2], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Grey Haven Solutions, Vancouver, Canada

Pure calcium has been experimentally shown to exhibit several stable phases across a range of high pressures. While many of these phases have been theoretically predicted using T=0 K ab inito calculations [1], the relative stability of the distorted simple cubic phases above 30 GPa at finite temperatures remains unclear. To address this ambiguity, we developed an Atomic Cluster Expansion (ACE) potential [2] for calcium, fitting it to a structural dataset generated using the ASSYST methodology outlined in [3]. Quantum-accurate finite-temperature free energies were determined using the Temperature Remapping Approximation (TRA) [4]. The resulting pressure-temperature phase diagram offers new insights into the phase stability of calcium at elevated pressures and temperatures.

[1] Ishikawa et al., https://doi.org/10.1103/PhysRevB.81.092104 [2] Bochkarev et al., https://doi.org/10.1103/PhysRevMaterials.6.013804 [3] Poul et al., https://doi.org/10.21203/rs.3.rs-4732459/v1 [4] Dsouza et al., https://doi.org/10.1103/PhysRevB.105.184111

MM 6.7 Mon 17:30 H10

Phase-stability Study of the Marcasite-Structure Solid Solutions (Fe, TM)Sb_2 (TM = Cr, Ni) Synthesized via Combinatorial Co-Deposition and Antimonization — •Martin Kostka[1], Luqman Mustafa[1], Maik Golombiewski[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Alfred Ludwig[2], Adreas Kreyssig[1], and Anna Böhmer[1] — [1]Experimental physics IV, Ruhr University Bochum, 44801 Bochum — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, 44801 Bochum

Transition-metal di-pnictides of the pyrite-marcasite family are model systems for crystal chemistry. We investigate phase formation and stability of transition-metal di-antimonides in the orthorhombic marcasite structure. We employ a two-step synthesis of granular films, using combinatorial co-deposition of the

transition metals and subsequent antimonization at different temperatures. This technique allows efficient exploration of substitution ranges and lattice parameter evolution within the marcasite structure. We investigate the formation and crystal structures of the (Fe,Ni)Sb_2 and (Fe,Cr)Sb_2 substitution series. We evidence the continuous substitution of $FeSb_2$ (class A marcasite) with Ni up to $Fe_{0.5}Ni_{0.5}Sb_2$, and a clear phase separation between $Fe_{0.5}Ni_{0.5}Sb_2$ and a Ni-rich $Ni_{1-z}Fe_zSb_2$ phase (class B marcasite). Cr-substituted $FeSb_2$ shows a subtle phase separation into an Fe-rich $Fe_{1-y}Cr_ySb_2$ and a Cr-rich $Cr_{1-z}Fe_zSb_2$-phase (both class A marcasite) when synthesized at 500°C, but not at higher Temperatures. We acknowledge support from DFG (TRR288,A02).

MM 6.8 Mon 17:45 H10

Investigation of glass formation in Pd40Ni40P20 metallic glass via fast scanning calorimetry — •Hongshuai Li, Sher Bahadur Raut, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Pd-Ni-P metallic glasses (MGs) exhibit exceptional glass-forming ability; in fact, Pd40Ni40P20 was the first bulk metallic glass-forming alloy discovered. Understanding glass formation in these materials requires exploring factors that impede correlated atomic motions in glass-forming liquids. This study investigates the atomic relaxation and thermal history of Pd40Ni40P20 MG, utilizing data from multiple cycles of heating around the glass transition temperature, activation energy determined by flash differential scanning calorimetry (DSC), and critical cooling rates. Additionally, we examine the effects of annealing time on the DSC signals at high heating rates of up to 1000 K/s. Our results demonstrate that adjustments in cooling rates and annealing duration significantly influence glass transition behavior and thermal stability. These findings enhance our understanding of the mechanisms underlying glass formation in Pd-Ni-P MGs and their potential applications in advanced materials.

MM 6.9 Mon 18:00 H10

Tuning excitonic transition by Cr doping and associated lattice softening in the vdW chalcogenide: Ta2NiSe5 — •Isha Isha[1], Koushik Chakraborty[1], Aditi Agrawal[1], M. Isobe[2], and Arvind Kumar Yogi[1] — [1]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We have successfully grown defect free ultra-high quality single crystals of Cr doped Ta2NiSe5, maximum of 10% at Ni site in the lattice. Our preliminary STM results unambiguous provide clear signature of CDW phase, vdW layers and the vdW gap for Ta2NiSe5 which was found to be ~3.5 Å. We found a clear anomaly at the critical temperature Tc = 326 K in our transport measurement over rod shaped crystals - a transition into an excitonic insulator ground state as reported for parent Ta2NiSe5 compound. It is noteworthy to highlight our finding that Cr doping significantly suppresses the insulating ground state and the 10% doping reduces the resistivity of three orders. In addition, our detailed high-temperature Raman scattering for parent as well as Cr doping reveals sharp Raman modes and significant shift and suppression for 230 cm-1 phonon mode which might be associated with electron-phonon coupling, which may helps in resistivity drop as evident in our transport data. In addition, our detailed Raman scattering study suggests the persistence of lattice softening which may be due to strong electron-lattice coupling, and the origin is presumably due to strong excitonic fluctuations.

MM 6.10 Mon 18:15 H10

Magnetic Imaging of the Local Insulator to Metal Transition in CaRuO by NV Magnetometry — •Hayden Binger[1], Cissy Suen[2], Elina Zhakina[1], Luke Turnbull[1], Yejin Lee[1], Young-Gwan Choi[1], Max Krautloher[2], Bernard Keimer[2], Claire Donnelly[1], and Uri Vool[1] — [1]Max Planck Institute for the Chemical Physics of Solids,Dresden, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

The current-driven insulator to metal transition in $Ca_2Ru_2O_4$ is a fascinating phenomenon where increasing current driven across a sample causes a smaller voltage difference to develop. While this transition has been well studied in bulk $Ca_2Ru_2O_4$ through transport, and recently investigated by ARPES, little is known about the local character of the transition - especially in nanoscale devices. In this work we utilize scanning NV magnetometry to measure the local magnetic field induced by the local current in 100 nm thick lamellas of $Ca_2Ru_2O_4$. We observe a nonuniform field distribution that reveals the local current channels, allowing us to image the local character of the insulator to metal transition in $Ca_2Ru_2O_4$.

MM 7: Materials for the Storage and Conversion of Energy

Hydrogen related Surface Effects

Time: Monday 15:45–17:00 Location: H22

MM 7.1 Mon 15:45 H22

Effect of stress induced nanohydride formation on dislocation nucleation and pinning in FeCr alloys — •Ali Tehranchi[1], Jing Rao[2], Lekshmi Sreekala[2], Jazmin Duarte[2], Gerhard Dehm[2], Jörg Neugebauer[2], and Tilmann Hickel[1] — [1]BAM Federal Institute for Materials Research and Testing, ali.tehranchi@bam.de, Germany — [2]Max Planck Institute for Sustainable Materials

The detrimental effects of hydrogen (H) on the mechanical properties of metals are universally acknowledged. However, the mechanisms behind these effects remain unclear. In situ nano-indentation experiments are powerful tools for probing the effect of H on the hardness and plasticity of metals. In this work, ab initio calculations and stress dependent phase diagrams in chemical potential space are used to clarify the effect of nanohydrides on the pop-in load of in situ nanoindentation of FeCr alloys. It is shown that the anisotropic stress field of the indenter with a radius of 170 nm facilitates the formation of nanohydrides with significantly lower elastic constants and containing high eigen shear strain. The shear stress associated with these inhomogeneous inclusions is responsible for the experimentally observed reduction in critical shear for dislocation nucleation and the pop-in loads in these indentation experiments. On the other hand, for indenters with a larger radius, the pop-in load is increased due to the pinning of the pre-existing dislocations by the same nanohydrides which are not capable to form underneath the indenter because of the lower magnitude of its induced stress field. The formation of nanohydrides under loading has significant implications for H-embrittlement and H-storage.

MM 7.2 Mon 16:00 H22

Spherical nanoindentation during electro chemical nanoindentation — •Verena Maier-Kiener, Stefan Zeiler, and Anna Jelinek — Montanuniversität Leoben, Leoben, Österreich

Nanoindentation enables efficient characterization of material flow behavior, offering reliable results with minimal effort. While established for hardness and Young*s modulus, its potential for deriving localized flow curves remains underexplored due to challenges in correlating spherical indentation and uniaxial data. A calibration procedure addressing tip imperfections allows strain-rate-controlled experiments and accurate constraint factor evaluation. Using an innovative in-situ electrochemical charging method, side-charging cell, it is shown that electrochemical charging increases hardness and flow stress while reducing the constraint factor, providing valuable insights into deformation behavior.

MM 7.3 Mon 16:15 H22

Hydrogen-based reduction of iron oxide surfaces studied by ab-initio calculations — •Ahmed Abdelkawy, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Max-Planck-Str.1, 40470 Düsseldorf

The production of pure iron from the iron oxide ores is a very energy-intensive process. Additionally, the dependency on carbon and carbon monoxide as reducing agents results in CO2 as an intrinsic byproduct of the reaction. Consequently, the steel industry is responsible for more than 6% of the global CO2 emissions. Using Hydrogen (H) as a reducing agent would result in water being released instead. Two important aspects in this context are (i) the relative thermodynamics stability of iron oxide facets under different conditions, as this will determine their abundance and (ii) the interaction of H with the oxide surfaces, as these will catalyse the reaction. This work, which is an initial step toward understanding the complex process of the H-based reduction of iron oxides, focuses on Hematite (Fe2O3). Using density functional theory (DFT) calculations we explore the surface stability of different facets under relevant thermodynamic conditions. Additionally, we use transition state theory to describe different H reaction paths and their activation barriers. Keeping in mind the impact the description of the electronic structure may have on the considered quantities, the calculations were performed using both GGA-PBE and GGA-PBE+U. While our results indicate that both methods result in the same preferential reaction path, the electron localization from the (+U) term results in a significant reduction in the activation barrier.

MM 7.4 Mon 16:30 H22

Atomic Cluster Expansion potential for hydrogen-based direct reduction of iron oxides — •Baptiste Bienvenu[1], Mira Todorova[1], Jörg Neugebauer[1], Matous Mrovec[2], Yury Lysogorskiy[2], Ralf Drautz[2], and Dierk Raabe[1] — [1]Max Planck Insitute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, 44780 Bochum, Germany

Modeling atomistic mechanisms underlying hydrogen-based direct reduction of iron oxides poses many great challenges, due to the combined structural and electronic complexities of the bulk materials, but also due to the involved chemical reactions. To allow for atomic scale modeling of such processes over the relevant length and time scales, an accurate yet affordable interatomic potential is needed.

Following our previous work, which focused on the development of an Atomic Cluster Expansion (ACE) potential for iron and its oxides, we present in this work the extension of the model to include hydrogen. Based on an extensive DFT-computed database encompassing both iron and its oxides in a wide range of atomic environments involving hydrogen, we fit the extended ACE potential, also including magnetic degrees of freedom. To demonstrate the capabilities of the ACE potential, we focus on its ability to capture some basic mechanisms involved in the hydrogen-based reduction of iron oxides in various environments, including iron oxides-hydrogen (reactions at surfaces, bulk defects), iron oxides-water (surface oxidation), iron-water (surface reactions) and iron-hydrogen (trapping, interactions with defects).

MM 7.5 Mon 16:45 H22

Investigating phase diagram and phonons in superconducting Lanthanum Hydride through an accurate treatment of anharmonicity and nuclear quantum effects — •Abhishek Raghav[1], Kousuke Nakano[2], and Michele Casula[1] — [1]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Paris, France — [2]Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Japan

Hydrogen rich materials with clathrate structures are an important class of superconducting materials. Lanthanum hydride (LaH_{10}) is one such material, demonstrated to show superconductivity at 250 K and 170 GPa. Phase diagram, phonon spectrum and electron-phonon coupling are important ingredients used to predict superconductivity, being of BCS type. However, computing these accurately for hydrogen clathrate materials requires including anharmonicity due to nuclear quantum effects (NQE). In this work, we use the path integral molecular dynamics (PIMD) and the stochastic self-consistent harmonic approximation (SSCHA) to study NQE and finite temperature on the phase stability and phonons. In order to speed up PIMD and SSCHA calculations, we employ a machine learning potential generated using MACE. This allows us to explore the theoretical LaH_{10} phase diagram over an unprecedentedly wide range of temperatures and pressures. We found that, when quantum effects are included, hydrogen cage symmetrization occurs at lower pressures than in classical simulations, placing the maximum of T_c measured in experiments close to the quantum transition region.

MM 8: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Lithium-based Materials

Time: Monday 17:15–18:30 Location: H22

MM 8.1 Mon 17:15 H22

Lithium diffusion pathways in modern solid state Li conductors — •Mykhaylo Monchak[1], Volodymyr Baran[2], Stefan Strangmüller[3], and Anatoliy Senyshyn[3] — [1]Institut für Angewandte Materialien, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Deutsches Elektronen Synchrotron, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

The rapid development of energy storage demands cheaper, more robust electrode and electrolyte materials with improved electrochemical performance. Energy storage and conversion primarily rely on diffusion-based processes, making understanding diffusion pathways crucial. However, determining diffusion pathways in polycrystalline (non-cubic) materials is challenging using bulk or local measurements. Theoretical approaches like molecular dynamics simulations face numerous computational limitations. Alternatively, diffusion processes can be predicted from crystal structures using scattering density maps (electron for X-ray or nuclear for neutrons). These maps analyzed via probability density functions or reconstructed through the maximum entropy method (MEM) are highly reliable. MEM is particularly effective for powder-averaged diffraction data, detecting weak structural disorders. This study applies high-resolution neutron powder diffraction and MEM analysis to explore state-of-the-art lithium conductors considered for application in all-solid-state Li-ion batteries, providing insights into their diffusion pathways and systematics.

MM 8.2 Mon 17:30 H22

"Effortless Embedding": Non-Parametric Solid-State Embedding for NMR Computations using All-Electron DFT — •Federico Civaia[1], Simone S. Köcher[2,1], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH, Jülich

Solid-state electrolytes are crucial in lithium-ion battery research, because of the pressing need for safe and durable high-energy storage solutions. Understanding Li-ion dynamics in these materials is essential for developing improved battery technologies. Owing to its non-destructive nature and sensitivity to atomic environments, solid-state nuclear magnetic resonance (SS-NMR) spectroscopy has become an invaluable tool for probing diverse Li-ion environments and investigating Li-ion mobility.

To facilitate the interpretation of experimental Li SS-NMR spectra, we are developing a method for computing NMR parameters of diamagnetic Li compounds using the linear-scaling, all-electron, density functional theory code FermiONs++ [1]. To allow the description of both crystalline and disordered materials, we employ a SS embedding method. In this regard, we present a consistent, non-parametric hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) methodology for systematic and reproducible structure generation and SS embedding calculations.

[1] J. Kussman *et al.*, J. Chem. Phys. **138**, 134114 (2013); J. Chem. Theory Comput. **11**, 918 (2015).

MM 8.3 Mon 17:45 H22

Insights into Li-ion battery cathode redox chemistry via charge transfer multiplet simulations of $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ — •Ruiwen Xie[1], Maximilian Mellin[2], Wolfram Jaegermann[2], Jan. P Hofmann[2], and Hongbin Zhang[1] — [1]Theory of Magnetic Materials Group, Department of Materials and Geosciences, Technical University of Darmstadt — [2]Surface Science Laboratory, Department of Materials and Geosciences, Technical University of Darmstadt

The evolution of electronic structure during discharging and charging processes with Li intercalation and deintercalation in transition metal oxide cathode materials involves changes in oxidation states, non-rigid band behavior, and oxygen's role in charge compensation, which significantly impact cathode performance. To gain deeper insights, we combine experimental x-ray photoelectron spectroscopy (XPS) at various voltages with many-body electronic structure simulations. The electronic structures of Li_xCoO_2 and Li_xNiO_2 were calculated using Density Functional Theory and Dynamical Mean-Field Theory (DFT+DMFT). We found that Li intercalation and deintercalation shift the hybridization between Co/Ni *d* and O *p* orbitals relative to the Fermi energy, altering Co/Ni *d* occupancy. Based on this, we performed XPS calculations using the multiplet ligand-field model in Quanty to revisit the transition metal 2p satellite structure evolution. This study provides crucial insights into the interplay between electronic structure and Li intercalation dynamics for enhancing cathode performance.

MM 8.4 Mon 18:00 H22

Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials — •Yuandong Wang, Yute Chan, Hao Wan, Kyeonghyeon Nam, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Garnet $Li_7La_3Zr_2O_{12}$ (LLZO) is a highly promising solid state electrolyte (SSE) for lithium batteries. However, its practical application faces challenges, primarily arising from Li dendrite formation and the impact of grain boundaries (GBs) on Li transport and stability. Amorphous LLZO combines several desirable properties like blocking Li dendrite growth, high Li mobility and high electronic impedance. Controlling amorphous domains between crystalline grains could therefore offer an intriguing approach to tune electrolyte performance. For this, an atomistic understanding of the interplay between composition, structure and the properties of LLZO glass-ceramics is crucial.

This study introduces a Machine Learning Interatomic Potential (MLIP) tailored to accurately represent amorphous and GB structures in LLZO. Developed through an iterative training protocol using simulated annealing, this MLIP includes diverse structures in its training set, ensuring comprehensive modeling of complex LLZO phases. The MLIP enables large-scale molecular dynamics simulations, allowing the construction of realistic amorphous and GB models, and providing a foundation for in-depth analysis of LLZO structural and electrochemical behavior.

MM 8.5 Mon 18:15 H22

Early Stage of Li Cluster Nucleation at the Li Anode-Solid Electrolyte Interface in Solid-State Batteries — •Yun An[1,2], Taiping Hu[2], Quanquan Pang[2], and Shenzhen Xu[2] — [1]Fritz-Haber- Institut der MPG, Berlin, Germany — [2]School of Materials Science and Engineering, Peking University, Beijing, China

Li dendrite formation inside all-solid-state lithium batteries (ASSBs) strongly impedes their practical applications. Despite this recognized challenge, a comprehensive understanding of the Li dendrite nucleation mechanism remains elusive. In particular, the initial sites of Li dendrite formation are still ambiguous: do Li clusters form directly at the Li anode surface, or do they nucleate at a distance from the Li metal surface?

Here, based on deep-potential molecular dynamics simulations combined with enhanced sampling techniques, we investigate the atomic-level mechanism of Li cluster nucleation sites in ASSBs. We observe isolated Li clusters initially forming inside the solid electrolyte interphase (SEI), located approximately 1 nm away from the Li anode/SEI boundary, rather than directly connected to the Li anode. The local electronic structure of the spontaneously formed SEI is a key factor enabling the Li cluster formation within SEI. Our work provides atomic-level insights into initial Li-dendrite nucleation sites in ASSBs and could guide future design for developing Li-dendrite-inhibiting strategies.

MM 9: Poster

Time: Monday 18:30–20:30 Location: P1

MM 9.1 Mon 18:30 P1

Well-defined nanostructures synthesized by optimized anodic aluminum oxide template — •Linfeng Su, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The template method has unique advantages in the design and synthesis of materials with specific nanostructures but with some disadvantages. In recent years, through in-depth research and improvement of its preparation methods, the five shortcomings of the traditional anodic aluminum oxide (AAO) template method, such as short-range order and long-range disorder, insulator, single-set of pores, large dead volume, and limited capability to tune pore shape and arrangement, have been successfully addressed by our group. Large-scale control of the shape, size, spatial configuration, and combination of in-plane and out-of-plane pores of well-defined nanostructures can be achieved, thereby broadening the diversity of nanostructures[1, 2]. In addition, we have improved the mechanical strength of the prepared AAO template, so that it can maintain the stability of the nanostructure under a pressure of 10 MPa[3]. The optimized AAO template method provides practical guidance for the design and preparation of catalysts under complex application conditions. [1] Nat. Commun., 2022, 13(1), 2435; [2] Nat. Nanotechnol., 2017, 12(3), 244; [3] Nat. Commun., 2020, 11(1), 299.

MM 9.2 Mon 18:30 P1

Ferroelectric perovskite oxides: PFM investigations of (001) surface — •Andrzej Jasicki[1], Marta Macyk[1], Llorenç Albons[2], Konrad Szajna[1], Martin Setvin[2], Dominik Wrana[1], and Franciszek Krok[1] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Growing demand for energy from green sources drives development in this sector. Hydrogen, as one of the most promising fuels, is mostly produced with the use of electricity during electrolysis, what lowers the overall efficiency of whole process. To reduce energy costs, one should search for an efficient water-splitting catalyst.

Although ferroelectric perovskite oxides show great potential in photocatalysis, it can be further enhanced via piezo- and pyrocatalysis. In order to understand their role in water-splitting process, a thorough investigation of ferroelectricity manifested at surfaces is necessary. Piezoresponse Force Microscopy (PFM), a method based on inverse piezoelectric effect, provides an opportunity to have a closer look into surface domain structure of such materials.

This poster displays PFM and SEM data obtained by investigations into domain structure on surfaces of single-crystalline, ferroelectric perovskites, namely KNbO3 and BaTiO3. Measurements on both polished and cleaved (001) surfaces were conducted in room temperature and under ambient atmosphere. Influence of different poling voltages and exposure to water is also discussed.

MM 9.3 Mon 18:30 P1

Pressure-induced hybridization changes in elemental silicon at Mbar pressure — Robin Sakrowski[1], Christoph J. Sahle[2], •Gordon Scholz[1], Leonie Tipp[3], Mirco Wahab[3], Sindy Fuhrmann[3], and Christian Sternmann[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221, Dortmund, Germany — [2]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [3]Institut für Glas und Glastechnologie, TU Bergakademie Freiberg, Leipziger Straße 28, 09599, Freiberg, Germany

Silicon, a fundamental semiconductor material, undergoes intriguing structural and electronic transformations when subjected to high pressure [1]. These changes are investigated using X-ray Raman scattering (XRS) spectroscopy on pure Si powder loaded into a diamond anvil cell for pressures up to 108 GPa. The XRS spectra of the Si $L_{2,3}$-edge are compared with ab-initio theoretical calculations based on the Bethe-Salpeter equation. Observations include an increase in coordination number from 4-fold to 12-fold and metallization. Additionally, changes in the occupation probability of d-states under pressure are noted, as silicon valence electrons from the 3s and 3p orbitals are transferred.

This work is supported by the BMBF projects 05K22PE2 and 05K22OF1. [1] J.S.Tse et al., J. Phys. Chem. C 118, 1161 (2014)

MM 9.4 Mon 18:30 P1

THz signatures of displacive phase transformation — •Nandita Bajpai[1], Michael Dittler[1], Ahana Bhattacharya[1], Alexander Kunzmann[2], Gabi Schierning[2], and Martin Mittendorff[1] — [1]Department of Physics , University of Duisburg — [2]Institute for energy and material process, University of Duisburg

Phase Change Materials are widely applied in contemporary technological advancements such as sensors, activators, and electronic devices. The Terahertz time-domain spectroscopy (THz-TDS) reflectivity and transmissivity measurements provide valuable insights into carrier dynamics such as mobility and carrier concentration. The temperature-induced phase change results in significant changes in reflectivity and transmissivity that are linked to the presence of free electrons.

Furthermore, the change in the complex conductivity points towards the predicted formation of a charge density wave (CDW) phase, which is a manifestation of periodic modulation of the electron density. This provides more details toward understanding the role of electrons in the phase transformation.

MM 9.5 Mon 18:30 P1

Impact of hyperthermal oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the adsorption rate and the angular distribution of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. It is found that the angular distribution depends strongly on the surface structure and the incidence angle. A higher ratio of specular reflection is found in case of smooth surfaces and large incidence angles.

MM 9.6 Mon 18:30 P1

Ultrafast phonon-mediated dephasing of color centers in hexagonal boron nitride probed by electron beams — •Masoud Taleb[1], Mario Hentschel[3], Harald Giessen[3], and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Defect centers in hexagonal boron nitride (hBN) have gained significant interest as room-temperature single-photon sources, with strong coupling to phonons evident in their photoluminescence and cathodoluminescence spectra. Despite extensive studies, the electron-phonon coupling dynamics and phonon-mediated dephasing of these centers remain underexplored. In this study we experimentally employed an electron-driven photon source (EDPHS) to generate a coherent superposition of phonon states, with the delay between electron and photon pulses controlled to measure dephasing times. The findings reveal an ultrafast dephasing time of 200 fs and a radiative decay of 585 fs at room temperature, contradicting other optical techniques reporting a decay of a few nanoseconds. This rapid dephasing is attributed to the efficient excitation of coherent phonon-polaritons in hBN by electron beams. The research demonstrates the capability of sequential CL spectroscopy for probing the ultrafast dynamics of single emitters in quantum materials, facilitating future applications in quantum networks and devices.

MM 9.7 Mon 18:30 P1

Raman spectroscopic studies on $NiFe_2O_4$-NiO-Ni and MgO-Steel composites as inert anode materials for aluminium molten salt electrolysis — •Felix Drechsler[1], Ulziikhuu Otgonbayar[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Nonferrous Metallurgy and Purest Materials, D-09599 Freiberg, Germany

The use of inert anodes in aluminium molten salt electrolysis offers positive environmental effects compared to the commercially used graphite anode, especially by avoiding CO, CO_2 and perfluorocarbon (PFC) emissions. Cermet anodes consisting of $NiFe_2O_4$, NiO, and Ni were manufactured by powder metallurgy and sintered at different conditions using the Spark Plasma Sintering (SPS) technique. Furthermore, another type of anode was produced using MgO and steel powder mixture to form metalloceramic composites. These anode materials were investigated by micro-Raman spectroscopy to identify phases formed during the sintering process, such as nickel ferrite spinels. Temperature-dependent Raman measurements were performed to examine the micro-structure behaviour of the anode materials at elevated temperatures.

MM 9.8 Mon 18:30 P1

Influence of the alloying elements on microchemistry and nanostructure of Sm-Co based permanent magnets — •Burçak Ekitli[1], Alex Aubert[1], Fernando Maccari[1], Nikita Polin[2], Xinren Chen[2], Esmaeil Adabifiroozjaei[3], Leopoldo Molina-Luna[3], Baptiste Gault[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Functional Materials, TU Darmstadt, 64287 Darmstadt, Germany — [2]Max-Planck-Institut for Sustainable Materials, Düsseldorf 40237, Germany — [3]Advanced Electron Microscopy, TU Darmstadt, 64287 Darmstadt, Germany

Sm-Co 2:17 magnets are high-temperature, high-performance magnets that are commercially available. Their hard magnetic properties are driven by a pinning mechanism, where the complex microstructure and microchemistry play an important role [1]. Since commercial 2:17 magnets consist of five alloying elements and three coherent phases, it is difficult to establish a common understanding of their intrinsic and extrinsic properties. In this study, we continue to investigate the 2:17 magnet system, focusing on a simplified alloy system that we initially introduced [2] by adding Cu to the alloy. Our study focuses on the quaternary Sm(Co,Cu,Zr)6.7 alloy, with four different compositions chosen based on varying Cu concentrations. We investigate the microstructural properties and their influence on the hysteresis of the Sm-Co 2:17 magnet in detail, using advanced characterization techniques such as MOKE, MFM, TEM, and APT. We reveal how Cu concentration influences the microstructure and phase formation, ultimately affecting the magnetic properties.

MM 9.9 Mon 18:30 P1

Bonding changes in solid nitrogen under high pressure — Gordon Scholz[1], Robin Sakrowski[1], Johannes Niskanen[2], Christoph Sahle[3], Leonie Tipp[4], Mirco Wahab[4], Melanie White[5], •Peter Schäfer[1], Ashkan Salamat[5], Sindy Fuhrmann[4], and Christian Sternemann[1] — [1]TU Dortmund, Dortmund, Germany — [2]University of Turku, Turku, Finland — [3]ESRF, Grenoble, France — [4]TU Bergakademie Freiberg, Freiberg, Germany — [5]University of Nevada Las Vegas, Las Vegas, USA

Nitrogen has a complex phase diagram with 15 detected solid molecular phases [1]. In this study, we tracked the electronic and structural changes of nitrogen under high pressure using a novel combined set-up for X-ray Raman scattering (XRS) and X-ray diffraction (XRD) at beamline ID20 at the ESRF exploiting the diamond anvil cell method.

In the pressure regime between ambient conditions and 80 GPa we are able to confirm the δ-phase, ϵ-phase and the ζ-phase with XRD. The corresponding XRS measurements at the nitrogen K-edge show significant changes in the bonding structure. These changes are interpreted via calculated XRS spectra based on molecular dynamic simulations which reveal a hindrance of free rotations of the N_2 molecules in the ϵ-phase.

This work is supported by the BMBF via the projects 05K22PE2 and 05K22OF1.

[1] Turnbull et al. Nat. Commun., 9:4717, (2018)

MM 9.10 Mon 18:30 P1

Grain boundary transformation induced by boron segregation — Xuyang Zhou[1], •Sourabh Kumar[2], Siyuan Zhang[1], Xinren Chen[1], Baptiste Gault[1], Gerhard Dehm[1], Tilmann Hickel[1,2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, 40237, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 12489, Germany

The segregation of solute atoms at grain boundaries (GBs) critically influences the mechanical properties of materials, including corrosion resistance and fracture toughness. This study examines structural transformations induced by minimal boron concentrations at Σ13 GBs in ferrite thin films. Two sample protocols were investigated: one with carbon as the sole solute and the other with carbon and boron co-segregation. Using ab initio calculations, we meticulously explored the competing Σ13 GB phases coexisting with defects and analyzed the energetics of solute segregation at the GB interface. A defect phase diagram was constructed to illustrate the influence of B concentration on GB structure evolution. We reveal that B segregation transforms the GB structure from flat to zigzag trigonal prisms by forming new chemical bonds, enhancing B-Fe bonding strength by 5%. This transformation doubles steel's fracture resistance and provides valuable insights into solute-driven GB phase evolution, contributing to innovative strategies for designing durable, high-performance steel.

MM 9.11 Mon 18:30 P1

Investigation of spin-crossover iron triazole complexes with carbon nanotubes — •Niloofar Azadegan[1], Marvin Dzinnik[2], Maximilian Kilic[3], Franz Renz[4], and Rolf Haug[5] — [1]Institute of solid state physics, Hannover, Germany — [2]Institute of solid state physics, Hannover, Germany — [3]Institute of inorganic chemistry, Hannover, Germany — [4]Institute of inorganic chemistry, Hannover, Germany — [5]Institute of solid state physics, Hannover, Germany

Iron triazole complexes exhibit spin-crossover (SCO) behavior, transitioning between low-spin and high-spin states under external stimuli, making them suitable for sensing and memory applications.

This study investigates carbon nanotubes (CNTs) decorated with iron triazole to enhance electronic and magnetic properties. Current-voltage measurements were performed on bare and decorated CNTs, followed by cryostat measurements under controlled conditions. Preliminary results suggest interactions between SCO behavior and CNTs, with ongoing analysis to explore their potential in advanced electronics.

MM 9.12 Mon 18:30 P1

Linking Characteristic Length Scale in Nanoporous Gold to Alloy Composition and Dealloying Parameters — •Celina Passig[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous metals display unique material properties due to their high volume-specific surface area and characteristic sizes of pores and ligaments. Although theories of structure formation exist, the process is not yet fully understood. Investigating nanoporous gold as model system will deepen the understanding of the underlying mechanisms, enabling a more precise manipulation of nanoporous structures and their mechanical and functional properties. Therefore, a series of small-angle X-ray scattering (SAXS) data was measured, comparing AuAg alloy compositions subjected to different dealloying potentials, durations, and electrolyte concentrations. Preliminary dependencies were formulated to investigate how these parameters influence the resulting characteristic length scale. This ex-situ and future in-situ analysis of microstructural evolution can be used to identify the underlying mechanisms by validating simulated results of the same dealloying processes, such as those presented by Li et al. [Acta Mater. 222 (2022) 117424.].

MM 9.13 Mon 18:30 P1

Inhomogeneities at different length scales in nanocrystalline Pd-Au prepared by inert gas condensation — Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[1,2,3], Jules M. Dake[4], Torben Boll[1], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and •Astrid Pundt[1,2] — [1]Institute of Applied Materials (IAM-WK), Karlsruhe Institute of Technology — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, Ulm University

Inert gas condensation (IGC) is currently the only viable method to prepare bulk samples of nanocrystalline (NC) palladium-gold (Pd-Au). The raw material is thermally evaporated in a vacuum chamber with a background pressure of 10e-8 mbar that has been backfilled with low-pressure inert gas. On collision with the inert gas, the evaporated material condenses into small particles, which are then collected on a rotating cold finger, scraped off and mechanically compacted into disk-shaped samples.

In this study, we investigate the different types of inhomogeneities in IGC Pd-Au on different length scales and compare them to samples prepared by arc melting. To this end, we apply a variety of methods to accurately characterize the composition, porosity, grain size, grain orientation and grain growth behaviour on multiple length scales. Finally, we attempt to explain the source of the inhomogeneities and verify by probing the IGC experimental setup via various experiments.

MM 9.14 Mon 18:30 P1

Development, Characterization and Catalytic Evaluation of New Nanosized metal complexes — •Tarek El-Dabea — Chemistry Department, Faculty of Science, King Salman International University, Ras Sudr, Sinai 46612, Egypt

A series of novel nano metal complexes involving Pd(II), Cu(II), Fe(III) and Ag(I) ions were synthesized using a Schiff base ligand in a bidentate coordination mode. The structural and molecular characteristics of these complexes were

thoroughly characterized via an array of spectroscopic and analytical techniques, confirming molecular geometry and stoichiometry. Solution stability and stoichiometry of the complexes were systematically evaluated, demonstrating stable metal-ligand coordination. Notably, the Pd(II) complex exhibited unique electronic characteristics, identifying it as a promising candidate for catalytic applications. Based on these results, the Pd(II) complex was tested as a catalyst for synthesizing Different multicomponent reactions. This was achieved through using microwave irradiation. The selection of Pd(II) was informed by its favorable catalytic profile and theoretical insights. Optimization trials demonstrated that the Pd(II) catalyst afforded high yield and efficiency under eco-friendly (H*O/EtOH) solvent conditions. Reusability assessments showed that the catalyst retained high activity for up to five cycles, with minimal performance decline afterward. A mechanistic pathway was proposed, highlighting Pd(II)'s ability for axial coordination, supported by theoretical evidence

MM 9.15 Mon 18:30 P1

Epitaxial Stabilization of Multifunctional Oxide, Oxynitride, and Telluride Thin Films using a Hybrid Pulsed Laser Deposition Technique — Pia Henning, Anna Tschesche, Shagun Thakur, Niklas Kohlrautz, Abhishek Sharma, Laura Pflügl, and •Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Materials science uses state-of-the-art thin film techniques, such as pulsed laser deposition (PLD) and molecular beam epitaxy (MBE), to artificially fabricate complex materials [1]. Epitaxial films with controlled defects and orientation are practical for modifying functionalities. We developed a hybrid PLD system attaching molecular beam sources (for elements with high vapor pressure) to fabricate multifunctional oxide, oxynitride, and tellurides. Additionally, gases are provided through a microplasma source. This setup makes a wide range of cation and anion engineering possible in complex materials. In this presentation, we will address challenges in the growth of thin films and how modifications in the defects and structure influence functional properties by taking examples of La_2NiMnO_6 (ordered magnetism and electrocatalysis), Cr_xTe (ferromagnetism and magnetic anisotropy), and $SrNbO_3$ (optical transparency and metallic conduction). Moreover, we will discuss how such a hybrid deposition system can be utilized to grow high-entropy materials and stabilize doping beyond the solubility limit. [1] A. Tschesche, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

MM 9.16 Mon 18:30 P1

EXAFS-driven Investigation of ZnO-Mn2O3 and ZnO-Mn2O3-rGO Nanocomposites: Unraveling Structural, Optical, and Electronic Properties — •Shaimaa A. Habib[1], Shehab E. Ali[2], Messaoud Harfouche[3], and Ahmed Awad[4] — [1]1.*Physics Department, Faculty of Science, Damnhour University, Damanhour 22516, Egypt — [2]Materials Science Laboratory, Physics Department, Faculty of Science, Suez Canal University, 41522, Ismailia, Egypt. — [3]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [4]Physics Department, Faculty of Science, Tanta University, Tanta 31527, Egypt

The structural, optical, and electronic properties of ZnO-Mn2O3 and ZnO-Mn2O3-rGO nanocomposites were investigated. The materials, synthesized via sol-gel and self-propagation methods, exhibited porous structures with crystallite sizes of 22-48 nm, as confirmed by XRD and SEM analyses. UV-Vis spectroscopy revealed that rGO incorporation reduced the optical bandgap from 2.63 eV to 1.86 eV and increased the Urbach energy from 1.91 eV to 2.55 eV. The Wemple-DiDomenico model showed a decrease in oscillator resonance energy from 6.64 eV to 6.15 eV and an increase in dispersion energy from 6.47 eV to 13.24 eV. EXAFS and XANES studies at SESAME synchrotron facility provided insights into the coordination environment and electronic structure of the metal centers. This comprehensive characterization establishes a foundation for applying these nanocomposites in optoelectronics, photocatalysis, and energy conversion applications, highlighting rGO's role in enhancing composite performance.

MM 9.17 Mon 18:30 P1

Electrochemical determination of the diffusion coefficient of intercalating species in host metals - conditions of applicability of potential step chronoamperometry — •Magdalena Seiler, Giorgia Guardi, Stefan Wagner, and Astrid Pundt — KIT, Karlsruhe, Deutschland

The diffusion coefficient is generally used to describe the diffusion of intercalating species such as lithium and hydrogen in host metals. It can be determined by a variety of methods, including electrochemical methods. Among these, permeation methods between front and back side of a sample are widely used. On the contrary, in potential step chronoamperometry only one side of the sample needs to be contacted, which is e.g. beneficial for thin film studies. In this work measurements using both methods are performed for hydrogen in palladium and compared to the literature. It is shown that the application of the potential step chronoamperometry approach gives correct results only under very specific restrictions regarding sample thickness and measurement period.

MM 9.18 Mon 18:30 P1

Synthesis, and Characterization of Li/Mn-Excess Cathode Materials for Li-ion Batteries. — •John Karuga[1], Mesfin Kebede[2], and Guido Schmitz[3] — [1]Institute of Materials Science, Department for Material Physics, University of Stuttgart — [2]Institute of Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa — [3]Institute of Materials Science, Department for Material Physics, University of Stuttgart

The study aims to mitigate O2 evolution, spinel phase, and unstable CEI formation common in Li/Mn-excess cathodes. The poster presents preliminary results of the pristine Li/Mn-excess cathodes, which are practical alternatives to LFP, NCA, and Ni-excess materials for high-performance Li-ion batteries. The Li2MnO3 phase in Li/Mn-excess cathodes stabilizes the crystal structure, contributes to the higher discharge capacities >250 mAh/g. Commercialization of Li/Mn-excess materials remains challenging due to undesired transformation from layered to spinel phase, O2 evolution, parasitic reactions with the LiPF6 electrolyte. The Li/Mn excess materials were prepared via solid-state synthesis. Characterization with SEM-EDS, Raman, HR-TEM, and XRD confirmed the development of a material of uniform nano-crystallites with well-layered structure and 0.472 and 0.2 nm interplanar distances, which correspond to the 003 and 104 planes. The CV analysis confirms that the redox reactions (Ni2+/Ni4+; Co3+/Co4+; Mn3+/Mn4+/5+/7+) are highly reversible. The charge transfer resistance is low, indicative of better Li+ diffusion and stable CEI.

MM 9.19 Mon 18:30 P1

Magnetic anisotropy and anomalous Nernst effect in cubic Fe4N films — •Karel Knížek[1], Jakub Vít[1], Mariia Pashchenko[1], Petr Levinský[1], Kyo-Hoon Ahn[1], Jaroslav Kohout[2], and Imants Dirba[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czechia — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czechia — [3]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany

Iron nitrides Fe(x)N are commercially important compounds because of their versatile magnetic, electrical, and mechanical properties. We have studied magnetic and transverse thermoelectric properties of Fe(4)N films prepared by magnetic sputtering. The well-known anisotropic magnetoresistance [1] and rectangular magnetization curves for thin oriented films led us to investigate magnetic anisotropy by rotating the sample in external magnetic field and measuring magnetization along the field. The signal is complex, exhibiting harmonics beyond the expected crystal symmetry. Moreover, the magnetic-field history crucially impacts the anisotropy. The results are quite distinct below and above the metamagnetic phase transition near 50K. The results of the magnetic measurements are compared with anomalous Nernst effect experiments and DFT calculations.

[1] M. Tsunoda et al., Applied Physics Express 2, 083001 (2009).

MM 9.20 Mon 18:30 P1

Thermoelectricity in Bi-directionally Strained $CsSnI_3$ Perovskite — •Michele Reticcioli[1], Mariangela Ruggeri[2], Giovanna D'Angelo[2], and Alessandro Stroppa[1] — [1]CNR-SPIN L'Aquila, Italy — [2]Università degli Studi di Messina, Italy

Thermoelectric materials play a pivotal role in energy sustainability, converting waste heat into electricity without moving parts or emissions. Recent advances spotlight metal halide perovskites, such as $CsSnI_3$, as promising candidates for eco-friendly thermoelectric applications due to their low thermal conductivity and high electrical efficiency. In this work, we explore the influence of bidirectional strain on the orthorhombic gamma-phase of $CsSnI_3$ using density functional theory (DFT), complemented by experimental insights from our collaborators. Strain effects, ubiquitous in thin films grown on mismatched substrates, are known to modify electronic structures and transport properties. Our findings reveal a peculiar dependence of the bandgap on strain direction and intensity. These changes directly impact the thermoelectric properties, including the Seebeck coefficient and figure of merit, emphasizing the interplay between strain-induced electronic modulation and thermoelectric performance. This study contributes to the growing understanding of strain effects in perovskites, offering valuable insights into their potential for thermoelectric applications.

MM 9.21 Mon 18:30 P1

GAP vs. MACE: Efficiency evaluation in a liquid electrolyte system — •Anton Beiersdorfer[1], Lisa Hetzel[1], Carsten Staacke[2], Florian Deissenbeck[2], and Christopher Stein[1] — [1]Technische Universität München, München, Germany — [2]Cellforce Group GmbH, Tübingen, Germany

Machine learning interatomic potentials (MLIP) have transformed molecular simulations, enabling complex materials to be modeled with increasing accuracy and efficiency. As MLIP models evolve, so does the demand for advanced computing architectures, particularly graphics processing units (GPUs), which can accelerate computations compared to traditional central processing unit (CPU) based systems. However, the high cost associated with GPU resources constrain access in both academia and industry, highlighting the relevance of comparing GPU-based and CPU-based MLIPs under real-world conditions.

To this end two popular MLIPs are examined: the GPU-accelerated MACE model and the CPU-based GAP model applied to a test system of a standard

battery electrolyte. The system is selected for its demanding electrostatic interactions in solution, which the MLIPs approximate by learning the local interaction patterns that contribute to the overall electrostatic behavior. Therefore, it represents a significant computational challenge and provides a rigorous benchmark for MLIP accuracy and efficiency. By focusing on these models, the study aims to reveal key differences in computational and numerical performance metrics and resource efficiency as well as in physical performance, particularly through comparisons to experimentally measured properties.

MM 9.22 Mon 18:30 P1

Navigating the Latent Space of Chemical Solid State Reactions in Hybrid Battery Interfaces — •Sina Ziegler, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

We explore the potential of rare earth lithium halides as a material-efficient, nanometer-thick cathode coating in contact with thiophosphate electrolytes. Traditional theoretical approaches, such as molecular dynamics (MD) and Monte Carlo (MC) simulations, are computationally intensive for larger systems, posing a challenge in simulating battery interfaces. To identify a suitable halide/thiophosphate combination, it is essential to determine an energetically feasible solid-state reaction pathway within the multidimensional phase diagram of these materials. We employ *ab initio* thermodynamics to assess the thermodynamic stabilities of the resulting solid-state electrolyte (SSE) and halide interfaces by screening the reaction-free enthalpies of potential interface reactions. An end-member analysis is then performed to evaluate possible compositions of interface products and secondary phases, using techniques such as Principal Component Analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), and autoencoders to identify linked reactions within the chemical latent space.

MM 9.23 Mon 18:30 P1

Structure and transport properties of Li3MCl6 superionic conductors — •Ziyan Zhang[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]Chair for Functional Materials,School of Natural Sciences, Technical University of Munich,85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

Modern society permanently requires more advanced, better performant, safer, and cost-effective energy storage solutions, where the all-solid-state battery (ASSB) concept based on lithium metal is closest to commercialization. Solid electrolytes are a key component of ASSB, defining its lifetime and performance. Halide-based solid electrolytes Li3MCl6 (M = transition metals, rare-earth metals) are emerging as promising materials for all-solid-state batteries due to their high ionic conductivity, electrochemical stability, and compatibility with lithium metal anodes. The current study deals with the systematic characterization of Li3MCl6 solid conductors with M = In, Zr, and Ti transition elements. The focus will be put on the optimization of synthesis routes (between solvent-mediated and mechanochemistry), composition control as well as enhancement of ionic transport. Comprehensive structural characterization, encompassing lab X-ray diffraction (XRD) with Rietveld refinement combined with differential bond-valence estimates of lithium diffusion pathways and differential scanning calorimetry, is performed to reveal the crystallographic details, microstructure, and lithium-ion dynamics.

MM 9.24 Mon 18:30 P1

Processing of non-conductive materials by electroerosion treatment. — •Anton Bespalov — Moscow, Russia

Electroerosion processes process only conductive materials, but it is possible to process non-conductive materials by applying a thin layer of metal to their surface. In this work, based on experiments, the possibility of destruction (processing) of tungsten carbide coated with a layer of 0.01 mm copper with a copper electrode using electric erosion machines is considered. As a result of the experiments, the destruction in the samples corresponding to the shape of the electrode was revealed, which proves the possibility of processing.

MM 9.25 Mon 18:30 P1

Structure formation and phase behavior of amine-water mixtures — •Lena Friedrich[1], Michael Paulus[1], Aurélien Perera[2], Martina Požar[3], Dirk Lützenkirchen-Hecht[4], Nicola Thiering[1], Jaqueline Savelkouls[1], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität, 44221 Dortmund, Germany — [2]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, F75252, Paris cedex 05, France; — [3]University of Split, Faculty of Science, 21000 Split, Croatia — [4]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

Amines are associating liquids that can form transient supramolecular structures via hydrogen bonding [1]. Adding of water can significantly alter the liquids' structure [2] and amine/water mixtures show an interesting phase behavior exhibiting a lower critical solution temperature (LCST) [3]. We studied linear, primary amines mixed with various proportions of water for a variety of temperatures by X-ray diffraction at BL8 and BL9 of DELTA (TU Dortmund). The structure factor prepeak shows a peculiar concentration and temperature dependence which resembles the different phase regimes ranging from disordered nematic via single liquid to two liquid phase. We thank the BMBF for funding via DAAD in the scope of the French-German collaboration PROCOPE 2024-2025 (Project-IDs 57704875 and 50951YA). [1] A. Perera et al., JPC B 44, 128 (2024). [2] L. Almasy et al., PCCP 21, 9317 (2019); [3] J. Glinski et al., J. Colloid. Interface Sci. 162, 129-134 (1994)

MM 9.26 Mon 18:30 P1

A Phase Change Material's Journey through its Energy Landscape — •Jakob Ballmaier, Sebastian Walfort, Elias Abele, and Martin Salinga — Universität Münster, Institut für Materialphysik

The concept of energy landscapes is highly successful in explaining structural dynamics of supercooled liquids and glasses. Locally stable configurations correspond to local minima of the total potential energy of the system in the high-dimensional phase space. During physical aging a glass can evolve towards lower local minima through a series of saddle points. Experimental observation of this is challenging, since in large systems several saddle points are passed within the shortest resolvable timescales.

Here, we track paths through the energy landscape of a nanoscopic volume of germanium telluride by following the temporal evolution of its electrical resistance. Two regimes turn out to be especially instructive: fast measurements of the resistance immediately after the formation of the glass as well as slower measurements at low temperatures, where the influence of individual relaxation steps on the resistance can be resolved.

MM 9.27 Mon 18:30 P1

Graphite Composites with Titanium as a Secondary Filler - Microstructure and Electronics — •Hoang Thinh Nguyen, Maria Gaudig, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, Institute of Physics, Group μMD, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

The bipolar plate (BPP) is a crucial component in electrolyzers and fuel cell stacks, serving to separate individual electrochemical cells while ensuring electrical conductivity, water distribution, and mechanical stability. However, the high costs associated with conventional materials like titanium or stainless steel demand the exploration of novel materials and fabrication methods. Graphite-based composites have already emerged as cost-effective alternatives for BPPs. In this work, we developed and characterized an innovative composite material that combines the high electrical conductivity of titanium with the affordability and lamellar structure of graphite to create titaniumgraphite composites. Microstructural analyses using scanning electron microscopy (SEM) and nano X-ray computed tomography revealed that titanium particles integrate gapless into the graphite matrix, enhancing the creation of continuous conductive pathways. Electrical conductivity measurements revealed interesting dependencies on filler composition: depending on the filler ratio, either titanium or graphite becomes the dominant contributor to the overall conductivity. These findings highlight the interrelation between particle morphology, structure, and filler ratio in optimizing the composite matrix for BPP applications.

MM 9.28 Mon 18:30 P1

Mesoporous Ti and TiCu network structures prepared by liquid metal dealloying — •Niklas Österle, Markus Ziehmer, Fabian Andorfer, and Carl E. Krill III — Institute of Functional Nanosystems, Ulm University, Germany

Metallic open-cell foams have emerged as promising functional and structural materials. The use of Ti and TiCu would extend the application of such foams into the medical field, as both materials are highly biocompatible, making them excellent choices for implants and prostheses. Combined with the porous structure of metallic foams, which facilitates the infiltration and adhesion of bone cells, the functionality and performance of prosthetic devices could be significantly improved.

In this work, we present the fabrication of mesoporous Ti and TiCu network structures via liquid metal dealloying. This technique enables the selective removal of Cu from TiCu precursor alloys within a Mg melt to form mesoporous structures. By varying the Mg-to-precursor mass ratio, we show that the chemical composition and morphology of the final network can be tailored. The network structure and morphology were investigated using 2D and 3D imaging, and EDS and XRD were employed for phase analysis. Various morphological structures can be linked to specific compounds in the TiCu phase diagram. Future investigations will focus on post-dealloying thermal coarsening.

MM 9.29 Mon 18:30 P1

Role of trace elements on the GP-Zone formation Al-Cu alloys — •Sandra Müller, Isidor Switalla, Johannes Berlin, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Both formation and dissolution of Guinier-Preston zones in Al-Cu alloys depend on the presence of excess vacancies. They are quenched in from the high temperature homogenisation treatment but will possibly disappear during the natural aging at ambient temperature. The lifetime of excess vacancies in pure

Aluminium is much shorter than that in Al-Cu alloys, where vacancies presumably are trapped in GP zones. Therefore, a small increase in temperature can lead to drastic changes in the microstructure of these materials by releasing the trapped vacancies. Resistometry is a simple online method to monitor changes in the microstructure of a metallic alloy, complemented by DSC and hardness measurement.In this work we focused on natural and slightly above room temperature artificial ageing of Al-Cu samples containing 2 - 4 wt.% of Cu. DSC gives rather clear evidence that precursor cluster of only very few atoms form before the GP-zones are detected. Those precursors and the GP zones formation can be suppressed or delayed by minor addition of vacancy-binding trace elements like Tin and Indium.

MM 9.30 Mon 18:30 P1

Irradiation Induced Defects in W-Re Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny Russell[1], Maximilian Suhr[1], Leon Chryssos[1], Lucian Mathes[1], Mikhail Zibrov[2], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [2]Max Planck Institute for Plasma Physics, 85748 Garching, Germany

The plasma-facing components in a fusion reactor have to withstand the irradiation of 14 MeV neutrons, which are released in the fusion reaction of deuterium and trithium. Tungsten is considered to be the most suitable plasma-facing material, due to its high melting point, high thermal conductivity and low erosion under fusion reactor operating conditions. In addition to radiation damage, neutron irradiation of tungsten creates transmutation elements such as rhenium. In this work, the effect of rhenium on the defect characteristics in self-ion irradiated tungsten is investigated. Self-ion irradiation is used to mimic the radiation damage caused by 14 MeV neutrons. Positron annihilation spectroscopy is used to provide non destructive, atomic scale resolution measurement of the irradiation damage. Coincidence Doppler broadening spectroscopy of the 511 keV annihilation line is used to provide element sensitive measurements of vacancy type defects. This allows us to test theoretical predictions that rhenium precipitates around voids.

MM 9.31 Mon 18:30 P1

Phases of AlN by machine learning potentials — •Simon Liebing, Oliver Heymer, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany

AlN is an important wide-band gap semiconductor with e.g. applications in high power electronics. Under high pressure (about 13 GPa) the wurtzite phase transforms to the rocksalt phase. Here, we attempt to simulate this phase transition as function of temperature and pressure by means of machine learned interatomic potentials trained on accurate density functional theory molecular dynamics data. In particular we will utilize use the open-source library FitSNAP [1] for atomistic machine learning in combination with the molecular dynamics code LAMMPS [2]. FitSNAP is used to provide fast interaction potentials with accuracy inherited from DFT. It already provides interfaces for popular open-source codes such as Quantum ESPRESSO[3], PyTorch and LAMMPS and it supports the state-of-the-art atomic cluster expansion (ACE) descriptors [4]. The ACE descriptors transform structural information into machine learning models. This enables us to carry out large-scale classical MD systems of AlN with thou- sands of atoms with DFT accuracy. The results will be compared to earlier works based on small unit cells using density functional theory. [5] References [1] Rohskopf et al., Journal of Open Source Software, 8 (84), 5118 (2023). [2] A. P. Thompson et al. Comp Phys Comm, 271 10817 (2022). [3] P. Giannozzi et al. J. Chem. Phys. 152, 15 (2020). [4] Drautz, R. Physical Review B, 99 (1), 014104 (2019). [5] S.Schmerler and J. Kortus Physical Review B, 89, 6, (2014).

MM 9.32 Mon 18:30 P1

Brittle to Ductile: Elasticity and Bonding in TiVN Hard Alloys — •Santiago Gómez, Ferenc Tasnadi, Magnus Odén, and Igor A. Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, 58183 Sweden

Hard alloys find extensive applications, such as in coating metal-cutting tools and turbine protective layers, among others. Despite the availability of effective alloys in the market, most remain intrinsically brittle. A critical aspect of alloy engineering is, therefore, the systematic exploration of hard but more ductile alloys with improved fracture toughness.

The low temperature dynamical instability of VN suggest an alloying pathway to improve the ductility of TiN. The idea has been realized by supporting experiments using micro-pillar fracture analysis. In this study, we are searching for novel materials descriptors to gain a better understanding of brittle and ductile behavior, all in an ideal sense suitable for modern data-driven materials science powered by Density Functional Theory (DFT) calculations.

Our findings reveal composition-dependent variations in elastic moduli and anisotropy. Brittle to ductile behavior transition is predicted when a certain composition of Vanadium is reached. Chemical bonding analysis, employing the Quantum Theory of Atoms in Molecules (QTAIM), provide insights into the electronic structure, highlighting trends in bond critical point densities and virial ratios for first-neighbor interactions. These results are contextualized against analogous systems such as $Ti_xAl_{1-x}N$, providing a comparative framework.

MM 9.33 Mon 18:30 P1

Modeling dislocation motion in aluminium alloys by DFT — Inna Plyushchay[1,2], Anna Pliushchai[2,3], Nebahat Bulut[2], Zhengqing Wei[2], and •Sibylle Gemming[2,4] — [1]Natl. Taras Shevchenko University of Kyiv, Ukraine. — [2]Inst. Physics, TU Chemnitz, Germany — [3]Natl. TU of Ukraine, Igor Sikorsky Kyiv Polytechnic Inst., Ukraine — [4]MAIN Center, TU Chemnitz, Germany.

Measured elastic moduli of bulk metals differ from the ideal theoretical values due to the presence of point and line defects as well as grain boundaries, and their joint action has successfully been studied by atomistic simulations. For low-doped alloys with additional elements in small quantities, a plethora of further interactions is obtained, whose classical description is hampered by the lack of suitable potentials for the interaction between different elements. We therefore employ first-principles calculations to determine the dopant-induced electronic structure change in and around the core region of the Shockley partial dislocation in Aluminium as a prototype fcc metal with substitutional Mg, Zr, and Si atoms as dopants. The results indicate that the radius of the first coordination sphere changes within a range of few percent and that all discernible changes in electron density are localized within the first coordination sphere of the impurity. A tendency for the formation of aluminide precipitates is obtained, which may nucleate at 0D, 1D, or 2D defect sites and stabilize local structure motifs which would not be formed in the unperturbed bulk phase.

MM 9.34 Mon 18:30 P1

Generalized susceptibility expressed by Wannier functions — •Dominik Váňa and Jaroslav Hamrle — Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague

The generalized susceptibility describes the tendency (energy stability) of the cubic phase to become modulated. A typical example is the modulation of Ni_2MnGa [1] which can undergo structural transformation from austenite to a modulated structure. The generalized susceptibility is calculated using occupation probability (Fermi-Dirac distribution), however, this approach omits the dependence which the coupling coefficient of the electron-lattice interaction has on electronic states. The goal of this work is to express generalized susceptibility with calculated coupling coefficients. As the first step, we express generalized susceptibility using Wannier functions, modifying the original approach of Motizuki [2], based on a linear combination of atomic orbitals.

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MM 9.35 Mon 18:30 P1

First-principles insight into the role of electronic band filling on thermodynamic stability and mechanical properties of tantalum-diboride-based solid solutions — •Annop Ektarawong[1], Kunpot Mopoung[1], Chayanon Atthapak[1], Thiti Bovornratanaraks[1], and Björn Alling[2] — [1]Chulalongkorn University, Bangkok, Thailand — [2]Linköping University, Linköping, Sweden

Owing to their superior stabilities and mechanical behaviors at high temperature, AlB_2-type metal diborides have increasingly been considered as promising hard and protective coating materials for cutting tools. In this presentation, we theoretically demonstrate how the thermodynamic stability and mechanical properties of metal diborides can feasibly be improved either through the presence of structural defects beyond the dilute limit or through the alloying process, focusing particularly on tantalum diboride. Our first-principles studies reveal the significant enhancement of the stability, stiffness, shear strength, and hardness of the diboride can directly be interpreted in terms of electronic band filling of the bonding and antibonding states of the material.

MM 9.36 Mon 18:30 P1

Unveiling the Origin of the Yield Stress Anomaly in L12 Intermetallics via Atomistic Approaches — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

We present an approach to studying the yield stress anomaly (YSA) in L12 intermetallics by bridging the electronic scale with large-scale molecular dynamics simulations, using machine-learning-based interatomic potentials. An ab initio database of temperature-dependent Gibbs energy for relevant planar defects in L12 Ni3Al was developed, covering the full temperature range of the YSA. Machine-learning interatomic potentials for Ni3Al, trained through a physically informed active-learning scheme, achieved accuracy comparable to DFT data and successfully modeled key dislocation behaviors in million-atom models. These MD results enabled the development of a phenomenological model that effectively explains YSA characteristics, offering new insights into the high-temperature performance of L12-strengthened high-entropy alloys.

MM 9.37 Mon 18:30 P1

Modelling and Descriptor-based Synthesizability Analysis of High-Entropy Materials — •Chen-Chen Er[1] and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [3]Duke University, Durham, USA

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic and thermal properties that are promising for applications in the energy and electronics sectors. HEMs include disordered ceramics such as carbides, nitrides, or oxides with ordered anion sublattices and disorder on the cation sites. There are typically five or more cation species to maximize configurational entropy.

Efficient modelling of the disordered systems is conducted based on an ensemble of supercells approach as implemented in the partial occupation algorithm (POCC) [1] within the AFLOW framework [2,3]. Predictive descriptors including the entropy forming ability (EFA) [4] and disordered enthalpy-entropy descriptor (DEED) [5] are crucial to assess synthesizability. Here, we present results for several high-entropy ceramics, including their electronic properties and synthesizability.

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MM 9.38 Mon 18:30 P1

An extended two-temperature model for copper — •Simon Kümmel and Johannes Roth — FMQ, University of Stuttgart, Germany

Since its introduction, the two-temperature model (TTM) has been a very powerful tool used to simulate material under strong electronic excitation following strong laser irradiation by coupled heat conduction equations for the electronic and lattice system.

Here, we present an implementation of the TTM, coupled to a molecular dynamics code, in which the heat capacity, the heat conduction, electron-phonon coupling parameter depend on the degree of excitation. We extend this model by also including an interatomic potential that depends on the degree of excitation and is capable of reproducing non-thermal effects predicted by electron temperature-dependent density functional theory calculations.

We investigate the influence and importance of each parameter in a case study applied to copper and compare our findings to experimental investigations.

MM 9.39 Mon 18:30 P1

Exploring Ionic Diffusion and Heat Transport Mechanisms in NASICON Materials: A Molecular Dynamics Study — •Insa F. de Vries and Nikos L. Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, sodium-ion batteries have emerged as both a potential replacement and a complement to traditional lithium-ion based energy storage systems [1]. However, ensuring the safety and reliability of any future battery system requires a controlled modelling and a thorough understanding of the thermal conduction characteristics, especially with respect to preventing overheating during operation.

Our study uses molecular dynamics calculations on members of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ family with different stochiometries (x=2.6, 3.4 and 3.8). For each stochiometry we use different cell geometries characterised by an order parameter. In order to reveal the influence of the sodium ion mobility on the heat transport, we calculate key transport properties, namely the sodium diffusion coefficient and the thermal conductivity. We start from a pre-established interatomic potential [2] and calculate the thermal conductivity using a Green-Kubo approach. We find that it peaks for the compounds with x = 3.4. Increased diffusion caused by small variations in the parameterisation of the sodium-oxygen interaction leads to simultaneous, equally directed changes in the thermal conductivity.

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[2] P. Kumar & S. Yashonath, J. Am. Chem. Soc. 2002, 124, 3828

MM 9.40 Mon 18:30 P1

Semiclassical transport in multiple Weyl points — •Ricardo Barbosa, Stuart Parkin, and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

We investigate transport contributions[1,2] in three-dimensional materials exhibiting multiple Weyl nodes[2,3], which are linear band touchings acting as point-like sources and sinks of Berry curvature in momentum space, often referred to as "Weyl-Berry monopoles". Specifically, we analyze the transport properties of CoSi[4,5], a chiral topologically nontrivial semimetal with band-touching points of higher-than-two-fold degeneracy and nonzero Chern numbers. Notably, at the Γ and R points, the band-touching nodes are four- and six-fold degenerate, respectively, with Chern numbers up to ±4. Using the Boltzmann transport equation[6], we investigate how these features give rise to unconventional electronic properties, focusing on the corresponding charge and node conductivities.

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MM 9.41 Mon 18:30 P1

A novel technique for measuring 3D thermal conductivity of carbon paper — •Oliver Roser[1], Achour Mahfoudi[1], Cornelius Hahn[1], and Andreas Griesinger[1,2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

Gas diffusion layers based on carbon paper are used in various types of fuel cells. They make a significant contribution to dissipating the heat loss generated in the catalyst layers and homogenizing the temperature field. The material structure causes strongly direction-dependent thermal conductivities. It is not possible to determine the direction-dependent thermal conductivity under operating boundary conditions using existing methods. We present a newly developed technique with which thermal conductivity can be determined in all spatial directions. Measurements of thermal conductivity in the sample plane are carried out under steady-state boundary conditions. When measuring thermal conductivity through the sample plane, we use a transient measurement approach. The apparatus developed for this purpose and its components are presented. We show how to set and control the application-related boundary conditions such as temperature, surface pressure, moisture content and filling gas. The thermal measurements and evaluation strategies are presented, and the achievable accuracy of the method is discussed. Finally, we show initial measurement results that demonstrate a significant impact of direction, temperature and moisture content on thermal conductivity of gas diffusion layers, depending on the material structure.

MM 9.42 Mon 18:30 P1

Low-temperature thermal conductivity of $YAlO_3$ and $YbAlO_3$ — Parisa Mokhtari[1,2,3], •Ulrike Stockert[3], Stanislav Nikitin[4], Leonid Vasylechko[5], Manuel Brando[2], and Elena Hassinger[3,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Faculty of Physics, Technische Universität Dresden, 01062 Dresden, Germany — [4]PSI Center for Neutron and Muon Sciences, 5232 Villigen PSI, Switzerland — [5]Lviv Polytechnic National University, Lviv 79013, Ukraine

$YAlO_3$ is a popular substrate, laser, and scintillator material used at temperatures down to those of liquid helium. A good thermal conductivity is required for many applications for instance to facilitate energy release in lasers or thermal coupling via substrates.

We present for the first time thermal conductivity data on $YAlO_3$ below 80 K, covering the T range from 2 K to 300 K. In addition, we have studied the thermal conductivity of YbAlO3 in the temperature window from 50 K to 300 K. Both materials are very good thermal conductors. The thermal transport in these electrical insulators is phononic and can be fitted by the Callaway model. We discuss our results with respect to the relevance of different scattering processes, the origin of the thermal conductivity anisotropy, and the influence of Y-Yb exchange on the thermal transport. Our results on $YAlO_3$ confirm the suitability of the material for applications requiring a low thermal resistance at temperatures down to liquid He.

MM 9.43 Mon 18:30 P1

(Very) high-temperature physics of selected Planckian metals — •Zuzanna Helena Filipiak[1,2] and Andrew P. Mackenzie[1,2] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, United Kingdom

Planckian dissipation is the mysterious phenomenon of an almost universal saturation of the electron scattering rate in many condensed matter systems despite their vastly different microscopics and strengths of electron interactions. In crystalline samples, the Planckian temperature dependence of resistivity is referred to as strange metallicity in the low-temperature regime and bad metallicity if the behaviour continues to high temperatures. Despite interest in such materials because of their unique physics, their high-temperature characteristics continues to be understudied. We developed two setups in which resistivity of a metallic sample is measured as a function of temperature (ranging from 2 to 1000 K), magnetic field (up to 12 T) and atmosphere (oxygen-rich, argon, high vacuum). Our results for selected single-crystal and thin-film samples of metallic delafossites, nickelates and ruthenates, incl. ruthenium dioxide, will be presented.

MM 9.44 Mon 18:30 P1

Fitting Tensorial Properties with MACE: a Study of $Li_2Ti_5O_{12}$ Electric Field Gradient Tensors — Elena Gelzinyte[1], Karsten Reuter[1], Christian Carbogno[1], and •Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Machine learning interatomic potentials, which serve as surrogate models for predicting a structure's energy and forces, have significantly accelerated atomistic simulations. Equivalent approaches have been applied to predict other structural or atomic properties, such as charges, dipole moments, and polarisabilities. One such framework is MACE, a higher-order equivariant neural network [1]. Due to the way its internal features are constructed, the output part of the model may be readily modified to suit the symmetry of the target property. In this presentation, we discuss the required modifications for fitting atomic tensorial quantities and the resulting model's applicability, limitations, and advantages. For illustration, we focus on the prediction of electric field gradient tensors (a per-atom traceless symmetric tensor) using a $Li_2Ti_5O_{12}$ data set [2]. We consider the improvement in fitting the tensorial properties directly, rather than derived scalar properties, and compare the modified MACE's results with those of λ-SOAP [3], discussed in [2].

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MM 9.45 Mon 18:30 P1

First-Principles Analysis of Spin-Disorder Resistivity and Its Temperature Dependence — •Fabian Engelke, Felix Schug, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität, Giessen, Germany

By means of Matthiessen's rule, one can decompose the electrical resistivity of materials into contributions of separate scattering mechanisms. Here, we present ab initio calculations of the electron-magnon scattering contribution to the specific resistivity of ferromagnetic materials within the supercell method. For that purpose, we model the spin disorder with an atomistic spin model described by a Heisenberg Hamiltonian. We then use the Landau-Lifschitz-Gilbert equation to describe the system's dynamics and introduce temperature effects utilizing Langevin dynamics. In the second step, we employ noncollinear density functional theory and the Non-equilibrium-Green's function formalism in a Koringa Kohn Rostocker (KKR) representation to calculate the conductance through slabs of varying thickness derived from the spin-configurations obtained in the first step. Subsequently, we calculate the specific resistivity by averaging over supercells and applying Ohm's Law. First results for Fe show good agreement with experimental data at high temperatures, highlighting the contribution of magnetic short-range order effects to the total temperature dependence of the specific electric resistance in the temperature regime above the Curie-Temperature.

MM 9.46 Mon 18:30 P1

Tuning intrinsic anomalous Hall effect from large to zero in two ferromagnetic states of $SmMn_2Ge_2$ — Mahima Singh[1], Jyotirmoy Sau[1], •Banik Rai[1,2], Arunanshu Panda[1], Manoranjan Kumar[1], and Nitesh Kumar[1] — [1]S N Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700106, India — [2]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden

The intrinsic anomalous Hall conductivity (AHC) in a ferromagnetic metal is determined by its band structure, with spin orientation being a key band structure tuning parameter. We study a layered tetragonal room temperature metallic ferromagnet $SmMn_2Ge_2$, which gives us the opportunity to study magneto-transport properties where both the *c*-axis and *a*-axis can be magnetically easy axes depending on the temperature range we choose. We show a moderately large fully intrinsic AHC up to room temperature when the crystal is magnetized along the *c*-axis. Interestingly, the AHC can be tuned to completely extrinsic with extremely large values when the crystal is magnetized along the *a*-axis, regardless of whether the *a*-axis is magnetically easy or hard. First principles calculations show that nodal line states originate from Mn-*d* orbitals just below the Fermi energy (E_F) in the electronic band structure when the spins are oriented along the *c*-axis. Intrinsic AHC originates from the Berry curvature effect of the gapped nodal lines in the presence of spin-orbit coupling. AHC almost disappears when the spins are aligned along the *a*-axis as the nodal line states shift above E_F and become unoccupied.

MM 9.47 Mon 18:30 P1

Rapid photobleaching of Yb-doped optical fibers exposed to gamma radiation by high energy ns pulsed laser — •Esra Kendir Tekgül and Bülend Ortaç — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Rare earth-doped optical fibers (OFs) have become one of the new high-power laser and sensor applications. Therefore, it is very important to protect such OFs from being exposed to external effects and to increase their reusability after these effects. Here, Radiation Induced Attenuation (RIA) and the Photo-darkening (PD) processes play an important role. The main source of the problem is the color centers formed in the OF. Preventing or recovering these formations before and after the production of OF is of great importance in both efficient and long-lasting systems.

To determine the behavior of Yb-doped OF, they are exposed to gamma radiation or PD. The important recovery process is photobleaching (PB) for defects due to the gamma radiation. In our study, a rapid and efficient PB process was achieved using a high-energy nanosecond pulse to recover existing and/or revealed color centers in OF that had been irradiated with 10 kGy of gamma radiation. The PB process was analyzed based on the wavelength and energy of the pulsed light source. The highest level was achieved with the 532 nm wavelength laser. The findings indicate that the recovery of color centers can reach up to 96% in a shorter duration (hours) compared to results from studies utilizing continuous lasers.

MM 9.48 Mon 18:30 P1

Design of a setup for conducting experiments synchronized with sample scanning — •Maksim Khasanov — Moscow, Russia

The paper focuses on designing equipment with an electronic drive for compressing samples during experiments, aimed at analyzing their internal structure using computed tomography. The manual compression system previously used prolonged the experiment due to time-consuming data processing. The new electronic system significantly reduces the time required by automating the compression process. The work includes the design of the compression apparatus and its electric drive, providing a more efficient and precise solution for experimental procedures.

MM 9.49 Mon 18:30 P1

Extreme stability of $CoCrFeMnNi_{60}$ multicomponent alloys after severe plastic deformation — •Lukas Musiol[1], Mohan Muralikrishna Garlapati[1], Shabnam Taheriniya[1], Lukasz Rogal[2], Sergiy Divinskiy[1], Harald Rösner[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Material Science, Polish Academy of Science, Reymonta 25 St., 30-059 Krakow, Poland

Thermal stability of a (CoCrFeMn)Ni60 multicomponent alloy is investigated using in-depth microscopic examination. The specific composition is chosen as a transition one from "high-entropy" to "concentrated alloy" behavior. Such compositional design mimics a conventional alloy design of solutes in the terminal solid solution range but in equiatomic concentrations. Along with the analyses of the homogenized samples, an analysis of compressed and rotary swaged samples was performed to investigate the influence of deformation on the phase stability. The phase stability is investigated at intermediate temperature for prolonged annealing times, which has given an in-depth understanding of the formation and growth of new phases or precipitates. Detailed microscopy analyses were performed to determine the phases and their composition. Overall, the (CoCrFeMn)Ni60 multicomponent alloy has shown a stable microstructure even after extreme deformation and after prolonged heat treatments. The phase stability results, in conjunction with deformation and microstructure, will be correlated and discussed in detail.

MM 9.50 Mon 18:30 P1

Influence of Supercell Size Effects on the Mechanical Properties and Electronic Structure of High-Entropy Transition Metal Diborides ($HETMB_2$) — Inna Plyushchay[2], •Nebahat Bulut[1], Anna Pliushchai[1,3], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine — [3]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"

Modeling various supercell sizes for high-entropy transition metal diborides ($HETMB_2$) holds the potential to overcome the computational challenges associated with their unique bonding configurations and complex compositions. First-principles calculations were used to predict the electronic and elastic properties of high-entropy transition-metal diborides after employing supercells with a variety of atomic configurations and complex compositions. We found that larger supercells allowed for clustering of atoms of the same metal type, as evidenced by broadening of the peaks in the histogram of interatomic distances. This, however, had no significant influence on the mechanical properties. The mechanical properties of $HETMB_2$ are determined by the number of electrons, size of atoms or polarizability. However, the average number of *d*-electrons per metal atom was found to be crucial because it affects the Fermi level position relative to the pseudogap, and this impacts the elastic properties strongly in comparison to the binary-TMB_2.

MM 9.51 Mon 18:30 P1

Ab initio calculations of defects in the Mg2Ge intermetallic — •Pavel Papež[1,2], Martin Friák[2], and Martin Zelený[1] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, v. v. i., Brno, Czech Republic

This work is focused on ab initio calculations of different types of defects in the Mg2Ge intermetallic in order to explain a higher concentration of Mg in exper-

imental samples. Our calculations employed VASP software and include antisite defects and vacancies on both sublattices and furthermore interstitial additions of both Mg and Ge, all in charge neutral state. The calculations were also done with the modified Becke-Johnson potentials to study their influence on the band-structure of this semiconductor. We have calculated their formation energies in regards to Mg rich and Ge rich chemical potential limits. The phonon calculations were done to acquire the defect equillibrium concentration and the evolutiuon of defect formation energies with temperature.

MM 9.52 Mon 18:30 P1

Glass transition and physical aging studies of a gold based Bulk metallic glass by means of flash scanning calorimetry — •Klara Otto[1], Valerio Di Lisio[2], Daniele Cangialosi[2], and Isabella Gallino[1] — [1]Technische University Berlin, Chair for Metallic Materials, Berlin, Germany — [2]DIPC, San Sebastián, Spain

Flash scanning calorimetry is used to study the glass transition of metallic glasses, during direct solidification from the melt [1,2] and by reheating with rates up to thousands of K/s. This enables the access to the supercooled liquid state by avoiding crystallization during the cooling stages.

Glassy materials relax over time when held below the glass transition temperature, to minimize their excess thermodynamic properties. A new methodology to compare the relaxation times related to the atomic mobility with those determined throughout glassy aging of a gold based metallic glass, is presented. Isothermal physical aging was performed to retrieve the temperature dependent timescales of the alpha relaxation. Additionally, the characteristic time of glassy relaxation are retrieved in a wide temperature range [3] complemented with fictive temperature analysis.

The combined data were plotted on an activation diagram, that relates relaxation times to the inverse of temperature. This allowed to investigate relaxation time scales spanning 7 orders of magnitude using a single experimental technique.

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MM 9.53 Mon 18:30 P1

Glass Forming Ability, Thermal and Magnetic Properties of the Multicomponent Fe-Mo-P-C-B-Si Metallic Glass for AM Applications — •Alejandro Lejtman Rotberg[1], Amirhossein Ghamivi[2], Lucas M. Ruschel[2], Izzi A. Ahmad[1], Uma Rajput[3], Purbasha Sharangi[3], Paola M. Tiberto[2], Ralf Busch[2], and Isabella Gallino[1] — [1]Technical University of Berlin, Chair for Metallic Materials, Ernst-Reuter-Platz 1, 10587 Berlin, Germany — [2]Saarland University, Chair of Metallic Materials, 66123 Saarbrücken, Germany — [3]INRIM, Strade delle Cacce 91, Torino, Italy

Efficient power-to-work conversion in electric vehicles (EVs) requires soft magnetic materials with low coercivity. Fe-based metallic glasses reduce power losses but struggle achieving casting thicknesses over 1mm due to limited glass-forming ability (GFA). Additive manufacturing (AM), like Laser Powder Bed Fusion (LPBF), provides solutions, with recent studies revisiting Fe-Si-B compositions for processability and performance [1-3]. This study evaluates the alloy Fe74Mo4P10C7.5B2.5Si2. X-ray diffraction (XRD) results of cast plates and ribbons determined the GFA. Thermal properties were analyzed via Differential Scanning Calorimetry (DSC) and Differential Thermal Analysis (DTA), while magnetic properties using Vibrating Sample Magnetometry (VSM). Results suggest the alloy's potential for AM production of soft magnetic components for EVs.[1] Thorsson, L., et al. Selective Laser Melting. Materials & Design.[2] Rodríguez-Sánchez, M., et al. Relating Laser Powder. Materialia.[3] Sadanand, S., et al. Laser Powder Bed Fusion. Journal of Laser Applications.

MM 9.54 Mon 18:30 P1

An atomistic study on the role of size and composition on the structural and thermodynamic properties of Al-Pd bimetallic nanoparticles during melting and solidification. — •Dario Gonzalo Escriba Quispe[1], Justo Alcides Rojas Tapia[1], and Gustavo Cuba Supanta[1,2] — [1]Universidad Nacional Mayor de San Marcos, Lima, Peru — [2]Universidad Privada del Norte, Lima, Peru

Bimetallic nanoparticles (NPs) of Al-Pd exhibit structurally complex phases, as well as quasicrystalline approximants to the Al-Mn-Pd system, which, combined with their controversial and complex phase diagram, makes them an interesting subject of study. In this work, using molecular dynamics, the structural and thermodynamic properties of Al(x)Pd(100-x) NPs at different sizes and compositions are calculated.

The processes of melting and solidification are simulated using the open-source LAMMPS package and a MEAM-type potential. It was found, through the calculation of heat capacity, that the melting temperature and size of AlPd, Al2Pd5, and Al1Pd4 NPs follow a linear behavior, in agreement with the scaling law. Additionally, the RDF graphs of AlPd NPs show that it is an ordered intermetallic compound, with structural parameters such as the crystal structure and lattice parameter matching those reported experimentally. The Al1Pd4 nanoalloy was explored, where it was found that the NP has an icosahedral shape. However, the atoms exhibit internal ordering with regions showing FCC and HCP crystal structures. Finally, other additional results such as MSD, common neighbor analysis (CNA), the Warren-Cowley parameter, excess energy, and phonon dispersion are presented.

MM 9.55 Mon 18:30 P1

An X-ray diffraction study of copper powder for laser-based powder bed fusion — •Eric Schneider[1], Robert Ortmann[2], Julia Frank[3], Fabienne Hellwig[3], Tobias Grimm[2], Michael Blüm[3], Lena Friedrich[1], Michael Paulus[1], Jaqueline Savelkouls[1], Jan T. Sehrt[2], Christian Sternemann[1], and Arne Röttger[3] — [1]Universität TU Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44227 Dortmund — [2]Ruhr-Universität Bochum, Universitätsstraße 150, D-44801 Bochum — [3]Bergische Universität Wuppertal, Bahnhofstraße 15, D-42651 Solingen

Additive manufacturing (AM) of components using laser-based powder bed fusion of metals (PBF-LB/M) has reached market maturity. This layer-by-layer process offers advantages over casting and subtractive methods, especially for producing complex parts with internal cavities and is promising to produce topology-optimized lightweight structures. However, the use of copper powders for PBF-LB/M based AM poses challenges due to its high thermal conductivity and reflectivity. The directed oxidation and reduction of the copper particle surfaces can improve both, the powders processability and reusability. In this study we investigate the oxidation of pre-treated copper powders in air and its controlled reduction using $Ar/2\%H_2$ atmosphere at different temperature conditions up to 350°C by X-ray diffraction at beamline BL9 of DELTA synchrotron radiation source in order to reveal information about induction times and change in Cu, Cu_2O, and CuO phase composition for industrial processing. This research is funded by the DFG via projects RO 4523/9-1, SE 2935/6-1, and STE 1079/9-1.

MM 9.56 Mon 18:30 P1

Linking Process Parameters and Heat Treatment to Microstructural Properties of PBF-LBM 316L Steel for Structural Hydrogen Use — •Tim Haag, •Kai Stefan Lagemann, Stefan Wagner, and Astrid Pundt — Institut für Angewandte Materialien - Werkstoffkunde (IAM-WK), Karlsruher Institut für Technologie (KIT)

Additively manufactured (AM) 316L steel produced by powder bed-based laser melting (PBF-LBM) can be considered for sophisticated applications in hydrogen technology. This project investigates the influence of manufacturing parameters and post-processing treatments, such as heat treatment, on the resulting microstructure and its implications for material properties. The objective is to optimise the manufacturing process in order to achieve components with minimal porosity. The microstructure is comprehensively analysed using advanced techniques, which reveal hierarchical features and a complex interplay of various microstructural elements, including multiscale porosity, varying grain orientations and subgrain dislocation cells. Heat treatments are applied to alter microstructural characteristics and assess their impact on material properties.

MM 9.57 Mon 18:30 P1

Analysis of the Crack Formation in Printed Nanosilver Using In Situ Bending Technique — •Lennart Schwan[1], Michaela Klöcker[1], Michael Feige[1], Laila Bondzio[2], Thomas Kordisch[1], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences and Arts — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics

3D printing is an emerging technology with a wide range of applications. The modern multi-material jetting process, as used in the Nano Dimension Dragonfly Pro LDM, makes it possible to print dielectric and conductive materials in a single process. In addition to electrical circuits such as coils, capacitors, etc., strain gauges can also be printed.

The change in resistance of strain gauges is usually caused by the change in the geometric dimensions of the conductive layer when it is deformed. In the case of the printed material examined in this study, it is also known that the material is permeated by cracks which cause a directional dependence of the electrical conductivity.

The objective of this study is to investigate how these cracks develop during bending and thus also contribute to the change in resistance. For this purpose, a test specimen is loaded under a three-point bending test using a special in situ bending module. In order to investigate the propagation and formation of the cracks, the bending module is positioned in a scanning electron microscope in order to analyze the cracks under loading with a sufficient image resolution.

MM 9.58 Mon 18:30 P1

Atomistic Simulation of Laser-based Powder Bed Fusion of Metals — •Aamir Siddiqui, Simon Kümmel, and Johannes Roth — FMQ, University of Stuttgart, Germany

Additive manufacturing technology applications continue to call for increased reproducibility and quality. The goal is to study the melting and solidification of an AlTi alloy and to create a framework that allows for further studies on arbitrary alloys and metals. Molecular dynamics provides an understanding of

the melting and ablation process, resulting in an understanding of different heat transfer mechanisms. The simulation framework makes it possible to see how changes in scanning speed and laser power affect the melting dynamics.

The melting process of alloys shows that a significant amount of argon gas becomes trapped inside the sample. The simulation of powder beds formed by spheres of varying sizes reveals holes that vanish under vacuum conditions, but persist when the simulation box is filled with protective gas, providing information on the creation of defects. By deforming the sample, the influence of gas pockets on the mechanical properties and the evolution of the lattice structure within the sample can be seen.

MM 9.59 Mon 18:30 P1

Nanoscale characterization of AM316L stainless steel for hydrogen application — •Gabriele Palazzo, •Felix Stierle, Kai Stefan Lagemann, Christian Kübel, Stefan Wagner, and Astrid Pundt — Karlsruhe Institute of Technology, Karlsruhe, Germany

Additive manufactured (AM) austenitic stainless steel 316L prepared by selective laser melting (SLM) is characterized by advanced nanoscale characterization techniques to examine its microstructural features. High-resolution scanning TEM (HR-STEM), selected area diffraction (SAD), and analytical methods such as energy-dispersive X-ray spectroscopy (EDX) as well as electron energy loss spectroscopy (EELS) are employed. Typical SLM printing structures (equiaxial and columnar cellular structure, nano-inclusions) are observed with atomic resolution both for as-built and tensile tested samples. The presence of silicon-manganese oxide nano-inclusions, preferential chromium and molybdenum segregation around them is revealed, as well as iron depletion and chromium enrichment along the cell boundaries. This peculiar multi-scale AM microstructure accounts for the unique mechanical properties of AM316L in terms of resistance and ductile behaviour, if compared to the conventionally manufactured counterpart, allowing to overcome the trade-off between strength and ductility.

MM 9.60 Mon 18:30 P1

Fine-tuning of machine learning interatomic potential for the prediction of phonon properties — •Jonas Grandel, Philipp Benner, and Janine George — Bundesanstalt für Materialforschung und Prüfung, Berlin

Accurate phonon predictions are critical for assessing material stability and thermal behavior, but traditional approaches based on density functional theory (DFT) are computationally expensive, motivating the need for accelerated alternatives. In this work, we investigate the performance of the machine learning interatomic potential MACE-MP-0 for predicting harmonic phonons and thermal properties. The focus is on fine-tuning MACE-MP-0 using various sets of rattled structures and different hyperparameter to identify the most effective strategy for improving model accuracy. We want to develop a general fine-tuning workflow based on the foundational model that can be used to fast and accurately generate phonons to predict both stability and thermal properties. For this purpose, a benchmark dataset was constructed using DFT consisting of a broad range of different crystal systems and mainly of phase change materials and thermoelectric materials. Each fine-tuned model targets one specific material, allowing to improve each material individually. The results demonstrate significant improvements in the prediction of phonon band structures, with a root mean square error (RMSE) reduced from 0.6 THz for the original MACE-MP-0 model to 0.3 THz for the fine-tuned models. In addition, performance in terms of computational speed was improved by up to a factor of 10 compared to traditional DFT-based phonon calculations.

MM 9.61 Mon 18:30 P1

Learning the Reduced Density Matrix Functional from Quantum Processors and Using Density Matrix Embedding Theory to Extend its Universality — •Martin Uttendorfer — Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Deutschland

The advent of quantum computing makes reduced density matrix functional theory (RDMFT) on an exact level viable. By directly applying RDMFT, derived from Levy-Lieb's constrained search, this work leverages quantum processors to overcome some of DFT*s shortcomings, enabling more accurate modeling of quantum chemical and condensed matter systems. The proposed approach incorporates quantum algorithms that utilize variational quantum eigensolvers (VQE), which is viable to be executed on near-term intermediate scale quantum devices (NISQ) in conjunction with machine learning techniques. This work examines the theory*s application to different particle types, including fermions, bosons, and hard-core bosons, highlighting the flexibility of the RDMFT framework. Additionally, density matrix embedding theory (DMET) is incorporated, allowing for a hybrid classical-quantum approach that extends the functional*s universality. This work presents a quantum algorithmic approach to obtain the functional and provides a computational strategy for studying complex many-body systems while keeping the use of limited quantum resources to a minimum.

MM 9.62 Mon 18:30 P1

Integrating Long-Range Interactions into Machine Learning Interatomic Potentials — •Tulga-Erdene Sodjargal[1,2], Egor Rumiantsev[1], Philip Loche[1], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modeling (COSMO), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Bio and Brain Engineering, Korea Advanced Institute of Science and Technology (KAIST), 34141 Daejeon, Republic of Korea

Machine learning-based interatomic potentials (MLIPs) often rely on the locality ansatz, calculating atomic energies based on a fixed cutoff radius. While effective for many systems, this nearsightedness can lead to inaccuracies when long-range interactions, such as ionic interactions, dominate. To overcome this limitation, we integrate Particle Mesh Ewald (PME) techniques into existing MLIP frameworks. Our extension is modular and plug-and-play, requiring minimal modifications to incorporate into various models. We demonstrate significant improvements in both simple architectures, such as Behler-Parrinello Neural Networks, and advanced models, including state-of-the-art graph neural networks like the Point Edge Transformer (PET).

MM 9.63 Mon 18:30 P1

pyiron - Automated Workflows for Materials Science — •Jan Janssen[1], Marvin Poul[1], Sarath Menon[1], Tilmann Hickel[2], and Joerg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The pyiron framework, originally developed for atomistic simulations in the field of materials science, has recently been extended beyond the atomistic scale to enable data-driven materials design on all scales and including experiments. As a central interface for materials acceleration platforms (MAP), pyiron couples simulation methods ranging from ab-initio methods of the electronic scale, to the atomistic scale of machine-learned interatomic potentials and up to the continuum scale of crystal plasticity modelling with interfaces for experimental equipment and machine learning.

On our poster, we give a brief overview of the recent developments in the pyiron project and highlight a series of materials science applications. These range from pyiron_workflow, our redesigned graph-based workflow engine, to executorlib for up-scaling workflows for high-performance computing (HPC) and the python workflow definition, a joined standard developed in collaboration with AiiDA and jobflow, the workflow engine of the materials project. At the same time, the poster will provide an opportunity to meet the pyiron developers and discuss ideas and future applications.

Read more about pyiron on our website: https://pyiron.org

MM 9.64 Mon 18:30 P1

Investigating the Impact of Optimization Algorithms on Element-Substitution Based Materials Discovery — •David Greten[1], Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

In this study, we investigate how different optimization algorithms affect the relaxation of inorganic structures using general-purpose machine-learned interatomic potentials (MLIPs) like MACE-MP-0. Assessing computational efficiency and relaxation quality via structural similarity and kernel distance metrics, we find that optimizer choice significantly influences performance and can lead to different equilibrium structures. Analyzing both DFT-relaxed structures from the Materials Project and element-substitution based trial structures, we highlight the optimizer's impact in different scenarios. Our findings emphasize the critical role of optimizer selection in large-scale computational materials science workflows, particularly in the context of element-substitution based materials discovery. This can hopefully guide the community towards choosing appropriate algorithms for efficient and reliable structure relaxations.

MM 9.65 Mon 18:30 P1

The APyT Package: From Raw Data to Three-Dimensional Reconstruction — •Sebastian Eich — Department for Materials Physics, Institute for Materials Science, University of Stuttgart

The APyT package is an advanced, open-source Python framework for evaluating atom probe tomography (APT) data. It offers a suite of modules that automate key steps in APT processing, from mass spectrum calibration to three-dimensional sample reconstruction. Its modular architecture ensures seamless integration with external tools through standardized input/output interfaces, supporting both Linux and Windows environments.

Key features include high efficiency with NumPy and Numba, a low memory footprint, and extensive documentation. The modules are highly automated, requiring minimal user input to achieve accurate results. The package also integrates SQL database management for raw measurement data and corresponding metadata.

The mass spectrum module automatically calibrates and detects peaks, producing high-resolution spectra. The mass spectrum fitting module further refines this by fitting spectra with an analytical function, automatically deconvolving overlapping peaks by incorporating isotope abundances. The recon-

struction module generates a 3D sample reconstruction, including automatic chemical identification and export capabilities. Future enhancements include a PyQt-based GUI to streamline access to all APyT modules in one application.

MM 9.66 Mon 18:30 P1

Relation between the electronic structure and X-ray absorption spectra discussed using multiple-scattering formalism — Hubert Ebert[1], •Sergiy Mankovsky[1], and Jan Minar[2] — [1]LMU of Munich, 81377 Munich, Germany — [2]University of West Bohemia, Pilzen, Czech Republic

Recently, the concept of crystal orbital overlap population (COOP) has been reconsidered [1] based on the finite difference method (FDM), representing the calculated x-ray absorption spectra (XAS) in terms crystal orbital overlap population functions. This allows to reveal the correlation between XAS and the formation of the bonding/antibonding states in solids. Following the idea suggested in Ref. [1], we demonstrate that this relation can be investigated in a very efficient way using the multiple scattering formalism for electronic structure calculations. In this representation, both, the density of states and the x-ray absorption function are determined by the site-diagonal scattering path operator $\tau^{00}(E)$ which can be expressed as $\tau^{00}(E) = t^0 + \sum_n \tau^{0n}(E)\, G^{n0}(E)\, t^0$, in terms of the single-site scattering matrix t^0, the site-off-diagonal operators $\tau^{0n}(E)$, and the structural Green function $G^{n0}(E)$. The second term determines in a pair-wise resolved way the fine structure of the electron density of states (DOS) $n(E)$ as well as the XAS absorption coefficient $\mu(E)$. The DOS and the normalized x-ray absorption coefficient are calculated for several representative systems and discussed in line with the idea of the COOP concept.

[1] M. Diaz-Lopez, *et al.*, J. Phys. Chem. A **124**, 6111 (2020)

MM 9.67 Mon 18:30 P1

Upgrading the Coincidence Doppler Broadening Spectrometer at FRM II — •Danny R Russell, Francesco Guatieri, Leon Chryssos, and Christoph Hugenschmidt — FRM II - Technische Universität München, München, DE

The coincidence Doppler broadening spectrometer (CDBS) at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) provides state-of-the-art, depth dependent detection of defects and chemical composition at the annihilation site. A monoenergetic positron microbeam (50 μm FWHM) is guided onto a sample where positrons annihilate with electrons. The Doppler broadening of the characteristic 511 keV annihilation peak is measured by observing both emitted photons simultaneously.

We present simulations and hardware design for an upgrade to the CDBS which will allow backscattered positron capture. Up to ~ 40 % of the incident positrons are backscattered when they reach the sample surface. The annihilation events occurring when these backscattered positrons return to the sample or annihilate in experimental hardware contribute unwanted signal to the measured spectrum which cannot be removed in data processing.

We use an in-house particle tracking code to design a positron dump that will capture backscattered positrons at an electrode outside detector lines of sight. This will reduce the unwanted signal by up to 50 % and improve the quality of CDBS data. Additionally, we apply the same code to optimize an electrostatic focusing lens, further increasing the spatial resolution of the instrument.

MM 9.68 Mon 18:30 P1

High-entropy alloy pre-screening for lead-free halide double perovskites from material databases — •Marina S. Günthert[1,2], Bernd Meyer[1], and Christoph J. Brabec[2] — [1]Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg — [2]Materials for Electronics and Energy Technology (i-MEET), FAU Erlangen-Nürnberg

Over the last decade, lead-free halide double perovskites with composition $A_2BB'X_6$ have emerged as an interesting class of materials for optoelectronics. Furthermore, it was suggested to introduce different ion ratios on each of the double perovskite sublattices, leading to a vast space of possible compositions.

Two criteria are applied to have a first fast filtering approach to reduce the number of combinations. First, the search is limited to non-toxic and non-f elements for a green chemistry approach. Second, we estimate the thermodynamic stability of the compounds by using a criteria recently proposed by Muzzillo *et al.* [1], which focuses on the entropy stabilization by using several elements on each sublattice. This method can be easily adjusted for halide double perovskites. We applied it first to the Materials Project database but it can also be extended to other databases such as NOMAD and OQMD. In the end, this pre-screening gives an idea, which elements on the different sublattices of the double perovskite are worth further exploration.

[1] C.P. Muzzillo, C.V. Ciobanu, D.T. Moore, High-entropy alloy screening for halide perovskites, Mater. Horiz. **11** (2024) 3662-3694

MM 9.69 Mon 18:30 P1

Effect of $4f$ occupancy on L_3 edge of Cerium — •Prathibha Chandrashekhar, Patrik Thunström, Felix Sorgenfrei, and Heike Herper — Department of Physics and Astronomy, Uppsala University, Sweden

The valence $4f$ electrons in Cerium exhibit a strong itinerant tendency, allowing them to exist in a mixed-valence regime, between localized and delocalized states. This regime hosts correlated electron phenomena which has profound implications on the material's magnetic, transport, and electronic properties. The shift in $5d$ orbitals to higher energy levels, due to reduced screening from delocalized $4f$ electrons, provides critical insights into electronic properties. We study this shift by probing $2p$ to $5d$ transition using X-ray Absorption Spectra(XAS). However, accurately modeling the light-matter interaction in such systems remains challenging due to the itinerant nature of the $4f$ electrons, strong core-hole effects, multiplet interactions, and hybridization dynamics. In this work, we employ advanced theoretical approach that combines density functional theory (DFT) with multiplet ligand-field theory (MLFT). This method enables computation of $L_{2,3}$-edges by constructing and solving single-impurity Anderson model (SIAM) derived from first-principles calculations. Additionally, we investigate sensitivity of the computed spectra to Slater integrals, hybridization effects, and core-hole relaxation, offering new insights into the intricate electronic behavior of Cerium-based systems. PC acknowledges partial funding from Horizon Europe MSCA Doctoral Network grant n.101073486, EU-SpecLab, funded by European Union.

MM 9.70 Mon 18:30 P1

Stability of AgI Polymorphs and the AgI(0001) Surface Reconstruction — •Angela Rittsteuer[1], Andrea Conti[2], Michael Schmid[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics, 1090 Vienna, Austria — [2]TU Wien, Institute of Applied Physics, 1040 Vienna, Austria

Silver iodide (AgI) is a compound widely used in cloud seeding due to its ability to act as an effective nucleating agent for cloud condensation. Under ambient conditions, AgI crystallizes in hexagonal or cubic close-packed structures, the most prominent polymorphs being the wurtzite and the zincblende structure. A comprehensive understanding of its groundstate structures and phase behavior is essential not only to optimize its role in cloud condensation but also to explore broader applications in solid-state chemistry and catalysis.

To investigate the stability of AgI polymorphs, we perform extensive benchmarking studies across various levels of theory. These include Density Functional Theory with different approximations for the exchange-correlation energy, hybrid Hartree-Fock Density Functionals, and the Random Phase Approximation, offering a hierarchy of accuracy. Building on recent atomic force microscopy studies of the wurtzite AgI(0001) surface, we further provide theoretical insights by developing a machine-learned force field and applying simulated annealing and parallel tempering to study the surface reconstruction.

MM 9.71 Mon 18:30 P1

Investigation of Lloyd's formula at finite electronic temperatures — •Christian Maas[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen

In DFT calculations within the Korringa-Kohn-Rostoker (KKR) Green's function formalism the integrated density of states is analytically given by Lloyd's formula. Its better l-convergence can be used for a precise determination of the Fermi energy and a charge density normalization. In the past it has been shown that for finite electronic temperatures the calculation of Lloyd's formula can in principle be done on the same energy mesh that is used for the calculation of the charge density [1]. These calculations require to numerically evaluate the derivative of Lloyd's formula. We show that it is possible to accurately determine the derivative without using additional energy mesh points. This is done by interpolating Lloyd's formula with cubic splines which in turn are used to calculate the derivative. We compare the method to calculations without electronic temperatures and show that the spline interpolation does not lead to a significant accuracy lost.

[1] R. Zeller 2005 J. Phys.: Condens. Matter 17 5367, https://dx.doi.org/10.1088/0953-8984/17/35/005

MM 9.72 Mon 18:30 P1

Fiber composite materials in construction of go-cart. — •Mikhail Brusnikin — Moscow, Russia

Lightweighting any vehicle, especially sports equipment, has always been a pertinent issue, and I aimed to determine how significantly material substitution would affect the mass of the power structure by using modern composite constructions instead of classical steel solutions, with the condition of maintaining the same torsional stiffness as the steel sample.

Fiber composite materials are currently at the forefront of technology in terms of stiffness-to-weight ratio and are sufficiently accessible for my research, which was focused on their application in a sports device such as a go-kart.

The assumptions regarding the weight of the final product, which were proposed at the beginning of the research, turned out to be erroneous. Even in the best-case scenario, the weight reduction of the construction was less than anticipated.

MM 9.73 Mon 18:30 P1

RuNNer 2.0: An Efficient and Modular Program for High-Dimensional Neural Network Potentials — •Alexander L. M. Knoll[1,2], Moritz R. Schäfer[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[3], Alea Miako Tokita[1,2], Gunnar Schmitz[1,2], Henry Wang[1,2], Richard Springborn[1,2], Marco Eckhoff[4], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, Universität Basel, Switzerland — [4]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland

Machine learning potentials (MLPs) have become an important tool for atomistic simulations in chemistry and materials science. As methods in this domain grow increasingly complex and mature, the creation of efficient and user-friendly libraries now receives a lot of attention. We introduce the second major release of RuNNer, an open-source, standalone software package designed for constructing and evaluating second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 integrates the entire workflow into a fully OpenMP- and MPI-parallel program: from generating atomistic descriptors, via training a specific machine learning model, to its application in molecular dynamics simulations.

MM 9.74 Mon 18:30 P1

Hybrid soldering: Interfacial flux-doping of Cobalt nanoparticles hindering the formation and growth of intermetallic compound (IMCs) layers — •Farzad Khodabakhshi[1,2], Irina Wodak[1], Andriy Yakymovych[1], Gerhard Wilde[2], and Golta Khatibi[1] — [1]Vienna University of Technology — [2]University of Münster

The study investigated hybrid nanocomposite soldering of copper components using a lead-free tin-based solder alloy (Sn-3.5 wt% Ag). To suppress the growth of intermetallic compound (IMC) layers, specifically Cu3Sn and Cu6Sn5, at the interface between the solder alloy and the copper substrate during reflow solidification, a modified flux containing cobalt nanoparticles was applied. The research focused on the effects of incorporating cobalt nanoparticles in different fractions, up to 1.0 wt%, on the microstructural development of the soldered joints and the formation of IMC layers. Additionally, the impact of post-soldering aging treatment, conducted at approximately 180°C for extended periods (up to around 20 days), was assessed. The study analyzed how the alloying of cobalt nanoparticles affected the structure of Cu3Sn and Cu6Sn5 IMC layers, as well as the Sn-based solder alloy. This was done using energy-dispersive X-ray spectroscopy (EDS) elemental mapping in conjunction with field emission-scanning electron microscopy (FE-SEM). Furthermore, the microstructural evolutions of the soldered joints, influenced by the contribution of Co-nanoparticles and the aging treatment, were characterized and discussed using electron channeling contrast imaging (ECCI) microscopy.

MM 10: Topical Talk: M. Salvalagio

Time: Tuesday 9:30–10:00 Location: H10

Topical Talk MM 10.1 Tue 9:30 H10

Understanding the impact of disconnection flow on microstructure evolution — •Marco Salvalaglio — TU Dresden, Dresden 01062, Germany

In polycrystals, which are composed of misoriented grains and grain boundaries (GBs), microstructure evolution primarily occurs through GB migration. It is widely accepted that GB migration is mediated by the flow of line defects with both step and dislocation characters, i.e., disconnections. Numerous phenomena associated with grain boundary (GB) motion can, in fact, be linked to disconnection flow. This presentation discusses novel fundamental aspects regarding how disconnection flow affects overall microstructural changes. First, with a continuum (phase field) model of GBs that accounts for disconnections, we demonstrate that the generation of internal stress (shear coupling) is the primary factor responsible for deviations from classical curvature-driven grain growth observed in recent experiments. The relative impact of other factors is also briefly discussed. Second, through atomistic simulations, a Markov chain model analysis, and an experimental proof of concept, we demonstrate that asymmetric GBs exhibit direction-dependent mobilities and unidirectional motion under oscillatory driving forces or cyclic thermal annealing. This behavior can be attributed to the microscopic structure of GBs affecting the nucleation barriers of disconnections. Additionally, our findings suggest that applying oscillatory driving forces and non-equilibrium thermal fluctuations accelerates grain coarsening in microstructures, a conclusion further supported by numerical simulations.

MM 11: Topical Session: Defects of Defects

Time: Tuesday 10:15–13:00 Location: H10

Topical Talk MM 11.1 Tue 10:15 H10

The role of disconnections in the shear-migration coupling of grain boundaries — •Marc Legros[1], Armin Rajabzadeh[1], Romain Gautier[2], Nicolas Combe[1], and Frédéric Mompiou[1] — [1]CEMES-CNRS, 29 rue Jeanne Marvig, 31055, Toulouse, France — [2]UMET, Université de Lille, Cité scientifique, 59655 Villeneuve d'Ascq

Grain-boundary (GB)-based plasticity is an alternative to classical, dislocation-based deformation. It is supposed to play a significant role in nanocrystalline metals (d<100 nm) for example, that contain a large proportion of GBs but virtually no dislocations. Among all the mechanisms potentially able to generate a permanent (plastic) deformation, the dominant one is the so-called shear-migration coupling. Despite a recent increase in simulations studies, its experimental characterization remains very scarce. Aside from experimental obstacles, the problem is very vast as real grain boundaries possess at least 5 degrees of freedom and contains a potentially infinite number of disconnections, a specific defect that combines step and dislocation characters.

Using both in-situ TEM experiments and molecular dynamic simulations (NEB Nudge Elastic Band), we have shown that shear-migration coupling involves the displacement of these disconnections. As dislocations in the crystal, the properties of these disconnections seem to guide the coupling mechanism of migrating grain boundaries. The overarching question becomes whether we should still consider a given GB as a crystalline defect or a network of its own, which mechanical properties (mobility, shear coupling) are governed by its nature or by its defects?

MM 11.2 Tue 10:45 H10

Atomistic simulation of point defects behavior inside grain boundaries — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — Ruhr University Bochum, ICAMS, 44801 Bochum, Germany

The properties of point defects play a key role in the description of many phenomena within grain boundaries (GBs), such as pre-melting or atomic diffusion. Compared to the bulk, point defects inside GB are characterized by low formation energy and high complexity. Thus, the thermodynamic/kinetic properties of GBs strongly depend on the behavior of point defects. To reveal general aspects of this relationship, we studied behavior of vacancies and self-interstitial atoms inside tilt grain boundaries for several metals (Ni, Al, Fe, Nb, Mo and W) using atomistic modeling. The simulations revealed that the self-diffusion along the tilt GBs at low/moderate temperatures is mostly driven by migration of self-interstitial atoms. However, heating leads to a change in the GB diffusion mechanism to a more complex exchange process, not related to specific defects, but similar to atomic diffusion in a liquid. This change is due to the disordering complexion transition of GBs, which also significantly affects GB mobility.

MM 11.3 Tue 11:00 H10

Impact of grain boundary defects on grain boundary diffusion and segregation of Cr in Ni bicrystal — Shraddha Sevlikar[1], Mohan G. Muralikrishna[1], Daniel Gaertner[1], Sergei Starikov[2], Tobias Brink[3], Daniel Scheiber[4], Daria Smirnova[3], Daniel Irmer[5], Bengü Tas[1], Vladimir A. Esin[5,6], Vsevolod I. Razumovskiy[4], Christian H. Liebscher[3,7], Gerhard Wilde[1], and •Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]ICAMS, RU Bochum, Germany — [3]MPI for Sustainable Materials, Düsseldorf, Germany — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria — [5]Mines Paris, PSL University, Évry, France — [6]Université de Lorraine, CNRS, Nancy, France — [7]RC FEMS, RU Bochum, Germany

Grain boundary diffusion of Cr in a near Sigma-11 Ni bicrystal is measured using the radiotracer technique. Opposite to expectations, two distinct contributions to short-circuit diffusion along the nominally single interface are distinguished and related to the existence of two macroscopic facets with distinct inclinations and, as a result, distinct structures. The segregation factor of Cr in Ni is found to be about unity, which is fully supported by ab initio calculations. Using classical atomistic simulations, Ni grain boundary self-diffusion rates are cal-

culated for the symmetric and asymmetric facets. An accelerated self-diffusion kinetics along the asymmetric facet is observed and attributed to the presence of disconnection-like defects. A heterogeneous mechanisms governing atomic migration across distinct facets is corroborated.

15 min. break

Topical Talk MM 11.4 Tue 11:30 H10

Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics — •Fadi Abdeljawad — Lehigh University, Bethlehem, PA, USA 18015

Interfaces greatly influence the physical properties and stability of materials microstructures. Of particular interest in crystalline solids are phenomena that occur due to anisotropic interfacial properties. In polycrystalline aggregates, several experimental observations revealed that an initially flat GB profile may facet into hill-and-valley morphologies with well-defined planes and junctions connecting them. Dislocation-like defects exist at facet junctions, which in general connect GB facets with different atomic structures and interfacial properties. Based on classical atomistic simulations and mesoscale modeling, we examine GB faceting transitions and subsequent facet coarsening dynamics. Our modeling framework accounts for anisotropic interfacial energies, and it incorporates junction energetics and their non-local interactions. The hallmark of our approach is the ability to independently examine the various factors affecting this interfacial instability. Theoretical and computational studies predict the dominant growth morphologies as a function of GB facet junction energies. Furthermore, atomistic and mesoscale simulations show that when accounting for junction energetics GB faceting and subsequent facet coarsening is akin to spinodal decomposition in bulk materials. In broad terms, our work provides an avenue to account for GB structural transitions in models of microstructural evolution.

MM 11.5 Tue 12:00 H10

Defect Phase Diagrams for Grain Boundaries in Mg: Chemical trends at Finite Temperatures — •Prince Mathews[1], Rebecca Janisch[2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum — [3]Federal Institute for Materials Research and Testing (BAM), Berlin

Lattice defects are known to directly influence the behaviour of materials. The framework of defect phase diagrams (DPDs) offers a powerful and knowledge-based approach for the tailored design of materials by controlling defect phases in competition to bulk phases. Using ab-initio methods and automized workflows, the DPD for the example of Ga segregation to Σ7 [0001] 21.78° (sym. plane 12-30) Mg grain boundary is calculated. It predicts a series of defect phase transformations, which turn out to be in good agreement with transmission electron microscopy experiments. Similar to bulk phases, the stabilities of defect phases can change with temperature. Therefore, different approaches to extend the DPD considering the relevant entropy contributions are discussed. A new sub-lattice model, which is focused on the statistics of grain boundary site column coverages, provides promising insights into temperature-dependent processes of defect phase transformations.

MM 11.6 Tue 12:15 H10

A computationally highly efficient analytical model for the description of defect phase diagrams — •Jing Yang, Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, D-40237, Germany

In this work, we propose an analytical thermodynamic model for constructing defect and surface phase diagrams. The model is capable of accurately describing the composition-temperature dependence of phase transitions on the surface, including order-disorder ones. It provides a promising alternative to the sublattice model, which is commonly used in the CALPHAD framework to describe solution phases with ordering, as we demonstrate using the system of Mg surface with Ca substitutions. First, as a foundational reference we construct the surface phase transition with grand-canonical Monte Carlo simulation coupled with cluster expansion. The system undergoes a transition from a solid solution (disordered) phase at high temperature, Ca-poor condition to an ordered defect phase with 1/3 Ca coverage. We then show that it is possible to accurately reproduce the critical transition condition with an analytical model assuming a Boltzmann distribution of the phase fractions. Finally, we compare our method with the sublattice model. The proposed method provides a computationally highly efficient and easy-to-parametrize analytical model for constructing defect phase diagrams.

Topical Talk MM 11.7 Tue 12:30 H10

Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling — •Helene Zapolsky[1], Gilles Demange[2], Yuri Borges Gomes Lima[3], Anastasiai Titova[4], and Renaud Patte[5] — [1]GPM, UMR 6634 University of Rouen, France — [2]GPM, UMR 6634 University of Rouen, France — [3]GPM, UMR 6634 University of Rouen, France — [4]GPM, UMR 6634 University of Rouen, France — [5]GPM, UMR 6634 University of Rouen, France

Very great interest in the structure of interphase interfaces between fcc and bcc crystals has historically arisen due to their technological importance in steels. These interfaces also play a crucial role in metallic nanomultilayers (NMLs), where the presence of numerous semi-coherent interfaces leads to a broad spectrum of novel and remarkable properties. One such system, the Cu/Mo NML, holds promise for thermal management applications due to the combination of copper's excellent thermal conductivity and molybdenum's low coefficient of thermal expansion. In these systems, defects at the fcc/bcc interface have a profound impact the thermal properties of the materials. Recently, the Quasiparticle Approach (QA), based on the phase-field methodology, has emerged as a powerful computational tool for modeling and predicting the atomic-scale structure of various interfaces. In this work, we employ atomistic modeling to examine the detailed structure of the fcc/bcc interface, exploring the relationship between this structure and the mode of interface propagation during displacive phase transformations in pure iron and in Cu/Mo NML.

MM 12: Materials for the Storage and Conversion of Energy

Non-Lithiumbased Materials, Characterisation and Simulation Methods

Time: Tuesday 10:15–13:00 Location: H22

MM 12.1 Tue 10:15 H22

Where Electrons Rest After Dark: Polaron Stability in Opto-Ionic 2D Niobium Titanate — •Christoph Dähn[1], Yang Wang[2], Risov Das[2], Bettina V. Lotsch[2], Karsten Reuter[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]MPI für Festkörperforschung, Stuttgart

Two-dimensional Niobium Titanate in alkaline solution is promising for opto-ionic energy applications, since it can store photo-generated charge carriers over macroscopic time scales. Although experiments suggest polarons to play a key role for charge storage, identifying the atomistic and electronic mechanisms active in this material has so far proved challenging, also due to the intrinsic disorder of this compound. In this work, we shed light on these aspects by performing hybrid density-functional theory calculations. In a first step, we explore the vast amount of possible lattice decorations resulting from the partial occupation of Ti-sites with Nb, from which we identify a representative set of stable configurations for this disordered material. In a second step, we investigate the stability of polarons at different lattice sites in these configurations. To qualitatively rationalize these results, a fuzzy classification scheme [1] is applied to group comparable polarons according to their local environment. This allows us to analyze how the local environment influences polaron stability and, in turn, long-term charge retention and its underlying mechanisms [2].

[1] K. C. Lai *et al.*, *J. Chem. Phys.* **159**, 024129 (2023).
[2] Y. Wang *et al.*, *J. Am. Chem. Soc.* **146**, 25467(2024).

MM 12.2 Tue 10:30 H22

Beyond Ion Dynamics: Efficient Charge Transport Simula- tions including Polarons at Battery Scales — •Matteo Rinaldi, Karsten Reuter, and Christian Carbogno — Fritz-Haber- Institut der MPG, Berlin

Polarons have long been recognized as fundamental for charge transport in battery materials - be it as charge carrier or as ion-transport enhancer [1]. Nonetheless, a quantitative modeling of polaron dynamics in such materials has, so far, remained elusive. On the one hand, the activated dynamics of polarons requires time and length scales that are inaccessible with first-principles methods. On the other hand, (machine learned) interatomic potentials do not capture electronic charge transport by construction. In this work, we overcome this hurdle by exploiting force-field models that explicitly account for the electronic viz. polaronic degrees of freedom in a semi-classical, adiabatic fashion. We demonstrate the viability of the approach for lithium titanium oxide (LTO), a prototypical anode material for which polaron hopping is known to play a decisive role [1]. To this end, we train an equivariant message-passing model to density-functional theory data obtained with hybrid functionals. By then performing large-scale molecular-dynamics simulations with this force-field, we investigate both ionic and polaronic transport in LTO as well as their dynamic coupling. We show that polarons diffuse orders of magnitude faster than ions and discuss the implications for the design of battery materials.

[1]M. Kick, C. Scheurer, and H. Oberhofer, ACS Appl. Energy Mater. 4, 8583 (2021).

MM 12.3 Tue 10:45 H22

Tuning electronic structure of CoNi LDHs via surface Fe doping for achieving effective oxygen evolution reaction — •Yunli Shi[1,2], Huaping Zhao[1], Junqi Li[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xian 710021, China

Cobalt and nickel-based layered double hydroxides (LDHs) are promising oxygen evolution reaction (OER) catalysts, but their performance is limited by poor conductivity and low intrinsic catalytic activity. In this study, CoNi LDHs were used as a matrix, with iron sites introduced onto the surface via cation replacement (Fe-CoNi LDHs). Unlike ternary Fe-CoNi LDHs synthesized through conventional one-step methods, the iron sites in Fe-CoNi LDHs are primarily located on the surface and edges of nanosheets, ensuring abundant exposure of reactive sites. Surface doping was found to optimize the coordination environment and electronic structure, reducing the binding energy between reactants and active sites. As a result, Fe-CoNi LDHs exhibit an overpotential of only 260 mV at 10 mA cm-2, demonstrating superior OER performance. This study elucidates the electronic structure and mechanism of enhanced activity, highlighting the potential of surface doping to advance electrocatalytic applications.

MM 12.4 Tue 11:00 H22

Ferromagnetic chiral hybrid organic-inorganic perovskites — •Muskan Nabi and Alessandro Stroppa — CNR - Institute for SuPerconductors, INnovative materials, and devices Italy

In recent years, chiral hybrid organic-inorganic perovskites where the organic cations are the *source* of chirality, have received great attention from the physics and chemistry community. Their functional properties enable the control of light, charge, and electron spins in the same materials. Here, we discuss the intriguing *chirality transfer mechanism* in newly synthesized ferromagnetic chiral hybrid inorganic perovskite and their interplay with magnetism. Although the organic cations are chiral and polar molecules, their arrangement in the crystal structure results in a chiral non-polar space-group P212121. Moreover, we discuss a new chirality order parameter such as the electronic chirality measure (ECM) aiming at quantify the molecular cation chirality taking into account ionic and electronic degrees of freedoms simultaneously. Also, the relation of ECM to physical properties of chiral hybrid perovskites will be discussed.

MM 12.5 Tue 11:15 H22

Enhanced Supercapacitor Performance of Sr-Doped Barium Stannate (BaSnO3) Nanostructures: Synthesis, Characterization, and Electrochemical Insights — Alaa Farid[1,2], •Diaa El-Rahman Rayan[1,3], Moataz Fayed[4], Saad Mohamed[4], Abdel Hakim Kandil[2], Mohamed Abd El-Nasser[2], and Mohamed Rashad[1] — [1]Central Metallurgical Research and Development Institute (CMRDI), P.O. Box: 87 Helwan, 11421, Egypt — [2]Chemistry Department, Faculty of Science, Helwan University, Cairo, Egypt — [3]Department of Physics, Deraya University, New Minia, Minya, Egypt — [4]Mining and Metallurgy Engineering Department, Tabbin Institute for Metallurgical Studies, (TIMS), Tabbin, Helwan, Cairo Egypt

This study investigates the structural, morphological, thermal, and electrochemical properties of Sr-doped barium stannate. The annealing of undoped BaSnO3 at various temperatures leads to the formation of cubic BaSnO3 phase predominating at 1100 ˚C. The increasing Sr ion doping induces lattice strain, with slight shifts in the (110) peak. HR-TEM analysis confirms high crystallinity with a significant reduction in particle size from 125.3 to 22.6 nm due to Sr doping. Electrochemical performance tests in a three-electrode configuration show that Sr doping significantly enhances charge storage capacity, with Ba0.8Sr0.2SnO3 achieving a maximum specific capacitance of 1902 F.g-1 at 1 A.g-1. Additionally, the device demonstrated an impressive energy density of 65.6 Wh.kg-1 at a power density of 1633.54 W.kg-1.

15 min. break

MM 12.6 Tue 11:45 H22

Advanced Electron Energy Loss Spectroscopy techniques in catalyst analysis — •Daniela Ramermann, Michael Poschmann, Christoph Göbel, Wenchao Wan, Elisabeth H. Wolf, Saskia Heumann, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr

Electron energy loss spectroscopy (EELS) is a powerful technique that gives access to the electronic structure of the sample, enabling analysis of elemental composition, chemical bonding and oxidation states. Combined with the high spatial resolution of a scanning transmission electron microscope, detailed analysis of a catalyst can be carried out, to gain knowledge about the structure-function relationship. In addition to spatially resolved oxidation state analysis, accessing spectra at higher energy losses than commonly used was recently reported.

We apply these techniques to investigate the oxidation states of a CuZn-based MeOH catalyst system spatially resolved, using self-measured standards. Furthermore, we give examples of the utilization of EELS at high energy losses on a Co-based ammonia decomposition catalyst.

MM 12.7 Tue 12:00 H22

Rapid Identification of Ion Migration in Solid-State Ion Conductors from Machine-Learning Raman Spectroscopy — Manuel Grumet[1], Takeru Miyagawa[1], Karin S. Thalmann[2], Tomáš Bučko[3,4], •Waldemar Kaiser[1], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Institute of Physics, University of Freiburg — [3]Faculty of Natural Sciences, Comenius University of Bratislava — [4]Institute of Inorganic Chemistry, Slovak Academy of Sciences

Raman spectroscopy is a rapid, non-invasive, and widely available technique that provides a fingerprint of atomic vibrations within solid-state materials. In this work, we demonstrate evidence of Raman signatures that arise from the migration of ions within solid-state ion conductors. We use a rapid computational framework, which consists of machine-learning molecular dynamics simulations [1] and machine-learned polarizability tensors [2], to predict finite-temperature Raman spectra of two classes of superionic conductors, i.e. AgI [3] and Na_3PnS_4 (Pn=P,Sb) [4]. Our simulation results indicate pronounced and broad low-energy Raman intensities due to the host lattice that are correlated with the diffusion of cations. These insights can open novel synergies with experiments to rapidly screen novel compounds for future battery materials. [1] Miyagawa, et al. J. Mater. Chem. A. 12, 11344-11361 (2024) [2] Grumet, et al. J. Phys. Chem. C, 128, 15, 6464-6470 (2024) [3] Brenner, et al. Phys. Rev. Mater. 4, 115402 (2020) [4] Brenner, et al. J. Phys. Chem. Lett. 13, 25, 5938-5945 (2022)

MM 12.8 Tue 12:15 H22

Ion Dynamics in Li-Garnet Electrolytes from Machine-Learning Molecular Dynamics and Raman Spectroscopy — •Takeru Miyagawa[1], Hyunwon Chu[2], Willis O'Leary[2], Manuel Grumet[1], Jennifer L.M. Rupp[1,2], Waldemar Kaiser[1], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology

Lithium lanthanum zirconate (LLZO) is a promising electrolyte compound for solid-state batteries. Despite subtle differences in the structural properties, its cubic phase, often stabilized by doping, strongly exceeds the tetragonal counterpart in its ionic conductivity. Here, we study the interplay of Li ion migration and host lattice dynamics in tetragonal and cubic LLZO, and compare the ion dynamics to Ta-doped LLZO, using machine-learning molecular dynamics benchmarked in our previous study [1]. We observe a strongly correlated Li-ion migration in the undoped cubic LLZO at increased temperatures, whereas the tetragonal phase showed no Li ion conduction. In contrast, Li ion hopping is the dominant mechanism in Ta-doped cubic LLZO. Additionally, we compute finite-temperature Raman spectra [2] of the LLZO materials and correlate them to experiments. Our predicted Raman results accurately align with measured Raman spectra, allowing us to reveal concrete vibrational motifs that may be utilized to screen LLZO films for the presence of the conductive cubic phase. [1] Miyagawa, et al. J. Mater. Chem. A 12, 11344 (2024) [2] Thomas, et al. Phys. Chem. Chem. Phys. 15, 6608-6622 (2013)

MM 12.9 Tue 12:30 H22

Extracting Gibbs free energies from local composition fluctuations in atom probe data — •Parisha Diwan, Jianshu Zheng, Rüya Duran, Guido Schmitz, and Sebastian M. Eich — University of Sttugart

In this work, thermodynamic fluctuation theory which is traditionally used for liquids has been extended to solids by incorporating an additional elastic work component to account for local composition variations, which is not present in liquids. In solids, composition fluctuations are quantified through the relative variance of the composition histogram, which is influenced by the evaluation volume size and interface effects. These fluctuations are key to determining the Gibbs free energy of mixing in solid alloys. The technique most suitable for identifying local composition fluctuations is Atom Probe Tomography (APT), which provides high-resolution, 3D spatial chemical information at the atomic level. This allows for the detection of local composition variations in solid materials, making it an ideal tool for the evaluation of the extended fluctuation theory. The study applies this theory to a Cu-Ni alloy, using experimental APT data and spatial frequency distribution analysis. By comparing the results with existing phase diagram data, the method demonstrates its effectiveness in extracting the Gibbs free energy of mixing from local composition fluctuations in solids. The comparison with the latest CALPHAD depiction of the miscibility gap further supports the reliability of the method, showing that the proposed approach can accurately predict thermodynamic properties in solid alloys based on atomic-scale data.

MM 12.10 Tue 12:45 H22

Nanoscopic Bubble Formation during Hydrogen Desorption: Insight from Simulations and Neutron Scattering at the Nanometer Scale and its Impact on Hydrogen Storage Performance — •Arnab Majumdar[1], Neslihan Aslan[1], Martin Müller[1,2], and Sebastian Busch[1] — [1]GEMS at MLZ, Helmholtz-Zentrum Hereon — [2]Kiel University

Chemical hydrogen storage using complex hydrides is promising; characterizing the process at various length scales is crucial for optimizing this approach. At the nanometer length scale and below, neutron scattering is a powerful non-destructive technique, in particular because of hydrogen's significant scattering interaction with neutrons. Additionally, neutrons scatter differently depending on the isotope, allowing deuterium to be used in place of hydrogen.

Small Angle Neutron Scattering (SANS) is suited for characterizing structures at the nanometer length scale. In situ measurements confirmed the occurrence of the hydrogen storage process but the measurements alone could not provide complete details about the processes.

Computer simulations were performed; the most suitable model described the nanoscopic structure using the probability distribution of different compounds. The evolution of initial to final probability distribution was modelled according to different chemical kinetic models. This approach qualitatively reproduces the experimental data, suggesting the presence of trapped gas at the nanometer scale during desorption. This key insight enables an estimate of volumetric performance at the engineering scale, which shows a good match with experiments.

MM 13: Topical Session: Defects of Defects

Time: Tuesday 14:00–15:30 Location: H10

Topical Talk MM 13.1 Tue 14:00 H10

Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles — •Eugen Rabkin and Jonathan Zimmerman — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa, Israel

Recrystallization of bulk metals plays a central role in materials processing, yet it has not been utilized so far for the synthesis of metal nanoparticles. In this work we describe the kinetics of recrystallization and related annealing phenomena in Pt nanoparticles. We uniaxially deformed the particles, annealed them both in-situ and ex-situ, and characterized their morphology and microstructure. Our findings reveal that new grains often nucleate within the parent particle, only to be rapidly reabsorbed back into it, with a strong correlation between this phenomenon and particle size. We propose a model that combines recrystallization and recovery through dislocation annihilation at the particle surface, predicting a critical size for recrystallization in nanoparticles. Finally, we propose a set of rules for nanoparticle recrystallization, mirroring the rules of recrystallization in bulk materials.

MM 13.2 Tue 14:30 H10

Hierarchy of defects in near-Σ5 tilt grain boundaries in copper studied by length-scale bridging electron microscopy — •Hui Ding[1], Anoosheh Akbari[2], Enze Chen[3], Harald Rösner[2], Timofey Frolov[4], Sergiy Divinski[2], Gerhard Wilde[2], and Christian H. Liebscher[5] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]University of M\"unster, Institute of Materials Physics, Münster, Germany — [3]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA — [4]{Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — [5]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundaries (GBs) are material imperfections that significantly impact material properties. In this study, we utilized aberration-corrected scanning transmission electron microscopy to examine the structure of a series of near-Σ5(310)[001] tilt grain boundaries in copper. Globally, the GB appears flat with no noticeable defects. On the atomic-scale, however, various types of GB defects are observed. When a slight deviation in the misorientation is introduced, a patterning emerges featuring characteristic structural units from the Σ5 (310) [001] and Σ5 (210) [001] tilt boundaries. The structural landscape of the GB becomes more complex when GB plane inclination is also present, such as a wavy morphology or staircase-like architecture. Our investigation into GB structure, particularly its inherent defects, is a prerequisite towards gaining atomic-scale insights into their potential impact on material properties.

MM 13.3 Tue 14:45 H10

Data-driven modelling of vacancy segregation to grain-boundaries — •Christoph Dösinger, Oliver Renk, and Lorenz Romaner — Montanuniversität Leoben, Department of Materials Science, Roseggerstraße 12, A-8700 Leoben, Austria

Both vacancies and grain-boundaries (GB) are important defects in materials. The vacancies can interact with the GBs which might lead to a formation of voids, as a result this might start the formation of pores or cracks. From atomistic simulations it is known that vacancies can be attracted to GBs, which indeed may act as sinks for the vacancies. However, such simulations, especially if performed using ab-initio, methods can be tedious and costly. In this work we apply machine learning (ML) methods to predict the segregation energies of vacancies to GBs, which give a measure how strongly a vacancy is attracted to specific sites at different GBs. For this ML approach each segregation site is described by its local environment which can be encoded by using for example Steinhardt or SOAP parameters. Together with the site-specific segregation energies a regression model, in our case a Gaussian Process, is trained. Previously we have shown that this approach can be used to predict the segregation of solutes to grain-boundaries. This method for prediction the segregation of vacancies is tested and applied to GBs in tungsten, for which a complete data-set is available for 15 different GBs (Σ3 – Σ43). By using this diverse set of GBs, it will be possible to predict the GB segregation of vacancies for general GBs or polycrystalline materials.

MM 13.4 Tue 15:00 H10

A high-throughput ab initio segregation study of light elements at Ni grain boundaries and their effects on cohesion — •Han Lin Mai[1], Jörg Neugebauer[1], and Tilmann Hickel[2] — [1]Max-Planck-Institut for Nachhaltige Materialien GmbH, Dusseldorf, Germany — [2]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

Segregation of alloying/tramp elements to grain boundaries (GBs) can drastically affect the properties of metallic alloys. We present a high-throughput density-functional theory-based study on the segregation of smaller elements, H, B, C, N, O, P, S, in a variety of FCC Ni GBs and their effects on cohesion. To support GB engineering efforts, we investigate the thermodynamics of segregation and calculate its effects on interface cohesion. These elements often play a significant role in engineering alloys, but their positioning at GBs is ambiguous and challenging to study. The study utilizes efficient and highly automated workflows using the integrated development environment pyiron. We discuss chemical and structural trends for segregation and cohesion at GBs for these elements. In order of segregation binding strength at GBs, the trend is approximately O > B, S > P > N = C = H. Elemental trends for maximum segregation binding strength across various GB models are largely consistent, enabling qualitative cross-element comparisons through small GB sets. However, conventional metrics, such as GB energy, are insufficient for predicting segregation strength or quantity for these elements.

MM 13.5 Tue 15:15 H10

Mechanistic Influence of Interstitial Solutes on Hydrogen Trapping at Σ5 GB in γ-Fe — •Poulami Chakraborty, Mauricio Rincon Bonilla, and Elena Akhmatskaya — Basque Centre for Applied Mathematics, Bilbao, Spain

The local variation of grain boundary atomic structures and chemistry caused by segregation of impurities influences the macroscopic properties of polycrystalline materials. Here, the effect of co-segregation of carbon and boron on hydrogen segregation at a Σ5 (210) [001] tilt grain boundary in γ-Fe phase is studied by density functional theory. The grain boundary structure predominantly features kite-like motifs, which are disrupted by atomic-scale defects. First-principles calculations indicate that carbon and boron exhibit the strongest segregation tendency. Their interaction with aluminum is notably repulsive, leading to aluminum depletion at the grain boundary. Subsequently, the effect of boron and carbon co-segregation is studied with the introduction of H at the GB. Our comprehensive investigation provides valuable insight in the interaction of interstitial impurities with substitutional solutes, which, strongly influences grain boundary composition and the properties of the interface.

MM 14: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 14:00–15:15 Location: H22

MM 14.1 Tue 14:00 H22

Multiscale defective interfaces for realizing Na-CO2 batteries with ultralong lifespan — •changfan xu, tzuchin huang, and yong lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The cycling capability of Na-CO2 batteries has been impeded by limitations in the kinetics of cathodic CO2 reduction/evolution reaction (CO2RR/CO2ER) as well as the challenging process of depositing/stripping metallic Na during cycling.[1-3] Herein, a "two-in-one" electrode with multiscale defective FeCu interfaces (CP@FeCu) is presented, improving the kinetics of CO2RR/CO2ER and modulating sodium deposition behavior.[4] The enhancement of sodiophilicity and catalytic properties is attributed to multiscale defective FeCu interfaces, as revealed by experimental and theoretical investigations. The defect and valence oscillation effects originate in multiscale defective FeCu interfaces, effectively facilitating reactant adsorption and Na2CO3 decomposition during CO2RR/CO2ER processes, along with exceptional cycling stability of 2400 cycles (4800 h) at 5 μA cm*2. Meanwhile, the CP@FeCu with high sodium affinity creates a uniform electric field and strong Na adsorption, promoting favorable nucleation sites for dendrite-resistant and durable anodes. This work provides scientific insights into the design of "two-in-one" electrodes, which are crucial for addressing challenges in sodium anodes and CO2 cathodes.

[1] Small 2023, 2206445
[2] Adv. Funct. Mater. 2023, 2300926
[3] Energy Environ. Mater. 2024, 7, e12626
[4] Adv. Mater. 2024, 2409533

MM 14.2 Tue 14:15 H22

Electro-chemo-mechanical behavior of a layered cathode material upon cycling — •Robert Löser[1], Yug Joshi[2], Roham Talei[1], and Guido Schmitz[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

The mechanical properties of lithium-ion cathode materials play a critical role in determining battery performance such as cycle life, durability, and safety, especially when the battery is under external pressure which is typical for all-solid-state batteries. This research investigates LiCoO2 (LCO), a prevalent hexagonal layer-structured cathode material, and explores its mechanical responses during de-/lithiation using sputter-deposited thin films and nanoindentation. The values of the experimental Young*s modulus in pure (101) and (003) lattice orientations are quantified to 337.1 * 8.7 GPa and 267.9 * 7.2 GPa, respectively, in the fully lithiated state. Furthermore, a substantial texture-dependent decrease in Young*s modulus upon lithium deintercalation is demonstrated, probably due to modification of the bonding interactions between the cobalt oxide layers. Delithiation also elevates the relative contribution of plastic deformation, indicating that dislocation glide becomes easier in deintercalated states. By extensive cycling, the Young*s modulus in higher lithiated charge-states decreases considerably which is most-likely due to irreversibility of phase transitions. The work provides valuable insight on the dynamic changes of the mechanical properties during electrochemical cycling of LiCoO2, which paves the way for all other layered cathode materials.

MM 14.3 Tue 14:30 H22

$MnTiO_3$ as a Carbon-Free Cathode for Rechargeable Li-oxygen Batteries — Doaa Ahmed[1,2], Wernfried Mayr-Schmölzer[1], Mustafa Çelik[3,4], Abdulkadir Kizilaslan[3,4], and •Gregor Vonbun-Feldbauer[1,2] — [1]Institute of Advanced Ceramics, TU Hamburg, Germany — [2]Institute of Soft Matter Modeling, TU Hamburg, Germany — [3]Research, Development and Application Center (SARGEM), Sakarya University, Turkey — [4]Department of Metallurgical and Materials Engineering, Engineering Faculty, Sakarya University, Turkey

Lithium-oxygen batteries (LOB) are promising energy storage systems due to their high theoretical energy density. However, their main challenges are the sluggish kinetics of oxygen reduction and evolution reactions (ORR/OER) and high charge overpotentials. To overcome these challenges, the development of a suitable catalyst is crucial. Here, $MnTiO_3$ was investigated as a carbon-free cathode catalyst using density functional theory (DFT) calculations and experimental approaches. DFT calculations revealed the coexistence of Mn and Ti energy levels near the Fermi level of $MnTiO_3$, which facilitates ORR/OER. This feature endows MnTiO3 with a bifunctional role in promoting battery performance. Our DFT-based investigation further elucidates the surface stability and catalytic properties of $MnTiO_3$. In addition, experiments confirm that the electrochemical reactions on $MnTiO_3$ follow a two-electron pathway. LOBs with $MnTiO_3$ exhibit a total overpotential of 1.18 V and 1.55 V from DFT and electrochemical measurements, respectively, and current densities up to 1 A/g.

MM 14.4 Tue 14:45 H22

Modeling and optical characterization of Lithium deposition on Copper current collectors — •Len Kimms[1], Tjark Ingber[2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH

In this contribution, we will present modeling results of the initial deposition of lithium metal on a copper current collector combined with experimental insights. Zero–excess lithium–metal batteries (ZELMBs) may offer higher energy densities, better safety, and reduced cost by reducing the amount of lithium employed in the cell. Instead of an excess of lithium as electrode, the anode is formed in situ during charging. When charging the battery, lithium is plated on the current collector directly. However, the lifespan of ZELBMs in practical applications is still limited by irreversible loss of active lithium. The loss is induced by the high reactivity of lithium which causes parasitic side reactions and dendrite growth during charging cycles. To uncover the mechanisms at play, the initial deposition of lithium metal has been experimentally investigated by plating varying amounts on a copper surface with different current densities. The deposits have been characterized by scanning electron microscopy (SEM) and laser scanning microscopy (LSM) in an automated way. Numerical simulations of a simple geometric model were employed to uncover the relevant mechanisms which govern the growth over different stages. Combining the experimental and numerical results, an effective description of the deposition has been found.

MM 14.5 Tue 15:00 H22

Preparation of Prussian blue analogue materials and their application to potassium-ion batteries — •Ping Hong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Prussian blue (PB) and its analogs (PBAs), with their unique open framework structure and chemical stability, have emerged as promising cathode materials for potassium-ion batteries (PIBs). PB and PBAs feature three-dimensional channels, facilitating rapid potassium-ion intercalation and de-intercalation, thus delivering excellent rate performance. Furthermore, its low-cost synthesis and environmentally friendly properties provide a strong foundation for potential commercial applications. Despite these advantages, the practical application of PBAs is hindered by challenges such as their high solubility in electrolytes and limited cycle stability and life. To overcome these limitations, we optimized synthesis techniques (by simple adjustment of the co-precipitation method) and structural design, leading to significant improvements in material performance. In addition, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. The improved PBA cathode exhibited remarkable cycling stability, showing almost no capacity decay after 500 cycles at a current density of 100 mA/g within the voltage range of 2.0-4.0 V. It maintained excellent cycling performance even under high current conditions, providing strong support for the advancement of high-performance PIBs.

MM 15: Invited Talk. C. Scheu

Time: Wednesday 9:30–10:00 Location: H10

Invited Talk MM 15.1 Wed 9:30 H10

Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties — •Christina Scheu[1], Ruben Bueno Villoro[1], Siyuan Zhang[1], Baptiste Gault[1], Duncan Zavanelli[2], and Gerald Jeffrey Snyder[2] — [1]Max-Planck-Institute for Sustainable Materials, Max-Planck-Str. 1, 40627 Düsseldorf, Germany — [2]Northwestern University, Clark Street 633, 60208, Evanston, USA

Grain boundary defect phases are known since more than three decades, but mostly the impact on mechanical properties was investigated. In our work we were able to correlate the atomic structure and chemical composition of grain boundary defect phases in different thermoelectric materials to the electrical and thermal properties. For example, we were able to show by atom probe tomography and scanning transmission electron microscopy that grain boundaries in p-type Ti(Co,Fe)Sb Half-Heusler thermoelectric materials possess a signifi-

cant Fe segregation and Co depletion compared to the bulk. Atomic column resolved scanning transmission electron microscopy images reveal that the grain boundary phase has a hexagonal close packed stacking compared to the face centered cubic stacking of the bulk with lattice distances differing from those of any known bulk phase. The grain boundary defect phase acts as fast charge carrier pathway providing a high electrical conductivity while simultaneously reducing the thermal conduc

MM 16: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 10:15–13:00 Location: H10

Topical Talk MM 16.1 Wed 10:15 H10

Microstructure and transport in model isotropic amorphous solids — •Peter Derlet — Condensed Matter Theory Group, Paul Scherrer Institut, Switzerland

Amorphous solids lack long range order, however structural heterogeneity can exist over intermediate length scales suggesting the notion of a glassy microstructure. Such spatial variations, whatever they may be, can also be related to variations in thermally driven structural fluctuation time scales. In this talk, I will present atomistic simulations of model isotropic (metallic) binary glass systems spanning the microsecond timescale, and discuss the resulting amorphous structure in terms of bond frustration, demonstrating that despite the strong disorder, a percolative region containing strong medium range order emerges that fundamentally affects transport and dissipation. Particular focus will be given to how such simulations can give insight into experiments probing arrested colloidal glasses obtained through isotropic compression, and structural decorrelation in a metallic glass probed by long-time x-ray photon correlation measurements.

MM 16.2 Wed 10:45 H10

Liquid-like versus Stress-Driven Dynamics in a Metallic Glass Former Observed by Temperature Scanning XPCS — •Maximilian Frey[1], Ralf Busch[1], and Eloi Pineda[2] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]Department of Physics, Institute of Energy Technologies, Universitat Politècnica de Catalunya - BarcelonaTech, 08019 Barcelona, Spain

Using high flux synchrotron radiation (ESRF, ID10), we study a Pt-based metallic glass former via X-ray photon correlation spectroscopy (XPCS) upon temperature scanning through the glass, glass transition and supercooled liquid (SCL). In the equilibrium SCL, the obtained intensity autocorrelation functions are well-described by a conventional Kohlrausch-William-Watts (KWW) model. Yet, in the glass and especially the glass transition region, this approach fails. Instead, we demonstrate that a multiplication of two KWW functions allows to describe the complex decay shape. Within the glass transition region, the fit parameters of the two separate KWW fits decouple massively. While one KWW component models the compressed shape of glass-typical non-equilibrium dynamics, the other fit maintains stretched liquid-like characteristics. We demonstrate that the compressed decay can be likely addressed to ballistic-like atomic motions while the stretched component apparently reflects (sub-)diffusive atomic motions, which are both superimposed in the non-equilibrium.

MM 16.3 Wed 11:00 H10

Non-monotonic hydrodynamic relaxations in a nanochannel — •Linnea Heitmeier[1,2], Thomas Voigtmann[1,2], and Jesper Schmidt Hansen[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, 51170 — [2]Heinrich Heine University, Universitätsstraße 1, Düsseldorf — [3]DNRF Center Glass and Time, IMFUFA, Department of Science, Systems and Models, Roskilde University, DK-4000 Roskilde

Nanotechnology is an active research field with applications in the everyday-life, electronics and medicine.

In my talk, I will present results of Molecular-Dynamics Simulations of a glass-forming liquid, which is confined in a nanochannel and excited with a sinusoidal force in order to probe the velocity relaxation on different lengthscales.

I show that the velocity relaxation behavior in different regions of the channel depends non-monotonically on the position of the fluid.

To explain the results, I will make use of the Maxwell-model for fluids, which states that a fluid behaves like an elastic solid on small timescales and like a viscous fluid on large timescales.

The simulation results can be recovered by this model, when using generalizations of this model:

On the one hand, a two-mode-Maxwell-model captures the contributions from the short-time dynamics and the slow structural relaxation to the viscosity. On the other hand, a spatially non-local generalization of the Maxwell-model allows to capture the velocity relaxation in the channel depending on different positions.

MM 16.4 Wed 11:15 H10

Structural Complexity and Atomic-Scale Dynamics in Metallic Glasses — •Emel Gurbuz and Elif Ertekin — University of Illinois Urbana-Champaign

Metallic glasses (MG) become prominent for their exceptional mechanical strength, corrosion resistance, and versatile processing capabilities, all strongly linked to their amorphous atomic structures. Despite extensive research, the interplay between structural motifs, their connectivity, and the resulting dynamic behavior during glass formation remains insufficiently understood.

This study uses molecular dynamics simulations to explore the dynamics of glass formation in MG systems with varying compositions (Fe_xZr_{100-x}, Co_xZr_{100-x}, Cu_xZr_{100-x}). By analyzing melt-quench trajectories, we identify key structural motifs, such as five-fold icosahedra, and examine their role in the "freezing in" process. Regions with rapid solidification and liquid-like behavior are characterized by tracking atomic diffusivity distributions over time. Remarkably, sequences of connected icosahedra persist as liquid-like regions even at low temperatures, facilitating ionic transport.

Our findings reveal critical insights into the mechanisms governing structural and dynamic complexity in MGs, advancing the understanding of their formation and potential for designing functionally optimized materials.

15 min. break

Topical Talk MM 16.5 Wed 11:45 H10

Structural relaxation and deformation of bulk metallic glasses — •Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

In metallic glasses, relaxation is discussed in the context of shear transformation zones, viscous flow, structural medium-range order (MRO) and even crystal nucleation. However, the structural origin of different relaxation modes and how these structures change during relaxation, rejuvenation or deformation is rather unclear. In order to address some of these related aspects, calorimetric measurements have been performed together with TEM-based analyses of the local medium range order structures before and after plastic deformation as well as after controlled thermal relaxation. The combined results of macroscopically averaging and spatially resolved analyses are discussed with respect of the correlations between relaxation, deformation and modifications of the MRO structure.

MM 16.6 Wed 12:15 H10

Tracing the Roots of Elastic Heterogeneity in Metallic Glass — •Reza Rashidi[1,2], Birte Riechers[1], and Robert Maass[1,2,3] — [1]Federal Institute of Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany — [2]Department of Materials Engineering, Technical University of Munich, 85748 Garchingen, Germany — [3]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Metallic glasses (MGs) show structural and temporal heterogeneities over a broad range of time and length scales. With the aid of atomistic simulations, we can explain these dynamic and structural fluctuations at the nanometer scale. Here, our focus shifts to the larger length scale of property variations and the ongoing exploration of their origin. In past work, we suggested that cooling constraints during solidification could lead to elastic heterogeneities and therefor an elastic microstructure on the scale of ~100 nm (Materials & Design 229 (2023) 111929). In this presentation, we further support this idea by examining various casting geometries and thermal histories, tracking how elastic decorrelation lengths change with sample size and position within the MG. We also find that thermal annealing reduces decorrelation length-scale gradients and smooths out fluctuations in modulus values (Scripta Materialia 255 (2025)116380). In concert with the nano-elastic property assessment, we leverage spatially-resolved scanning nanobeam diffraction in the search for a structural origin of elastic microstructure.

MM 16.7 Wed 12:30 H10

Yield surfaces of glass-forming fluids — •Stephan Domann[1,2] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Heinrich-Heine-Universität

The yielding of amorphous solids depends in principle on the geometry of the deformation applied to the solid. This defines a ”static” yield surface in the state of principal stresses that is typically described by empirical models (such as von Mises, Tresca, Drucker-Prager etc). In a similar vein, approaching the glass transition from the fluid side, the flow stresses approach a dynamical yield stress,

defining the dynamical yield surface as the geometry of the flow is varied. Owing to the difficulty of imposing arbitrary steady deformation geometries, both experiment and simulation data are scarce.

We will discuss an approach to model yield surfaces that is rooted in a first-principle theory originally developed by Fuchs and Cates, the combination of mode-coupling theory of the glass transition with the integration-through transients framework (ITT-MCT). Using suitable simplifications, we recover some of the well-known empirical yield surface descriptions as limiting cases. It also sheds light on the qualitative differences arising between models of the upper-convected and the lower-convected type. We also performed non-equilibrium molecular-dynamics simulations of a model glass former to determine the dynamical yield surface. Surprisingly, this attains a shape that is in qualitative agreement with the lower-convected model, although common expectation is that upper-convected models are more canonical in emerging from microscopic descriptions of glass forming fluids.

MM 16.8 Wed 12:45 H10

Unveiling the Asymmetry in Density within the Shear Bands of Metallic Glasses — •Harald Rösner[1], Arabinda Bera[2], and Alessio Zaccone[2] — [1]Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Milan, Department of Physics "A. Pontremoli", via Celoria 16, 20133 Milan, Italy

Plastic deformation in metallic glasses at room temperature leads to the development of shear bands due to shear localization. In many experiments, shear bands have shown local density variations along their path, with a distinct imbalance in magnitude between local densification and dilation. However, a comprehensive mechanistic understanding or theory to explain this asymmetry has been lacking until now. Here, we introduce a new model [1] that consists of a sequential arrangement of alternating topological charges, generating a dipolar field. The resulting microscopic displacement field, when integrated into the deformation gradient tensor, provides an accurate analytical solution for the observed imbalances in the density variations. The implications of this model are discussed, highlighting the potential to elucidate a broader range of observations in shear bands.

[1] H. Rösner, A. Bera, and A. Zaccone, Phys. Rev. B, 110(1), 014107 (2024).

MM 17: Development of Calculation Methods

Machine Learning, DFT

Time: Wednesday 10:15–12:45 Location: H22

MM 17.1 Wed 10:15 H22

Premature Convergence, It's Nothing to be Embarrassed About: Solving Performance Issues with Swarm-Based Global Optimization to Generate Pt Nanoparticle Ensembles — •Julian Holland[1], Malgorzata Makos[3], Difan Zhang[4], Mal-Soon Lee[3], Roger Rousseau[3], Chris-Kriton Skylaris[2], and Vanda Glezakou[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Southampton, Southampton, UK — [3]Oak Ridge National Laboratory, Oak Ridge, USA — [4]Pacific Northwest National Laboratory, Three Cities, USA

Swarm-based global optimisation (GO) algorithms have proven successful in exploring potential energy surfaces (PESs) of chemical systems. However, they are often limited by their serial implementation. Our GO software, pyGlobOpt, uses an asynchronously parallel artificial bee colony (ABC) methodology, mitigating this limitation. We enhance pyGlobOpt further by tuning parameters against a new, general, ensemble generation assessment criterion. Using this criterion, we were also able to demonstrate how to overcome premature convergence, an issue pervading the use of the ABC algorithm for some systems, using a clustering-based methodology. We demonstrate that using the clustering algorithm alongside tuned pyGlobOpt parameters can lead to a 5-fold increase in the number of unique low-energy structures found as well as more than halving the average energetic distance from the global minimum. We produce ensembles of thermodynamically relevant Pt nanoparticles with varying hydrogenation using our enhanced software and compare to experimental results.

MM 17.2 Wed 10:30 H22

Charge Equilibration in Machine Learning Potentials — •Martin Vondrak[1,2], Johannes Margraf[1], and Karsten Reuter[2] — [1]Bayreuth University, Bayreuth, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Machine learning (ML) techniques have recently been shown to bridge the gap between accurate first-principles methods and computationally cheap empirical potentials. This is achieved by learning a mapping between a system's structure and its physical properties. To this end, state-of-the-art models typically represent chemical structures in terms of local atomic environments. This inevitably leads to the neglect of long-range interactions (most prominently electrostatics) and non-local phenomena (e.g. charge transfer), resulting in significant errors in the description of e.g. polar molecules or materials in non-isotropic environments. To overcome these issues, we are developing ML frameworks for predicting charge distributions in molecules based on Charge Equilibration (QEq). Here, atomic charges are derived from a physical model using environment-dependent atomic electronegativities. In this presentation, we will demonstrate strategies for creating long-range interatomic potentials on the example of Kernel Charge Equilibration (kQEq) models combined with local Gaussian Approximation Potentials (GAP). An alternative approach, incorporating QEq into the equivariant MACE neural network scheme will also be discussed.

MM 17.3 Wed 10:45 H22

Development of on-the-fly kinetic Monte Carlo framework with neural network potentials for surface chemistry — •Tomoko Yokaichiya, Tatsushi Ikeda, Koki Muraoka, and Akira Nakayama — The University of Tokyo, Tokyo, Japan

It is established that adsorbate-adsorbate lateral interactions in heterogeneous catalysis significantly influence adsorption and activation energies. To further our understanding of the degree to which such lateral interactions affect catalytic properties, we develop an "on-the-fly" adaptive kinetic Monte Carlo (kMC) simulation scheme. The scheme proceeds by energetically evaluating each configuration, including its local adsorbate-rich environment, using a neural-network potential then stores them to a database for efficient reuse in later kMC iterations. We apply this scheme to the industry-relevant interactions of H adsorption and diffusion on Pd and Pt surfaces as well as CO oxidation on Pt surfaces. With this scheme, we are able to elicit the extent lateral adsorbate-adsorbate interactions influence surface reactions and diffusion.

MM 17.4 Wed 11:00 H22

DECAF: An Open Source Local Atomic Environment Classifier — •King Chun Lai, Sebastian Matera, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Classification of local atomic environments (LAEs) is an inevitable task in most atomic-scale modeling and simulation. The reason is trivial, atoms' characteristics are predominantly determined by neighbors within a limited radius. The task itself, however, is abstract and error-prone due to the diversity of structures and the often ambiguous relationship between geometry and atomic behaviors. To address these issues, we have developed the open-source package DECAF during the last years [1]. DECAF automatically identifies equivalence groups within atomic structure datasets on the basis of the LAEs. We showcase the usage of the DECAF package on a set of nanotructures. We explain the theoretical background as well as the influence of different options to control the outcome. A particular feature is DECAF's ability for out-of-sample classification, identifying LAEs that differ from any groups in the training set. We provide examples where this has been exploited such as automatic process exploration [2] or active learning.

[1] Lai *et al.*, J. Chem. Phys **159**, 024129 (2023). DOI: 10.1063/5.0160369 Available: https://gitlab.mpcdf.mpg.de/klai/decaf
[2] Lai *et al.*, ChemRxiv (2024). DOI: 10.26434/chemrxiv-2024-jbzr7

MM 17.5 Wed 11:15 H22

Accurate TDDFT Excited-State Spectra Across the Full Spectral Range — •Matthias Kick and Troy Van Voorhis — Massachusetts Institute of Technology, Cambridge, MA, USA

Theoretically, electronic excitations can be obtained by analyzing the frequency components of the time-dependent dipole moment obtained from real-time time-dependent density functional theory (RT-TDDFT) simulations. Yet, an exact treatment of electronic excitations in large systems with TDDFT is computational prohibitive. Super-resolution techniques such as compressed sensing typically fail due to the presence of a quasi-continuum of electronic excitations. We present a new approach where we combine exact short-time dynamics with approximate frequency space methods. As a prototypical test system, we use an organic dye-molecule adsorbed on a semi-conductor quantum-dot surface. We calculate the entire electronic absorption spectrum of this system and find that our approach can accurately capture narrow features and a quasi-continuum of states at the same time. We see a reduction of the required amount of data points up to a factor of 20 compared to standard Fourier analysis. By doing so, our

method allows us to study electronic properties of large systems in ways that are not currently possible.

15 min. break

MM 17.6 Wed 11:45 H22

Beyond-DFT Machine-Learning Interatomic Potentials and Applications to Covalent-Organic Frameworks — •Yuji Ikeda, Axel Forslund, and Blazej Grabowski — University of Stuttgart, Germany

Covalent-organic frameworks (COFs) are nanoporous crystalline materials composed of covalent organic secondary building units (SBUs), primarily composed of light elements such as C, N, O, and H. Many COFs exhibit a quasi-two-dimensional layered structure, stabilized by van der Waals (vdW) interactions. Machine-learning interatomic potentials (MLIPs) offer an exciting opportunity to explore COFs, enabling access to extended time and length scales in molecular dynamics (MD) simulations. To accurately model vdW interactions, MLIPs must be trained on datasets that include these effects, often derived from vdW-DFT functionals. However, vdW-DFT methods are essentially semi-empirical, with parameters calibrated for experimental agreement, raising concerns about their transferability. Instead, we propose generating training data from post-Hartree-Fock methods, such as coupled-cluster (CC) calculations, which are non-empirical and provide beyond-DFT accuracy. By utilizing MLIPs trained on these high-accuracy datasets, we aim to investigate the structural properties of COFs in unprecedented detail.

MM 17.7 Wed 12:00 H22

Performance and limits of finite-temperature DFT for SiO2 — •Axel Forslund, Jong Hyun Jung, Blazej Grabowski, and Yuji Ikeda — Institute for Materials Science, University of Stuttgart, Germany

Silicon dioxide (SiO2) is a widely studied compound, yet far from fully understood. It exists in a variety of different phases, several of which are dynamically stabilized. These structures require dynamic vibrations of the atoms to not transform, and pose a challenge from an atomistic modeling point of view. Even in recent publications where state-of-the-art machine-learning interatomic potentials (MLIPs) have been used, the predictions differ significantly from experiments. For example, the transition between the two dynamically stabilized phases beta-quartz and cristobalite is very sensitive, and a single meV/atom shift can change the transition by 100 K. Not only the accuracy of the MLIP and the method for free-energy calculations matters, but also the underlying ab initio data play a crucial role. We demonstrate this sensitivity, and provide a simplified, yet precise method of estimating the quartz-cristobalite transition temperature. This approach is accurate enough to closely estimate the transition temperature using new density-functional-theory (DFT) functionals, and we demonstrate this for several functionals and on-top corrections. Our method is also efficient enough for using the random-phase approximation (RPA), which provides a transition temperature in very good agreement with the average CALPHAD value, and thus serves as a benchmark for the development of improved DFT functionals.

MM 17.8 Wed 12:15 H22

DSKO: Dancing through DFTB Parametrization — •Artem Samtsevych, Yihua Song, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Density Functional Tight-Binding (DFTB) offers a computationally efficient alternative to *ab initio* methods, bridging between the accuracy of DFT and the speed of semiempirical models. The approximate nature of DFTB makes its reliability highly dependent on parameter quality. While recent advancements have significantly improved the parametrization of the so-called repulsive potential, the parametrization of the so-called electronic part of the DFTB interaction remains relatively simplistic and underdeveloped.

Here, we present our in-house DFTB Slater-Koster Optimizer (`DSKO`), a novel DFTB parametrization framework that aims at producing highly accurate and transferable electronic parameter sets, under rigorous physical constraints. By incorporating robust optimization algorithms and physics-informed loss functions, `DSKO` generates parameters that align well with high-level DFT references, particularly in predicting electronic properties like density of states (DOS) and band gaps. The versatility of `DSKO` facilitates the application of DFTB to a wide spectrum of materials science challenges, from catalysis to energy storage, paving the way for routine high-fidelity semiempirical simulations.

MM 17.9 Wed 12:30 H22

A Fundamental Study of Slater-Koster Tables in Density Functional Tight-binding within Trial Nickel Oxides Systems — •Yihua Song, Artem Samtsevich, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institut

Density-Functional Tight Binding (DFTB), a semiempirical approximation to Density Functional Theory (DFT), is widely used thanks to its undoubtful computational efficiency, which allows to access large scale systems out of reach for DFT, while keeping adequate accuracy and direct electronic structure information. To be mentioned, even with non-spin polarized and non +U reference, the optimized parameters are able to be highly transferable to spin-polarized, DFTB+U and large scale calculations without any pain. The speed advantage in DFTB originates from precalculating distance dependent two-center interaction integrals for each atomic species pair, following the Slater-Koster (SK) principle[1]. In a fundamental study of the prototypical system Ni/NiOx, we test the hypothesis of adapting the SK integrals depending on the local environment. Considering a trial structure containing Ni in different oxidation states simultaneously, we find that assigning to each Ni "type" its optimal SK parametrization significantly improves the description of the band structure and density of states. Generalizing this concept opens a promising way towards adaptive, reliable, machine-learnable SK parameters.

MM 18: SYMD contributed

Time: Wednesday 10:15–13:15 Location: H23

MM 18.1 Wed 10:15 H23

Relation Between Element Specific Chemistry and Basis Set Size of Machine Learned Interatomic Potentials — •Haitham Gaafer, Jan Janssen, and Joerg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

Machine learned interatomic potentials (MLIP) have gained popularity in materials science for their scalability and accuracy on par with the Density Functional Theory (DFT) training data. Based on the linear scaling with the number of neighbors, the primary focus in the recent years was increasing the flexibility of MLIPs to further improve their accuracy, as demonstrated by approaches such as Neural Network potentials and the Atomic Cluster Expansion (ACE). The Bessel functions and Chebyshev polynomials gained popularity as basis sets to represent the atomic bonds and orbitals. Nonetheless, the connection between an MLIP's basis set and its capability to represent the chemical complexity of various elements is not yet well understood.

In this study, we use ACE, as implemented in the Pacemaker software package, to investigate three non-magnetic transition metals (i.e., Al, Au, and Cu). For each element, we parameterize computationally efficient ACE potentials based on a minimal basis set to achieve a given root-mean-square error (RMSE) across both training and testing datasets. We find that the complexity of the MLIP primarily depends on the scaling of the per-atom energy distribution rather than the chemical complexity of the elements. Consequently, it is primarily a numerical effect rather than a chemical effect.

MM 18.2 Wed 10:30 H23

Physics-Based Generative Models: Enhanced Structure-Property Sampling in Inverse Materials Design — •Patricia König[1], Nicolas Bergmann[1], Piero Coronica[2], Chiara Panosetti[1], Hanna Türk[1], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computational and Data Facility, Munich

Data-driven approaches for the inverse design of novel materials with desired properties have become a key tool in materials discovery. Here, we introduce a framework using physics-based Generative Adversarial Networks for enhanced structure-property sampling via latent space design.

We are interested in sampling structures of two chemical systems associated with different relevant physical quantities, like the work function in the electrochemical adsorption of iodide and hydroxide on copper surfaces, and the oxygen chemical potential in the CO to CO_2 conversion over an amorphous RuO_2 catalyst. As part of our framework, we track and evaluate the structural diversity and convergence of our generator with machine-learning interatomic potentials and quantitative metrics. This enables a high throughput and cost-effective evaluation of structural guesses and their related properties to leverage the full potential of generative models. Concluding, we are showing on two model systems how to explore a vast chemical space of datasets with sparse areas, particularly structures with high free energies in transition states and diverse amorphous surface structures, thereby advancing the understanding and design of novel materials.

MM 18.3 Wed 10:45 H23

Active learning-based automated construction of Hamiltonian for structural phase transitions: a case study on $BaTiO_3$ — •Mian Dai[1], Yixuan Zhang[1], Nuno Fortunato[1], Peng Chen[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas 72701, USA

The effective Hamiltonians have been widely applied to simulate the phase transitions in polarizable materials, with coefficients obtained by fitting to accurate first-principles calculations. However, it is tedious to generate distorted structures with symmetry constraints, in particular when high-ordered terms are considered. In this work, we implement and apply a Bayesian optimization-based approach to sample the potential energy surface, automating the Hamiltonian construction by selecting distorted structures via active learning. Taking $BaTiO_3$ (BTO) as an example, we demonstrate that the Hamiltonian can be obtained using fewer than 30 distorted structures. Follow-up Monte Carlo simulations can reproduce the structural phase transition temperatures of BTO, comparable to experimental values with an error < 10%. Our approach can be straightforwardly applied on other polarizable materials and paves the way for quantitative atomistic modelling of diffusionless phase transitions.

MM 18.4 Wed 11:00 H23

Comparing linear and deep learning surrogate models of materials electronic structure — •Valdas Vitartas, Chen Qian, James Kermode, and Reinhard Maurer — University of Warwick, Coventry, UK

The self-consistent electronic Hamiltonian matrix from Density Functional Theory (DFT) gives access to the electronic band structure and the density of states of a material, albeit at a large computational cost. Over recent years, several surrogate models based on linear parametrization and deep learning have been proposed to efficiently learn the electronic Hamiltonian as a function of the configuration and composition of materials. In this work, we compare two such models, the ACEhamiltonians [npj Comput. Mater. 8, 158] and MACE-H. Both provide a representation of the Hamiltonian in atomic orbital basis in terms of an equivariant many-body expansion of local atomic environments. In the case of ACEhamiltonians, the model parametrization is linear; for MACE-H, the representation serves as input to a message-passing neural network. The models are trained on reduced, valence-only Hamiltonian matrices for bulk gold and silicon generated from all-electron DFT via an approximately eigenspectrum-conserving transformation. We discuss the inherent strengths and weaknesses of the models by illustrating their accuracy, performance, data efficiency, and their ability to predict electronic quantities of interest for out-of-distribution configurations.

MM 18.5 Wed 11:15 H23

MACE-H: Equivariant Hamiltonian prediction with many-body expansion message passing — •Chen Qian, Valdas Vitartas, James Kermode, and Reinhard J. Maurer — University of Warwick, UK

The machine learning prediction of Kohn-Sham Density Functional Theory (DFT) Hamiltonians has the potential to accelerate the prediction of electronic properties, such as electronic band structures and electron-phonon coupling, while avoiding computationally expensive self-consistent field iterations. We introduce the MACE-H graph neural network, which combines the MACE body-order expansion message passing scheme with node-degree expansion blocks to efficiently generate messages that incorporate all relevant SO(3) irreducible representations. This model achieves high accuracy and high computational efficiency in capturing the local chemical environment. We demonstrate the model performance using several open materials benchmark datasets for 2D materials, achieving sub-meV prediction errors on matrix elements. Moreover, we discuss how the many-body expansion achieves higher data efficiency and examine its effect on out-of-distribution prediction for nanostructures featuring long-range interactions. To assess prediction outputs, we analyze the correlation between errors and hermiticity. The high computational efficiency and accuracy make the model a good candidate for electronic structure prediction in large-scale systems and high-throughput material screening.

15 min. break

MM 18.6 Wed 11:45 H23

Inferring Structure-Property Relationships with Artificial Intelligence: A Lignin Case Study — •Matthias Stosiek and Patrick Rinke — Technical University Munich, Munich, Germany

The potential of lignin as an abundant, underutilized biopolymer is increasingly being realized. A key challenge for the targeted production of lignins remains the poorly understood relation between lignin properties and its complex structure. Artificial intelligence (AI) methods could reveal such structure-function relationships but remain elusive in biomaterials research.

Structurally diverse lignins are extracted from birch wood combining the Aqua Solv Omni (AqSO) biorefinery process and AI-guided data acquisition[1]. Each lignin sample is characterized with 2D nuclear magnetic resonance (NMR) spectroscopy. A total of 95 collected NMR spectra are complemented with measurements of key lignin properties such as the antioxidant activity.

To establish structure-function relationships, we first correlate regions of the NMR spectra with the corresponding property measurements. Subsequently, we use RFR feature importance analysis to identify structural features that correlate with each property and provide a chemical interpretation of our findings. For instance, we find that a higher number of β-O-4 bonds leads to a lower surface tension in water indicating a more linear lignin structure. Our structure-inference approach is designed to be general and applicable to a wide range of materials and characterization data.

[1] D. Diment et al., ChemSusChem 2024, e202401711.

MM 18.7 Wed 12:00 H23

Machine learning electrostatics: Open challenges from batteries to proteins — •Max Veit — Technische Universität Darmstadt, DE

Long-range interactions such as electrostatics have long been a concern in developing accurate, efficient machine learning potential energy surfaces (ML-PES). Such potentials have now become established as a powerful technique allowing simulations of complex structures and processes with unprecedented realism and accuracy. However, the most widespread and successful methods to date do not incorporate any interactions beyond a fixed cutoff range, typically a few coordination shells. First, we need to ask the question of how methods with such an obvious limitation can be so successful, even applied to systems where long-range electrostatic interactions are known to be relevant. Second, we need to ask what approach, among the many proposed over the last decade or so, is the most appropriate if we want to incorporate long-range interactions in an accurate, efficient, and physically appropriate way. We investigate these questions in the context of a technologically relevant, experimentally accessible test system: lithium-intercalated graphite or nearly-graphitic nanoporous carbon. We first discuss the characteristics of this system that make it uniquely suited to machine learning simulation, then turn to the difficulties involved in defining what exactly makes a "good" electrostatic model, or long-range model in general, in the context of machine learning potentials, and finally discuss the implications for other systems – such as complex biomolecules – just out of the current reach of ML-PES simulations.

MM 18.8 Wed 12:15 H23

Data driven prediction of relative stability of binary and ternary TCP phases. — •Mariano Forti, Ralf Drautz, and Thomas Hammerschmidt — Interdisciplinary centre for advanced materials simulation, Ruhr-University Bochum

The study of precipitation of topological close packed(TCP) phases is of primary importance for the performance of superalloys. However, the structural complexity of these intermetallic compounds and the chemical complexity of the superalloys with typically up to ten elements hampers the exhaustive sampling of chemical space by density-functional theory (DFT) calculations. We overcome the related computational limitations by combining machine learning (ML) techniques with descriptors of the local atomic environment of the TCP phases and the use of interatomic potentials to predict phase properties with high precision. We illustrate our methodology studying the relative stability of the complex phases R, P, M and δ in binary and ternary systems produced from the main components in Co, Ni and Fe based superalloys.

MM 18.9 Wed 12:30 H23

Inverse Materials Design with Large Language Models — •Jan Janssen and Joerg Neugebauer — MPI for Sustainable Materials, Düsseldorf, Germany

Large language models (LLM) are trained on a vast amount of scientific literature to learn the included semantic, conceptional, and statistical relationships. The LLM applies these relationships to generate responses in natural language based on the context of the conversation. This raises the question: Can a LLM replace a scientist? Or how does the thought process of a scientist differ from the statistical approach of the LLM? Can the LLM make us better scientists?

We benchmark the capabilities of current LLMs to design new materials using atomistic simulations. While the required Python programming is challenging for the LLM and suffers from hallucination, this can be addressed with an agent-based approach by providing the LLM with a series of simulation workflows for the pyiron workflow framework. With these simulation workflows the LLM is not only capable to calculate material properties but can also invert the process and leverage statistical models to identify alloying compositions which match a pre-defined materials property, enabling inverse materials design.

Our benchmarks highlight the importance of developing scientific workflows. The more a workflow reduces the technical and scientific complexity of studying a given materials property the easier it is to use for LLMs and scientists alike. In this way LLMs also help us as scientists to validate and improve our scientific workflows. https://github.com/jan-janssen/LangSim

MM 18.10 Wed 12:45 H23

Workflow Utilities within the NOMAD Infrastructure: Lowering the Barrier to FAIR Data Management for Computational Materials Science — •J.F. Rudzinski[1], E. Boydas[1], N. Daelman[1], B. Mohr[1], J.M. Pizarro[1], T. Bereau[2], C. Draxl[1], L.M. Ghiringhelli[3], M. Girard[4], D. Usvyat[5], R. Valenti[6], and S. Botti[7] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]Dept. of Mater. Sci. and Eng., FAU Erlangen — [4]Max Planck Inst. for Poly. Res., Mainz — [5]Inst. für Chem., HU Berlin — [6]Inst. für Theor. Phys., GU Frankfurt/M — [7]RC-FEMS, Ruhr Uni. Bochum

NOMAD [nomad-lab.eu] [1] is an open-source, community-driven data infrastructure, focusing on materials science data. The NOMAD software can automatically extract data from the output of over 60 simulation codes, has been extensively expanded to support advanced many-body calculations and classical molecular dynamics simulations, and allows straightforward specialization via a rapidly developing plugin-based ecosystem. Both standardized and custom complex simulation workflows not only streamline data provenance and analysis but also facilitate the curation of AI-ready datasets. This contribution will focus on recently developed workflow functionalities and utilities within the NOMAD infrastructure. These advances enable highthroughput interfacing with the NOMAD repository, opening improved discovery pipelines by leveraging the benefits of NOMAD's comprehensive and FAIR-compliant data management system [2].

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 18.11 Wed 13:00 H23

Freedom of design: towards in silico design of molecules with desired quantum-mechanical properties — •Leonardo Medrano Sandonas[1], Alessio Fallani[2], Julian Cremer[3], Alexandre Tkatchenko[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, Germany. — [2]University of Luxembourg, Luxembourg. — [3]Pfizer Worldwide R&D, Germany.

The rational in silico design of chemical compounds requires a deep understanding of both the structure-property and property-property relationships that exist across chemical compound space (CCS), as well as efficient methodologies for defining an inverse property-to-structure mapping. In this presentation, we will discuss these relationships in the CCS sector spanned by small [Sci. Data 8, 43 (2021)] and large [Sci. Data 11, 742 (2024)] drug-like molecules, highlighting the existence of the "Freedom of design" principle [Chem. Sci. 14, 10702 (2023)]. The insights gained are subsequently leveraged to design molecules with desired properties. To this end, we first developed a variational autoencoder (VAE) approach and demonstrated that CCS can be parameterized using a finite set of quantum-mechanical (QM) properties [Nat. Commun. 15, 6061 (2024)]. We showcased the capabilities of this method by conditionally generating de novo molecular structures, interpolating transition paths for chemical reactions, and providing insightful insights into property-structure relationships. We expect our work will contribute to the development of advanced generative frameworks that enhance the in silico design and identification of molecules for specific chemical processes.

MM 19: Invited Talk: L. Bourgois

Time: Wednesday 15:00–15:30 Location: H10

Invited Talk MM 19.1 Wed 15:00 H10

Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys — •Laure Bourgeois[1,2], Nikhil Medhekar[2], and Matthew Weyland[1,2] — [1]Monash Centre for Electron Microscopy, Monash University, Victoria, Australia — [2]Department of Materials Science and Engineering, Monash University, Victoria, Australia

Solid-state precipitates are key components of many materials, and none more so perhaps than of lightweight alloys such as aluminium. These precipitates are often deeply buried inside the alloy matrix due to having at least one dimension at the nanoscale or even sub-nanoscale. These precipitates are also, in most cases, metastable phases that do not exist in a monolithic state, thus constituting difficult objects to characterise at the atomic scale. In this contribution we present the structural determination of several precipitate phases in lightweight alloys, including the classic Al-Cu, Al-Au and Al-Ag systems. Using a combination of scanning transmission electron microscopy and atomistic simulations, we reveal the existence of new interfacial structures and precipitate phases, and propose atomic-scale models for the mechanisms of nucleation and growth. This includes unexpected pathways for the formation of desired strengthening precipitates. These insights are used as a starting point to predict the precipitation behaviour of other, largely unexplored, alloy systems.

MM 20: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 15:45–18:30 Location: H10

Topical Talk MM 20.1 Wed 15:45 H10

Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting — •Paola Tiberto — INRIM, Torino, Italy

Amorphous soft-magnetic materials play an important role as core constituents in improving the energy transformation efficiency of electrical machines and passive electrical components. Although the melt-spinning process remains the main technique for obtaining amorphous soft-magnetic ribbons with remarkable soft magnetic properties, new and efficient production methods based on additive manufacturing have been developed in recent years, enabling the direct synthesis of larger elements. Ribbons were obtained by a conventional melt-spinning process while 3D-printed samples were produced by additive manufacturing via Selective Laser Melting (SLM) using powder of the same alloy as a precursor. In this study, we investigate the hysteresis properties of amorphous Fe-Si-B-based alloys in ribbon shape and 3D-printed bulk samples produced by different casting techniques. The SLM processing conditions have been observed to play a crucial role in the microstructure of the printed parts and, therefore, in their magnetic properties, due to their dependence on morphology. The effect of different printing parameters on magnetic properties, such as laser power and scan speed, has been studied. This study highlights the critical link between microstructure engineering through manufacturing techniques and the resulting magnetic performance, offering insights into optimizing both for enhanced energy efficiency in magneto-electrical applications.

MM 20.2 Wed 16:15 H10

Advancements in Developing Fe-Based Metallic Glasses for Additive Manufacturing of Soft Magnetic Components — •Amirhossein Ghavimi[1], Maryam Rahimi Chegeni[1], Purbasha Sharangi[2], Uma Rajput[2], Gabriele Barrera[2], Enzo Ferrara[2], Paola Tiberto[2], Isabella Gallino[3], and Ralf Busch[1] — [1]Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany — [2]INRIM, Strade delle Cacce 91, Torino, Italy — [3]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

This research aims to create suitable Fe-based soft-magnetic amorphous alloys for the 3D printing of motor components. Since a fully amorphous structure of the 3D-printed parts is expected to improve motor efficiency, i.e. increase magnetic softness and decrease energy losses, the glass-forming ability (GFA) is enhanced through the judicious change of the alloy chemical composition while maintaining competitive soft magnetic properties. The GFA of the compositions was studied by evaluating the critical casting thickness (dc) of the samples. Subsequently, XRD, DSC and DTA were used to characterize the structure and thermal behavior of the samples. The magnetic properties were determined by means of VSM in addition to the evaluation of losses. The eutectic zone of the Fe-Si-B system was experimentally determined. Evaluation of quaternary and quinary component alloys involved studying the effects of promising elements such as phosphorous and nickel on GFA and magnetic properties.

MM 20.3 Wed 16:30 H10

Ni-Nb-(Ta)-P-Based Bulk Metallic Glasses: The Origin of Glass Formation Based on Thermodynamics, Kinetics, Structure and Crystallization Behavior — •Lucas M. Ruschel and Ralf Busch — Chair of Metallic Materials, Saarland University, 66123, Saarbrücken, Germany

Ni-Nb-based bulk glass-forming alloys are among the most promising amorphous metals for industrial applications due to their incomparable combination of strength, hardness, elasticity and plasticity. A successful approach in alloy development is so-called minor alloying, where metallic glasses with improved properties and enhanced GFA are produced, if the proper minor alloying element is chosen for the respective base alloy. Here, minor additions of P to the

binary Ni-Nb system increase the GFA up to a record value of 5 mm, which surpasses the binary $Ni_{62}Nb_{38}$ alloy by 150 %. The partial substitution of Nb by Ta further boosts the GFA up to 6 mm. To elucidate the origins of the significant improvement in GFA, key properties such as the thermodynamics and kinetics of the system are studied, including the driving force for crystallization and the kinetic slowdown of viscosity during the transition from the equilibrium liquid to the glassy state. The primary precipitating phase, critical for glass formation, is identified by high-energy synchrotron X-ray diffraction (HEXRD) under containerless electrostatic levitation conditions. Complementary low-temperature HEXRD experiments reveal the structural evolution across a wide temperature range, offering a comprehensive understanding of the mechanisms responsible for the enhanced GFA.

MM 20.4 Wed 16:45 H10

Mechanical Behavior of Phase-Separated Zr-Al-Fe-Y Metallic Glasses for Prospective Implant Applications — •Devinder Singh[1,2], Parthiban Ramasamy[1], Anna Sophie Jelinek[3], Christoph Gammer[1], Zaoli Zhang[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben, Austria — [2]Amity School of Applied Sciences, Amity University Uttar Pradesh, Lucknow India — [3]Department of Materials Science, Montanuniversität Leoben, Jahnstraße 12, Leoben, Austria

Phase separation arises from the substitution of Y in Zr70-xAl12.5Fe17.5Yx (x=0-25 at.%) metallic glasses (MGs), resulting in the formation of nano-amorphous domains within a glassy matrix. The glasses with x > 10 show a typical liquid phase separation-induced two-glassy phase (Zr-rich and Y-rich) morphology with droplet-like microstructures. Atom probe tomography (APT) analysis confirms the formation of nanometer-sized Y-enriched clusters for x=15 and 20. The micro-hardness and nano-hardness are found to be in the range of 4.58-5.73 GPa and 5.22-6.11 GPa. The Zr-based MGs exhibit Young's moduli in the range of 81-91 GPa, which are lower than that of Co-Cr-Mo, 316L SS and Ti-6Al-4V commercial implant alloys. Evaluation of the cytocompatibility of the MG ribbons reveals high metabolic activity and well-spread human gingival fibroblast (HGF) cells on the surface of x=10 and 15 samples. Thus, the two glassy-phase Zr-based MGs free of toxic elements (Ni and Cu) exhibit suitable mechanical properties and biocompatibility for implant applications.

15 min. break

Topical Talk MM 20.5 Wed 17:15 H10

Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations — Johannes Sandberg[1,2,3], Leon F. Granz[2,3], and •Thomas Voigtmann[2,3] — [1]Universitë Grenoble-Alpes, Grenoble, France — [2]Heinrich-Heine-Universität, Düsseldorf, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

The microstructure that forms during solidification of metallic melts greatly influences the material properties. It depends crucially on the microscopic transport properties, and the initial phase selection in the cricial nucleus. Simulation of these phenomena faces two contradictory demands: while the relevant length and time scales match well that of classical molecular dynamics simulations, the sensitive dependence on details of the interatomic interactions is only captured in much smaller-scale quantum-mechanical simulations. In recent years, machine-learned interaction potentials have helped to reconcilce these requirements, allowing MD simulations to be performed with almost DFT-like accuracy.

I will present results that we have obtained using high-dimensional neural network potentials (HDNNP) to the case of Al-Ni melts and nucleation processes therein. Crucially, we assess the performance of the HDNNP by comparing to structural and dynamical experimental data of the liquids at different compositions. This reveals also how the level of DFT closure chosen in the quantum-mechanical simulations used to train the network influences the prediction of thermophysical quantities.

MM 20.6 Wed 17:45 H10

Study of solidification behaviour of undercooled Zr-Ni-Cu melts — •Chu Yu[1,4], Fan Yang[2], Dirk Holland-Moritz[2], Yindong Fang[1,4], Ivan Kaban[3], Stephanie Lippmann[4], and Peter K. Galenko[1] — [1]Otto Schott Institute of Material Research, Friedrich Schiller University Jena, Jena, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Cologne, Germany — [3]Leibniz IFW Dresden, Institute for Complex Materials, Dresden, Germany — [4]Institute of Applied Physics, Friedrich Schiller University Jena, Jena

We investigate the solidification behaviour of the glass-forming $Zr_{50}Cu_{35}Ni_{15}$ alloy employing different levitation techniques. The primary phase solidified from the undercooled melt has been found to be independent of the degree of undercooling up to a level beyond the hypercooling limit, as observed by time-resolved X-ray diffraction. The crystal growth velocity has been measured employing electromagnetic levitation (EML), where solidification occurs under stronger fluid-flow conditions compared to previous studies employing electrostatic levitation (ESL). In both cases the observed growth velocity increases with increasing undercooling, before reaching a plateau at undercoolings between 260-320 K. However, at small undercooling the growth velocities measured with EML are slightly higher than that in ESL. The solidification kinetics is discussed in terms of different crystal growth models, taking into account the effect of fluid flow. The works is supported by DFG, DLR, ESA via MULTIPHAS-project Nr. 50WM1941, and ProChance-exchange Program of the FSU Jena.

Topical Talk MM 20.7 Wed 18:00 H10

The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys — •Ralf Busch — Saarland University, Saarbrücken, Germany

According to basic hard sphere models Pt should replace Pd in the Pd42.5Cu27Ni9.5P21 alloy. But Pt42.5Cu27Ni9.5P21 shows significant structural differences compared to the Pd based alloy. To study the differences, we prepared a series of (Pd-Pt)42.5Cu27Ni9.5P21 alloys replacing Pd with Pt. We assess the thermodynamic functions revealing that the driving force for crystallization increases with the increase of the Pt content, which is in line with the decreasing critical casting thickness. The Pt-richer alloys are thermodynamically more fragile than the Pd-rich alloys, which is revealed by a larger specific heat capacity and a faster drop of the configurational entropy in the Pt-richer alloys. High energy XRD (HEXRD) studies reveal that the structure of the Pt rich alloys is dominated by its change in medium range order whereas the Pd-rich alloy is dominated by extraordinary short range order. The mechanical properties change drastically from a ductile behavior on the Pt-rich side to an embrittlement with increasing Pd content and decreasing Pt concentration. Nano-indentation investigations together with the HEXRD studies reveal that the embrittlement with increasing Pd-content can be connected to the structural changes. We used XPCS to study the atomic dynamics of the alloys as a function of temperature and wave vector.

MM 21: Interface Controlled Properties, Nanomaterials and Microstructure Design

Time: Wednesday 15:45–18:30 Location: H22

MM 21.1 Wed 15:45 H22

Plateau-Rayleigh-type failure mode of porous films and interconnects near massive substrates: mitigation strategies — •Gideon Henkelmann[1], Xinyan Wu[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Optical and Electronic Materials, Hamburg University of Technology, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum hereon, Geesthacht, Germany

Nanoporous thin films are under study as functional materials for actuation, photonics, catalysis, energy storage and as semiconductor interconnects. However, these thin films tend to self-detach from their substrate. The same failure mode is also observed in sintered silver paste, a widely used electronics interconnect material. In this work, we discuss the origin of the underlying instability. Based on those insights, we derive a mitigation strategy that depends on gradient in porosity. Combining experiment with kinetic Monte Carlo simulation, we validate the strategy and optimize the composition profile. An exponential gradient is found optimum, and this is rationalized by theory. Our approach greatly improves the structural stability of nanoporous thin films, enabling their more reliable use in advanced applications.

MM 21.2 Wed 16:00 H22

Compressive behavior and connecting topology of monolithic nanoporous niobium — •Seoyun Sohn[1,2], Shan Shi[3,1], Jürgen Markmann[1,2], Stefan Alexander Berger[1], and Jörg Weissmüller[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany

This study investigates the mechanical behavior of nanoporous (NP) Nb fabricated through liquid-metal dealloying, with an eye on the role of structure size and topology. Results from X-ray nanotomography and macro-compression tests confirm that coarsening degrades yield strength and that Young's modulus deviates from scaling laws previously developed for NP Au made by dealloying in aqueous media. Our analysis reveals that the scaled genus, a measure of network connectivity, of NP Nb observed from the tomographic reconstructions is lower than what has been reported for NP Au. This reduced connectivity provides an obvious explanation for the low modulus of NP Nb. Furthermore, the structural

dispersion implies that additional structural descriptors should be acknowledged to account for the mechanical differences between liquid-metal dealloyed materials and those synthesized via conventional aqueous dealloying.

MM 21.3 Wed 16:15 H22

Unravelling the metal-support interaction of sub-monolayer Pt thin films on manganese oxide via photoelectron spectroscopy — •Manuela Arztmann[1], Raul Garcia-Diez[1], Johannes Frisch[1], and Marcus Bär[1,2,3,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Energy Materials In-Situ Laboratory Berlin, Germany — [3]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

In heterogeneous catalysis, metal-support interactions (MSI) have been shown to greatly influence the selectivity and activity of catalysts, with reducible supports as preeminent examples. The various oxidation states accessible for manganese oxide allow to accommodate different amounts of oxygen vacancies, making it a promising support with tunable properties for catalysis. Studies show that the oxidation state of manganese is closely linked to its promoter capabilities in catalysis, though the MSI is not well understood so far. In this 'in-system' study, the chemical and electronic structure of the interface between Pt and manganese oxide was investigated by XPS/UPS as a function of Pt surface coverage. The thin film model catalysts were prepared by e-beam evaporation in a system directly connected to the XPS/UPS setup, enabling precise control of the Pt thickness from sub-monolayer levels to thick metal-like Pt layers, allowing for a systematic study of the property evolution in the near surface region without leaving vacuum conditions. Our results reveal an enhanced reduction of the manganese oxide with increasing Pt surface coverage indicating significant MSI.

MM 21.4 Wed 16:30 H22

Optical and electrical properties of borophene and borophene/silicon junction — •yaser abdi[1,2], masoud taleb[1], alireza eskandari[2], zahra alavi[2], mohsen moayedi[2], and nahid talebi[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany — [2]Department of Physics, University of Tehran, 1439955961 Tehran, Iran

Borophene, a 2D monolayer of boron atoms, possesses unique properties that have led scientists to conclude that it could be an excellent alternative to graphene in future electronic device applications. In this talk, which is based on our recent work on synthesis [1] and characterization [2] of optical [3] and electrical properties of borophene and borophene/silicon Schottky junction, I will discuss about the growth of borophene using a chemical vapor deposition approach and investigation of its optical and electrical behaviors. Leveraging advanced deep-subwavelength cathodoluminescence spectroscopy, we reveal the extreme anisotropic optical response of borophene in the visible range[3]. Finally, direct growth of borophene on silicon to make Schottky junction will be explained and some opto-electrical measurements will be presented. The optoelectronic response of a borophene/silicon-based detector is approximately ten times higher than that of detectors fabricated by transferring 2D materials onto silicon, due to the excellent junction formed by the direct growth of borophene on silicon.

[1] ACS Applied Materials & Interfaces 2021 13 (7), 8844-8850 [2] ACS Applied Nano Materials 2024 7 (11), 13712-13719 [3] arXiv preprint arXiv:2404.13609v2

MM 21.5 Wed 16:45 H22

Atomistic computer simulations of the influence of grain boundary phases on segregation — •Tobias Brink, Dongjin Kim, and Gerhard Dehm — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The properties of polycrystalline materials are often strongly affected by grain boundary (GB) segregation. Segregation energies, in turn, strongly depend on the available segregation sites and their atomic environments in the GB. At the atomic level, however, GBs are not only distinguished by their macroscopic, crystallographic parameters: different GB phases (or "complexions") can coexist even along the same GB and consequently affect available segregation sites. Similar as for bulk phases, the equilibrium atomic structure and chemistry of GBs changes based on temperature, pressure, concentration, chemical potential, etc.

Here, we investigate Ag segregation to [111] tilt GBs in Cu with hybrid molecular dynamics/Monte Carlo computer simulations using EAM potentials. These GBs are of interest because they exhibit two GB phases, "pearl" and "domino". Depending on the misorientation, either the pearl or the domino phase can more easily accommodate Ag segregants. As a consequence, the GB phases not only display distinct segregation behavior, but the stability of the GB phases is now also a function of the Ag excess concentration. An outlook on the effects of other segregants will be given and comparisons to experimental results will be discussed.

MM 21.6 Wed 17:00 H22

Characterizing the strength and stability of grain boundaries in Ni alloys by atomistic simulations — Reyhaneh Ghassemizadeh, •Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of the adhesion and mechanical stability of interfaces between two grains in a microstructure of a material from atomistic calculations remains a challenge. A possible approach to systematically address this issue is an idealized cleavage simulation analyzed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. With this approach, we analyze the stability of GBs in Alloy 718 using density functional theory calculations and thereby distinguish the influence of the different alloying elements on the strength of these interfaces. Furthermore, we systematically examine the influence of oxygen at the GBs and thereby shed light on the respective segregation-induced embrittlement in polycrystalline Ni systems. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 21.7 Wed 17:15 H22

Ce-doped Ni-based nanocrystal ribbons for Near-Perfect Infrared Absorbers — •Timuçin Emre Tabaru[1], Ali Karatutlu[2], Iremnur Duru[1], and M. Fatih Kilicaslan[3] — [1]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey — [2]Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University Ankara 06800, Türkiye — [3]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, 58000 Sivas, Turkey

Absorption properties of Ni-based ribbons prepared with a composition of 75 % Ni, 10 % Cr, 8 % Si, 5 % Fe, 2 % B, and %1 Ce-doped were investigated in the infrared region. The ribbons were prepared by melt spinning, and the samples exhibited a nanocrystalline structure due to rapid solidification. The total absorbing effectiveness of the Ni-based ribbons reached a maximum of about %93 at 3-5 *m mid-wave infrared (mid-IR) window when the ribbons were doped with Ce causing an approximate 5% improvement in the mid-IR absorption. Overall, the composite films provide over 80% IR absorption at the wavelengths from 3 *m to 25 *m. Due to the superparamagnetic behavior of the Ni-based composite film suggesting a decrease in electrical conductivity, a high impedance allows such high IR absorption over a large EM spectrum. This indicates that Ce-doped Ni composite film can be a good candidate for thermal emitters and infrared imaging, and for integrating into small-pixel uncooled infrared detectors.

MM 21.8 Wed 17:30 H22

Tracking the emergence and persistence of abnormal grain growth in the commercial aluminum alloy AA5252 using 3D X-ray microscopy — •Helmuth-André Schulz-Harder[1], Jules M. Dake[1], Wolfgang Ludwig[2], Haixing Fang[2], Pierre-Olivier Autran[2], Karolína Gutbrod[1], Markus Ziehmer[1], Madlen Atzen[1], Thomas Wilhelm[3], Volker Schmidt[3], and Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Germany — [2]The European Synchrotron (ESRF), Grenoble, France — [3]Institute of Stochastics, Ulm University, Germany

The origin of abnormal grain growth (AGG) remains unclear despite decades of investigation, even though this phenomenon has far-reaching implications for a wide range of industrial applications. A significant challenge lies in the scarcity of time-resolved 3D data on AGG. To address this, we acquired a time series of 3D maps of the commercially available aluminum alloy AA5252 using synchrotron-based diffraction-contrast tomography (DCT). The reconstructed grain maps reveal the presence of extreme abnormal grains, the evolution of which could be observed over time and traced back nearly to the point of emergence. To further explore the influence of second-phase particles (known to be present in AA5252) on the growth of abnormal grains, we conducted complementary phase-contrast tomography (PCT) measurements. The combination of these datasets provides new insight into the locations where abnormal grains emerge and the mechanism(s) driving their persistent growth advantage.

MM 21.9 Wed 17:45 H22

Direct Laser Writing of metallic material utilizing the principle of sensitized triplet-triplet upconversion — •Kristin E. J. Kühl[1] and Georg von Freymann[1,2] — [1]University of Kaiserslautern-Landau, 67663 Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern

Direct Laser Writing (DLW) is a versatile technique for fabrication of microstructures, which is constantly evolving. Conventional DLW uses two photon absorption to form polymers from monomers via a photochemical reaction. Current research is leaning towards new materials, such as different kinds of metal which satisfy different demands on the physical properties of structures like electric conductivity or ferromagnetism, as well as the application of different photochemical reactions to provide more opportunities in the implementation of the printing process.

In this talk a novel approach to Direct Laser Writing of metallic materials is presented. For this purpose, photochemical compounds and principles were investigated via different methods and applied in a home built setup for Direct Laser Writing. A sensitized triplet-triplet annihilation upconversion process (sTTA-UC) is used to generate the energy required for the photochemical reduction of nickel. Since efficient sTTA-UC is usually limited to deoxygenated materials, a solvent is used that has the property of generating a local deoxygenated area upon excitation by a sensitizer. These three processes are combined to enable Direct Laser Writing of 2D nickel structures.

MM 21.10 Wed 18:00 H22

Friction coefficient and work function investigation of transition-metal dichalcogenide — •Malik Al naabi, Shuyu Huang, Antoine Hinaut, Ernst Meyer, and Thilo Glatzel — University of Basel, Basel, Switzerland

Despite extensive research on the tribological properties of MoS2,the frictional characteristics and electronic properties of other members of the transition-metal dichalcogenide (TMD) family have remained relatively unexplored. To understand the effect of the chalcogen on the tribological behavior of these materials and gain broader general insights into the factors controlling friction at the nanoscale, we compared the friction force behavior for a nanoscale single asperity sliding on MoS2, MoSe2, WS2, and WSe2, in bulk using friction force microscopy (FFM). Additionally, we used Kelvin probe force microscopy (KPFM) to investigate the work function. All the materials were cleaved in the nitrogen glovebox.

MM 21.11 Wed 18:15 H22

Nano-scale precipitations in NiTi-based alloys after laser powder bed fusion: FIB/STEM and APT analyses — •Farzad Khodabakhshi[1], Raphael Freundl[2], Eric A. Jägle[2], and Gerhard Wilde[1] — [1]University of Muenster — [2]Universität der Bundeswehr München

Phase formation and nano-scale precipitation during laser powder bed fusion (LPBF) of a NiTi/Nb powder mixture were characterized throughout the matrix of NiTi using advanced microscopy techniques. The study employed focused ion beam (FIB) preparation combined with scanning transmission electron microscopy (STEM) and atom probe tomography (APT). Different nano-scale phases formed through in situ alloying and their interfacial coherence with the NiTi-based alloy were examined using atomic-scale high-resolution microscopy. Subsequent nano-scale elemental mapping and chemical analysis were performed by APT. The results indicated significant changes in the contributions of in situ formed phases when altering the fraction of niobium. Low fractions of Nb can modify the intrinsic structure of NiTi precipitates. Changing the grain boundary energy helps shift these precipitates toward the interiors of grains rather than remaining at the boundaries. Conversely, increasing the niobium fraction towards the eutectic composition results in the formation of a new structure comprised of precipitates with a specific ternary composition within the NiTi alloy matrix due to LPBF deposition.

MM 22: Materials for the Storage and Conversion of Energy

Time: Wednesday 15:45–16:45 Location: H23

MM 22.1 Wed 15:45 H23

Understanding Stability of Ni-rich NMC cathodes using beyond DFT many-body calculatations — •Hrishit Banerjee[1,2,3,4], Clare Grey[2,4], and Andrew Morris[3,4] — [1]University of Dundee — [2]University of Cambridge — [3]University of Birmingham — [4]The Faraday Institution

High energy density Ni-rich $LiNi_aMn_bCo_cO_2$ (NMC) cathodes undergo degradation in the form of O loss from the surface of NMC particles. O loss increases with Ni content and higher voltages. Our first-principles study examines the redox behavior of transition metals and O in NMC cathodes as a function of (de)lithiation. Despite Ni, Mn, and Co K-edges calculated using GW Approximation showing an excellent match with experimentally obtained XANES, we demonstrate that the ionic model of ascribing shifts in the XANES to changes in metal oxidation states is inappropriate. In these cases, which are characterised by strong covalency between the strongly correlated transition metal and oxygen, Dynamical Mean-Field Theory calculations are essential to calculate charges and hence assign oxidation states accurately. Due to a charge transfer from O p to Ni d, a ligand hole forms on O in Ni-rich regions. The individual Ni charge remains fairly constant throughout the charging/discharging process. In contrast, O has dual redox behavior, showing greater involvement in redox in Ni-rich regions while showing negligible redox involvement in Ni-poor regions. The dual behaviour of O in terms of participation in the redox process explains the overall higher relative stability of lower Ni content NMCs compared to Ni-rich NMCs or $LiNiO_2$ in terms of O loss.

MM 22.2 Wed 16:00 H23

Splitting Water Without Falling Apart: Accelerating the Understanding of NiFeV LDH via Design of Experiments and Machine Learning — •Juan Manuel Lombardi, Charles Pare, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

The development of sustainable energy technologies requires efficient, affordable, and durable electrocatalysts. Ni-based layered double hydroxides (LDHs) doped with Fe and V are promising candidates for the oxygen evolution reaction in anion exchange membrane water electrolyzers (AEMWE) due to their tunable structure and exceptional redox properties. However, the mechanisms by which dopants influence catalytic and structural properties are not fully understood, mainly due to the challenges posed by their humongous configurational space. In this study, we efficiently explore the thermally accessible configurations within the complex configurational space of γ-phase Ni LDHs doped with Fe and V. To maximize information gain, we sample the composition space using Design of Experiments (DoE), leverage machine learning interatomic potentials (MLIPs) to sample these configurations, and refine the results with Density Functional Theory (DFT) calculations for first-principles quality predictions. By combining these tools, we develop an optimal protocol to elucidate how the dopants influence material properties. This integrated methodology reveals pathways for optimizing NiFeV LDH compositions, enhancing energy conversion efficiencies while ensuring long-term stability.

MM 22.3 Wed 16:15 H23

Benchmarking exchange-correlation functionals for accurate computational predictions of metal organic frameworks — •Julia Santana Andreo, Joshua Edzards, Holger-Dietrich Sassnick, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics

Metal-organic frameworks (MOFs) have attracted significant attention due to their structural and chemical flexibility which makes them relevant for a wide range of technological applications, from gas storage to photocatalysis. The substitution of metal nodes and the functionalization of organic linkers can significantly expand the range of available MOFs, enabling the design of tailored properties for specific applications. While atomistic ab initio simulations can significantly contribute to explore this vast configurational space, it is mandatory to assess whether and how common approximations of density-functional-theory calculations affect the description of the structural, electronic, and vibrational properties of computationally predicted compounds. With the example of MOF-5 and its recently predicted functionalized variants [1] , we find that R2SCAN offers the optimal trade-off between accuracy and computational costs to describe electronic and vibrational properties in these materials.

[1] J. Edzards, H.-D. Saßnick, J. S. Andreo and C. Cocchi, J. Chem. Phys. 160, 184706 (2024)

MM 22.4 Wed 16:30 H23

Assessing the Bulk Stability of Oxygen Evolution Reaction Catalysts using Crystal Field Theory and Orbital Analysis — •Katarina Kretschmer[1], Michael Eikerling[1,2], and Tobias Binninger[1] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52072 Aachen, Germany

Proton exchange membrane water electrolysis (PEMWE) is an effective method for producing green, i.e. carbon-neutral hydrogen. At the PEMWE anode catalyst, water molecules are split to form oxygen molecules in the so-called oxygen evolution reaction (OER). Iridium oxide (IrO2) and ruthenium oxide (RuO2) are recognized as highly effective catalysts for the OER.

In this talk, I will discuss the electronic properties governing the bulk stability if IrO2 and RuO2. Utilizing density functional theory (DFT) calculations, the stability of both oxide materials is assessed from the perspective of crystal field theory and bond orbital analysis. The orbital overlap between the metal (iridium or ruthenium) and oxygen atoms in the lattice and the population of the emerging bonding or antibonding orbitals is analyzed, which can either contribute to or counteract the stability of the IrO2 and RuO2 lattices. This analysis will lead to the definition of electronic descriptors for predicting the bulk stability of transition metal oxide catalysts.

MM 23: Phase Transformations

Time: Wednesday 17:15–18:30 Location: H23

MM 23.1 Wed 17:15 H23

study on solid/liquid interfacial energy of Al-Cu alloys and its anisotropy under a static magnetic fields — •Chenglin Huang[1], Peter Galenko[2], Rainer Backofen[3], Ken Elder[4], Sansan Shuai[1], Jiang Wang[1], and Zhongming Ren[1] — [1]State Key Laboratory of Advanced Special Steel, School of Materials Science and Engineering, Shanghai University, 200444, P. R. C — [2]Department of Physics and Astronomy, Friedrich Schiller University of Jena, 07743, Germany — [3]Institute of Scientific Computing, Technische Universität Dresden, 01062 , Germany — [4]Department of Physics, Oakland University, Rochester, MI, 48309-4487, USA

In recent decades, external magnetic fields have been widely used in materials processing to control microstructure and optimize properties. Key phenomena include magnetic levitation, crystallographic orientation changes, magnetically induced phase transitions, and TEMHD. External magnetic fields also impact thermophysical properties such as phase transition temperatures, resistivity, viscosity, diffusion, and surface tension. These effects are closely linked to interface changes, where properties differ from the bulk. Despite their importance, quantitative studies on solid/liquid interfaces under magnetic fields remain limited. Accurately measuring interfacial energy and anisotropy, and exploring atomic-scale behavior under magnetic fields, are key challenges. This research systematically investigates the effects of external magnetic fields on interfacial energy and its anisotropy in Al-Cu alloys, offering theoretical and practical insights for controlling solidification under such fields.

MM 23.2 Wed 17:30 H23

From electronic structure to thermodynamic phase diagrams with automated workflows — •Sarath Menon[1], Marvin Poul[1], Tilmann Hickel[2], Ralf Drautz[3], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]Ruhr University Bochum

Phase diagrams are useful for understanding coexistence lines, phase stability, and phase transitions under varying thermodynamic conditions. Calculating phase diagrams involves determining the Helmholtz and Gibbs free energies of different phases and their dependence on thermodynamic state variables - a task that is both intricate and computationally demanding.

In this work, we introduce automated workflows for the calculation of Helmholtz and Gibbs free energies, incorporating configurational entropy, and provide accompanying computational tools. A key component of our approach is the alchemical transformation method, where atomic species are systematically altered along a thermodynamic path to evaluate free energy changes with composition.

We demonstrate the effectiveness of this methodology using an Atomic Cluster Expansion (ACE) machine-learning interatomic potential, parametrized using the ASSYST method, to generate unbiased *ab initio* structure datasets, and compute the phase diagram of the Au-Cu system. Our workflows are independent of the interatomic potential and the material system, making them readily transferable and paving the way for making the computation of thermodynamic phase diagrams a routine task in the field of atomistic simulations.

MM 23.3 Wed 17:45 H23

Phase formation at an interface between Ni and Sn layers during a soldering process — •Sandra Gaertner, Sergiy V. Divinski, Harald Rösner, and Gehard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

Soldering is a method for creating permanent bonds between metal parts, often resulting in the formation of intermetallic compounds. The transition to lead-free solder, driven by environmental regulations, has increased the interest in Sn-based solder alloys. However, the soldering process for interconnects involves complex processes related to material transport, phase stability, phase formation, and kinetic aspects of phase transformation. In this study, we investigated the interdiffusion and diffusion-controlled phase formation in a SnSb-solder alloy between a Ni-based layer with a small amount of Si and a Cu substrate, employing SEM and TEM. Analysis of the untreated states revealed a lamellar-type structure of the Ni-based layer, characterized by a uniform distribution of elements, while the solder alloy exhibited a β-Sn matrix and a SbSn phase. Following the soldering process, we observed the formation of various intermetallic compounds like CuSnNi and SnCu, encased within the β-Sn matrix. The SbSn phase remained as small inclusions. Moreover, the Ni-based layer initially shrank, resulting in a residual thin film that displayed an increased Si content compared to its untreated counterpart. This study highlights the intricate mechanisms involved in Cu transport from the substrate through the solder material. Alongside Sn, Cu drives the transformation of the Ni-based layer, ultimately leading to its complete consumption.

MM 23.4 Wed 18:00 H23

Temperature-modulated dilatometry as a tool for studying precipitation kinetics in alloys — •Marcel Simhofer[1], Philipp Brunner[1], Jiehua Li[2], Wolfgang Sprengel[1], and Roland Würschum[1] — [1]Inst. of Mater. Phys., NAWI Graz, Graz Univ. of Technol., Graz 8010, Austria — [2]Inst. of Casting Res., Montanuniv. Leoben, Leoben 8700, Austria

Temperature-modulated dilatometry is implemented as a tool for studying phase equilibration processes in alloys. As a case example, the phase equilibration between the saturated solid solution Al(Mg) and intermetallic Al_3Mg_2 in the Al(Mg) binary alloy is studied. The varying solubility of Mg in Al upon temperature modulation causes a modulation of the relative fractions of the two phases, which can be in-situ monitored by dilatometry owing to their different atomic volumes. The phase shift between the length change caused by phase equilibration and the applied sinusoidal temperature variation yields access to equilibration kinetics. The observed variation of the phase shift with the modulation frequency is quantitatively analyzed in the framework of a simple kinetic model, revealing that the equilibration process is controlled by the diffusion of Mg in Al.

M. Simhofer et al., J.Alloys&Comp. 1010 (2025) 176984

MM 23.5 Wed 18:15 H23

Formation mechanism of bicontinuous structure during peritectic melting of TiAg — •Zhongyang Li[1], Lukas Lührs[1], Tobias Krekeler[2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Electron Microscopy Unit, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Reverse peritectic reactions, and specifically the peritectic melting of TiAg, have been proposed as dealloying-like processes that produce quite similar microstructures but avoid the restrictions on sample size inherent in liquid-metal dealloying (LMD). Here, studies of the microstructure evolution during peritectic melting of TiAg suggest a formation mechanism that is not LMD-like but rather relies on liquid film migration. The process starts with wetting of the TiAg grain boundaries by the alloy melt. Successively, both Ti and Ag continue to dissolve from one side of, while β-Ti deposits on the other side and the liquid film sweeps the pristine TiAg crystal. TiAg-Ti interfaces with well-defined orientation relationship and with concentration gradients support this picture, as does the phase morphology in partly decomposed samples. The process generates a bicontinuous structure with a solid Ti skeleton, interpenetrated by the Ag-rich melt, which is conserved even after coarsening. This study clarifies the mechanism of peritectic melting in TiAg, and it may provide a basis for identifying other alloy systems suitable for producing bicontinuous microstructures by that process.

MM 24: Members' Assembly

Welcome to this general meeting of the DPG-SKM division MM! All of you, presenters of MM talks or posters and other interested participants of this conference, are cordially invited to this meeting. We will come together in a relaxed atmosphere, supported by drinks and pretzels (at least) for personal exchange. The poster prizes will be awarded during the Members Assembly. The current conference will be discussed and your feedback is very welcome. We will ask for your suggestions for future topical sessions in MM and symposia as well as for invited speakers. Take this opportunity to share your ideas regarding our MM program for our next DPG spring meeting.

Time: Wednesday 18:45–20:45 Location: H10

All members of the Metal and Material Physics Division are invited to participate.

MM 25: Invited Talk: D. Rodney

Time: Thursday 9:30–10:00 Location: H10

Invited Talk MM 25.1 Thu 9:30 H10

Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments — •David Rodney — Institut Lumière Matière, Université de Lyon, France

Brittleness limits the structural use of ceramics, but zirconia stands out due to transformation-induced plasticity (TRIP) between tetragonal and monoclinic phases. This stress-driven transformation enables up to 7% plastic deformation in single-crystalline ceria-doped zirconia, offering potential for high ductility. However, understanding the TRIP effect remains incomplete.

To address this, we combined in situ Laue micro-diffraction experiments at synchrotron facilities with atomistic simulations. Existing interatomic potentials fail to capture zirconia's complex polymorphism. We thus developed neural network interatomic potentials (NNIP) using DeepMD-kit for pure and ceria-doped zirconia. These NNIPs align well with ab initio data on thermodynamic, mechanical, and dynamical properties, accurately modeling phase stability, elastic properties, and energy barriers.

Using the NNIPs, we simulated the uniaxial compression of tetragonal ceramics, exploring stress-strain behavior, phase transformations, and deformation mechanisms across various compression directions. Simulations are confronted with the in situ experiments and the phenomenological theory of martensitic transformation. Key factors, including size, temperature, strain rate, and pre-existing defects, are critically analyzed, providing a comprehensive understanding of stress-induced phase transformations in zirconia ceramics.

MM 26: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Thursday 10:15–11:45 Location: H10

MM 26.1 Thu 10:15 H10

Influence of sulfur on the amorphous structure, high temperature viscosity and solidification of Zr-based bulk metallic glass formers — •Bastian Adam, Oliver Kruse, Lucas Mathias Ruschel, Maximillian Frey, Nico Neuber, and Ralf Busch — Chair of Metallic materials (LMW), Saarbrücken, Germany

The usage of the element sulfur in Bulk Metallic Glass (BMG) synthesis was recently introduced by Kuball et al. and lead to increased research interest into these new family of BMG [1]. Here we report on the influence of sulfur on the A2B type intermetallic composition (Zr50Ti16.6Ni18.3Cu15) that was characterized by container-less electromagnetic melting under microgravity within the 43rd & 44th TEMPUS parabolic flight campaigns by the German aerospace center (DLR). The investigation is accompanied by structural investigations of the amorphous solid and liquid that were conducted with the help of an electrostatic levitation device to observe the structure and solidification in an in-situ wide-angle scattering diffraction experiment at the German electron synchrotron (DESY) in Hamburg.

[1]A. Kuball, O. Gross, B. Bochtler, and R. Busch, Sulfur-bearing metallic glasses: A new family of bulk glass-forming alloys, Scr. Mater., 2018.

MM 26.2 Thu 10:30 H10

Structure and dynamics of Ni-Nb alloy melts upon sulfur addition — Nicolai Grund[1], Dirk Holland-Moritz[1], Saba Khademorezaian[2], Lucas P. Kreuzer[1,3], Nico Neuber[4], Lucas M. Ruschel[4], Hendrik Voigt[2], Johanna Wilden[1], •Fan Yang[1], Sergiy Divinski[2], Ralf Busch[4], Andreas Meyer[1], and Gerhard Wilde[2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [2]Institute of Materials Physics, University of Münster, Münster, Germany — [3]Heinz Maier-Leibnitz-Zentrum, Technische Universität München, Garching, Germany — [4]Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

We investigated the change in the structure and dynamics of a Ni-Nb bulk metallic glass upon sulfur addition on microscopic and macroscopic scales. With the sulfur concentration of 3 at.%, where the composition $Ni_{58}Nb_{39}S_3$ exhibits the best glass forming ability in the investigated sulfur concentration range, both the equilibrium and undercooled melt dynamics remain almost unchanged. Only in the glassy state sulfur seems to result in less decoupled mass transport to the viscosity of the undercooled liquid, where the Ag tracer diffusion coefficient is slower in the ternary alloy. With the structural disorder introduced by alloying sulfur, the improved glass forming ability is attributed to geometrical frustration, where crystal nucleation requires a depletion of sulfur and hence long range diffusion, as long as no primary sulfur-containing crystalline phase is involved.

MM 26.3 Thu 10:45 H10

Probing Medium-Range Order in Metallic Glasses with 4D-STEM — •Birte Riechers[1] and Robert Maass[1,2,3] — [1]Federal Institute of Materials Research and Testing (BAM), Germany — [2]University of Illinois at Urbana-Champaign, USA — [3]Technical University of Munich, Germany

Medium-range order (MRO) in metallic glasses (MGs) plays a crucial role for their applicability, as it significantly affects their mechanical properties. Important details of the MRO were revealed by micro-second long atomistic simulations, that have shed light on the temperature- and time-dependent evolution of MRO, especially in connection to the emergence of a network of specific structural motifs (JALCOM 821, 153209, 2020; Acta Mater. 267, 119730, 2024).

While these insights help to understand the effect of MRO evolution, the experimental validation remains challenging. To test these findings, we employ 4-dimensional scanning transmission electron microscopy (4D-STEM) (Ultramicroscopy 232, 113405, 2022) to analyze both the first and second diffraction shells of MGs. By examining the diffraction symmetries at these length scales, we aim to uncover the dominant structural features associated with MRO.

MM 26.4 Thu 11:00 H10

Structural evolution during annealing in a Zr-Cu-Al bulk metallic glass by X-ray absorption spectroscopy — •Andrea Fantin, Reza Rashidi, Birte Riechers, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding structural evolution in the time-temperature-transformation diagrams of bulk metallic glasses (BMGs) is crucial to tackle common challenges in glass science such as embrittlement and mechanical failure. Preliminary extended X-ray absorption spectroscopy fine structure (EXAFS) measurements carried out at the Zr and Cu K-edges on a typical Zr-Cu-Al system allowed following the evolution of element-specific bond lengths, static and dynamic disorder, and nearest-neighbor numbers as a function of temperature and time. Data on the as-cast BMG, on further annealed BMG at two different temperatures (0.9Tg and 1.02Tg) and at different holding times was collected (ex-situ) at the BM-08 beamline, ESRF, finally showing two different behaviors depending on the temperature used, which will be described in terms of EXAFS fitting parameters during the presentation.

MM 26.5 Thu 11:15 H10

Thermodynamic, kinetic and structural study of Pt42.5CuxNi36.5-xP21 alloy variations — •Ziyu Ling[1], Maryam Rahimi Chegeni[1], Nico Neuber[1], Sergey Kasatikov[2], Amirhossein Ghavimi[1], Andrea Fantin[3], Isabella Gallino[4], and Ralf Busch[1] — [1]Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes — [2]Helmholtz-Zentrum Berlin für Materialien und Energie Elektrochemische Energiespeicherung — [3]Bundesanstalt für Materialforschung und -prüfung, Berlin — [4]Lehrstuhl für Metallische Werkstoffe,TU Berlin

The thermodynamic and kinetic properties of Pt42.5CuxNi36.5-xP21 glass-forming liquids are studied via differential scanning calorimetry and Flash DSC (Mettler Toledo). The kinetic fragilities of the alloys are determined from relaxation times measured in a broad heating rates range using a Tg shift method and the relaxation time of the deeply undercooled liquids determined via a step-response method. Furthermore, the specific capacity heat (Cp) as a function of temperature for the glassy, liquid and crystalline state of the chosen alloys are determined. The thermodynamic fragility is assessed from the 'Cp jump' at Tg and the driving force for crystallization is calculated using fitting parameters of thermodynamic functions derived from Cp data. Then the glass forming ability of the alloy liquids is evaluated based on their critical cooling rates and TTT-diagrams. The interfacial energy is obtained by JMAK fitting with TTT-diagrams. Moreover, the alloy ribbons were investigated by synchrotron X-ray scattering experiments at DESY for structural study and by XPS and NEXAFS at BESSY for energy state information of each elements.

MM 26.6 Thu 11:30 H10

Temperature dependence of cooperativ fluctuations in supercooled glass-forming metallic melts — •Jürgen Schawe[1], Min Kyung Kwak[2], Mihai Stoica[1], Eun Soo Park[2], and Jörg Löffler[1] — [1]ETH Zürich, Laboratory of Metal Physics and Technology, Zurich, Switzerland — [2]Seoul National University, Department of Materials Science and Engineering, Seoul, Republic of Korea

The behavior of a supercooled glass-forming metal alloy depends on the cooperative atomic fluctuations caused by the dynamic heterogeneities in the melt. These spatial and temporal heterogeneities form dynamic clusters, which are re-

gions of cooperative rearrangement (CRR). The time and temperature dependence of the CRR characterizes the α-relaxation. In this study, the correlation length ξ, characteristic of the CRR, is derived for Pt57.4Cu14.7Ni5.3P22.6 and Pd43Cu27Ni10P20 bulk metallic glasses by fast differential scanning calorimetry in a temperature range between the glass transition temperature Tg and Tg + 50K. It appears that while the composition of the alloy influences the macroscopic α-relaxation and vitrification kinetics, typically defined by Tg, as well as the limiting temperature of the Vogel-Fulcher-Tammann-Hesse equation and the fragility index, it has no significant influence on the correlation length of the cooperative atomic motions. In agreement with many other materials, ξ at Tg is about 3 nm for both metallic glasses. The temperature dependence of ξ correlates with the apparent activation energy of the α-relaxation and is the reason for their non-Arrhenius behavior.

MM 27: Transport in Materials: Diffusion, Charge or Heat Conduction

Machine Learning, Quantum Theory

Time: Thursday 10:15–13:00 Location: H22

MM 27.1 Thu 10:15 H22

Modelling Heat Transport in Metal-Organic Frameworks with Machine Learned Potentials — •Martin Klotz[1], Florian Lindner[1], Sandro Wieser[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria

Many of the envisioned applications of porous metal-organic frameworks (MOFs), like gas storage or catalysis, involve exothermal processes. This requires the materials to efficiently dissipate heat. It is, thus, vital to gain a fundamental understanding of how structural and chemical modifications impact heat-transport in such systems. Here, we chose MOF-74/Zn as parent system for which we calculated the anisotropic thermal conductivity using approach to equilibrium molecular dynamics simulations. For these, we applied machine-learned force field potentials, as they surpass DFT simulations by orders of magnitudes in terms of speed and classically parametrized force field potentials in terms of accuracy. Subsequent to thoroughly benchmarking and testing the employed methodology, we studied structure-to-property relationships for MOF-74 derivatives, systematically varying the node metal and the linker structure.

MM 27.2 Thu 10:30 H22

Predicting 2D conventional superconductors — Thalis H. B. da Silva[1], Théo Cavignac[2], Tiago F. T. Cerqueira[1], •Hai-Chen Wang[2], and Miguel A. L. Marques[2] — [1]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [2]Universitätsstr. 150

We perform a large-scale search for two-dimensional (2D) superconductors by using electron-phonon calculations with density-functional perturbation theory combined with machine learning models. In total, we screened over 140k 2D compounds from the Alexandria database. Our high-throughput approach revealed a multitude of 2D superconductors with diverse chemistries and crystal structures. Moreover, we find that 2D materials generally exhibit stronger electron-phonon coupling than their 3D counterparts, although their average phonon frequencies are lower, leading to an overall lower transition temperature (T_c). Despite this, we discovered several out-of-distribution materials with relatively high T_c. In total, 105 2D systems were found with $T_c > 5$ K. Some interesting compounds, such as CuH_2, NbN, and V_2NS_2, demonstrate high T_c values and good thermodynamic stability, making them strong candidates for experimental synthesis and practical applications. Our findings highlight the critical role of computational databases and machine learning in accelerating the discovery of novel superconductors.

MM 27.3 Thu 10:45 H22

Modelling complex proton transport phenomena - Exploring the limits of fine-tuning and transferability of foundational machine-learned force fields — •Christian Dressler[1], Malte Grunert[2], Jonas Hänseroth[1], Max Grossmann[2], and Erich Runge[2] — [1]TU Ilmenau, Institute of Physics, Theoretical Solid State Physics — [2]TU Ilmenau, Institute of Physics, Group of Theoretical Physics 1

The solid acids CsH_2PO_4 and $Cs_7(H_4PO_4)(H_2PO_4)_8$ pose significant challenges for the simulation of proton transport phenomena. In this talk, we present the use of the recently developed machine-learned force field MACE to model proton dynamics on nanosecond timescales for these systems and compare its performance with long-term ab initio molecular dynamics (AIMD) simulations. The MACE-MP-0 foundation model shows remarkable performance for all observables derived from molecular dynamics simulations, but minor quantitative discrepancies remain compared to the AIMD reference data. However, we show that minimal fine-tuning - fitting to as little as 1 ps of AIMD data - leads to full quantitative agreement between the radial distribution and autocorrelation functions of MACE force field and AIMD simulations. Long-time AIMD simulations are unable to capture the correct qualitative trends in diffusion coefficients due to their inherent time scale limitations. In contrast, we demonstrate that accurate and convergent diffusion coefficients, consistent with experimental data, can only be reliably achieved through multi-nanosecond molecular dynamics simulations utilizing machine-learned force fields.

MM 27.4 Thu 11:00 H22

Understanding thermal transport in organic semiconductors using machine learned force fields — •Florian Unterkofler[1], Lukas Reicht[1], Lukas Legenstein[1], Sandro Wieser[2], Michele Simoncelli[3], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria — [3]Columbia University, New York (USA)

Organic semiconductors (OSCs) are key materials for optoelectronic devices such as solar cells and organic light-emitting diodes (OLEDs). While the properties related to charge transport of OSCs are relatively well understood, we still lack an understanding of the fundamentals of the heat transport in those materials. To study the atomistic origins of heat transport, we developed a strategy for calculating the thermal conductivity of complex organic crystals employing non-equilibrium molecular dynamics (NEMD) simulations with highly accurate, system-specific, machine-learned Moment Tensor Potentials (MTPs). These MTPs are trained on ab initio data obtained from on-the-fly active-learning molecular dynamics simulations.[1]

We then simulated the thermal transport in pentacene with NEMD to analyze the heat conduction in real space at an atomistic level and to identify heat-transport bottlenecks. Alternatively, we also use the MTPs to accurately calculate thermal conductivities arising from the particle-like propagation and the wave-like tunneling of phonons in reciprocal space. Both approaches are consistent and agree with available experiments.

[1] npj Comput Mater 10, 18 (2024)

MM 27.5 Thu 11:15 H22

Influence of Defects and Layer Twisting on Phonon Dynamics in Bilayer Graphene and MoS_2 Using Machine Learned-Force Field Calculations — •Sabuhi Badalov[1,2] and Harald Oberhofer[1,2] — [1]Department of Physics, University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

In crystalline materials, thermal, mechanical and even electronic properties are often described in terms phonon spectra and dynamics. These, can, to a large degree be influenced by even minute structural changes, such as through defects or by altering the relative alignment of a material's layers. By means of a state-of-the-art machine learning-augmented force field approach, we carry out extensive phonon calculations to understand how the defect density and layer configurations influence the phonon spectra in bilayer graphene and MoS_2. Our results highlight an interplay of phononic phenomena with the materials' Moiré patterns with major consequences on the transport properties of these materials. Moreover, we explore the possibility of phonon-mediated superconductivity through the electron-phonon coupling in topologically nontrivial phonon states. While this is still ongoing research, our results so far not only further the understanding of phonon dynamics in 2D materials, but also offer a solid foundation for future investigations into harnessing topological phonons for advanced electronic and thermal control technologies.

15 min. break

MM 27.6 Thu 11:45 H22

Thermoelectric quantum transport simulations via the time-linear nonequilibrium Green's function method — •Riku Tuovinen[1] and Yaroslav Pavlyukh[2] — [1]Department of Physics, University of Jyväskylä, Finland — [2]Institute of Theoretical Physics, Wroclaw University of Science and Technology, Poland

Thermoelectric transport focuses on understanding charge and heat flow in quantum systems. While measuring electron current is relatively straightforward, nanoscale heat flux remains challenging to quantify [1]. Heat and charge exhibit fundamental differences, as highlighted by electron transport analysis within the nonequilibrium Green's function theory [2]. In the time-linear formulation, based on the generalized Kadanoff-Baym ansatz (GKBA), open system dynamics are described using an embedding correlator, enabling the calculation of time-dependent currents via the Meir-Wingreen formula [3]. However, calculating heat currents presents challenges, particularly within the wide-band limit

approximation (WBLA), which can result in divergent energy integrals. Besides the mathematical issues, the WBLA's reliability depends on the physical properties of the leads. To address these limitations, we present thermoelectric quantum transport simulations using the time-linear GKBA method without relying on the WBLA [4].

[1] J. P. Pekola and B. Karimi, Rev. Mod. Phys. 93, 041001 (2021).
[2] M. Ridley et al., J. Phys. A: Math. Theor. 55, 273001 (2022).
[3] R. Tuovinen et al., Phys. Rev. Lett. 130, 246301 (2023).
[4] R. Tuovinen and Y. Pavlyukh, in preparation (2024).

MM 27.7 Thu 12:00 H22

Sublinear in temperature transport in kagome metals: interplay of Dirac cones and Van Hove singularities — •Nikolai Peshcherenko[1], Ning Mao[1], Claudia Felser[1], and Yang Zhang[2,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Kagome metals are known to host Dirac fermions and saddle point Van Hove singularities near Fermi level. With the minimal two-pocket model (Dirac cone + Van Hove singularity), we propose a semiclassical theory to explain the experimentally observed sublinear resistivity in Ni_3In and other Kagome metals. We derive the full semiclassical description of kinetic phenomena using Boltzmann equation, and demonstrate that internode electron-electron interaction leads to sublinear in T scaling for both electrical and thermal transport at low temperatures. At higher temperatures above the Dirac node chemical potential, thermal and electric currents dissipate through distinct scattering channels, making a ground for Wiedemann-Franz law violation.

MM 27.8 Thu 12:15 H22

Phonon induced heat transfer between gold nanogap electrodes — •Yuki Hanamura, Kazuma Kishimoto, Mizuki Tada, Ryo Yamada, and Hirokazu Tada — Graduate School of Engineering Science, Osaka University, Japan

Recent studies have observed anomalous increases in thermal conductance in nanogaps narrower than a few nanometers [1]. Theoretical models attribute this phenomenon to electron tunneling effects and propagation of lattice vibrations due to mechanical interactions between the electrodes, i.e., phonon transport [2]. Experimental difficulties in the nanoscale have prevented us from sufficiently understanding the heat transfer mechanisms.

We have developed a device to measure both thermal and electrical conductance across nanogap electrodes. The device comprises a suspended structure with Micro Electro Mechanical System (MEMS) based actuators to tune the gap distance. We observed increased thermal conductances in sufficiently separated nanogaps, even in the absence of electron tunneling, suggesting phonon transport as the dominant mechanism [3]. We will show the effects of electrode gap distance and temperature on heat transfer across the nanogap.

[1] M. Pascale et al., Appl. Phys. Lett. 122, 100501 (2023).
[2] T. Tokunaga et al., Phys. Rev. B 104, 125404 (2021).
[3] Y. Hanamura et al., Nanoscale, in press.

MM 27.9 Thu 12:30 H22

Hydrodynamics of Lorentz symmetric systems: a quantum Monte Carlo study — •Adrien Reingruber[1], Kitinan Pongsangangan[2], Fakher Assaad[1], and Maksim Ulybyshev[1] — [1]Universität Würzburg, Würzburg, Germany — [2]Mahidol University, Bangkok, Thailand

We present a study on the hydrodynamic behavior of charge current in a Lorentz symmetric sys- tem: graphene at charge-neutrality. The momentum flow is completely decoupled from the charge current in this regime, since the electrons and holes propagate in opposite directions with exactly equal distribution functions. Instead of Navier-Stokes equations for the velocity field, we derive sim- ilar equations directly for the charge current. This eliminates the need for any coupling between the velocity field and charge current to explain the experimentally observed hydrodynamic flow profiles in graphene at half-filling. In this framework, the current diffusion coefficient replaces viscosity. To support this, we performed an extensive quantum Monte Carlo study, directly simulating samples with disordered edges using the underlying microscopic interacting quantum Hamiltonian. For the first time, we observe hydrodynamic behavior of the charge current in such simulations, extract- ing current profiles and a current diffusion coefficient whose temperature dependence qualitatively agrees with predictions from Boltzmann transport theory.

MM 27.10 Thu 12:45 H22

Transport coefficients of Weyl semimetals: the contribution of plasmons — •Kitinan Pongsangangan — Mahidol University, Bangkok, Thailand

This work investigates the contribution of plasmon, a collective mode arising from the dynamical screening of the long-range coulomb interaction, to thermoelectric responses as well as shear viscosity of Weyl semimetals using Boltzmann-equation approach. We find that plasmons make a noticeable contribution to the thermal conductivity and shear viscosity in an appropriate temperature window. We propose that this effect could be potentially observed in, for example, TaAs and NbAs.

MM 28: Mechanical properties

Strengthening Mechanisms

Time: Thursday 10:15–11:30 Location: H23

MM 28.1 Thu 10:15 H23

Parameterising edge dislocation trajectories in Ni-based superalloys with uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry, United Kingdom

The extraordinary strength exhibited by Ni-based superalloys at high temperatures is attributed to the presence of nanoscale precipitates in their microstructure, which hinder dislocation motion. In our work, we study edge dislocation-precipitate interactions using Molecular Dynamics (MD) simulations with classical effective potentials. The motion of a pair of edge dislocations moving under shear between pure Face-Centred Cubic (FCC) Ni into Ni3Al with an L12 structure is simulated using MD, where Ni is used to represent an idealised γ solid solution phase and Ni3Al for the γ' precipitate phase. The obtained trajectories are parameterised and Differential Evolution Monte Carlo (DE-MC) is used to determine parameter distributions. These distributions are then used to quantify the uncertainty in the model outputs, namely the dislocations' positions and velocities. The present approach yields physically meaningful parameters and accordingly, offers a means of extracting quantitative information from the atomistic scale that can be used to inform larger length scale simulations of dislocations. Using DE-MC as a sampling approach also means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties.

MM 28.2 Thu 10:30 H23

Atomistic Modelling of Solid Solution Strengthening in the Mg-Al-Ca System — •Erik Bitzek and Marvin Poul — MPI SusMat, Düsseldorf, Germany

Solid solution strengthening is one of the most important strengthening mechanisms for engineering alloys. It is caused by solutes impeding the glide of dislocations and is therefore best studied using atomistic simulations. While the interaction strength of individual solute atoms with dislocations in Mg has been well-studied with density functional density (DFT) calculations, the combined impact of multiple solute species on dislocation glide has not been extensively investigated. Furthermore, the prediction of the critical resolved shear stress requires additionally a statistical treatment and a continuum elastic model for the dislocation line.

Here we present atomistic simulations of basal dislocations gliding in Mg with different concentrations of Al, Ca, and mixtures of Al and Ca. These large-scale simulations were enabled by a newly-developed machine learning interatomic potential that allows for near-DFT accuracy. Using MD/MC simulations of different heat treatments, we show that Al-Ca clusters can form, which influence the solid solution strengthening by reducing the concentrations of individual solutes and through an antagonistic effect of Al and Ca on the stress field of these clusters.

MM 28.3 Thu 10:45 H23

Normal stress effect on the slip system of Mg alloys with long-period stacking ordered structures — •Naoki Uemura[1] and Ryosuke Matsumoto[2] — [1]Nagamori Institute of Actuators, Kyoto University of Advanced Science, Kyoto, Japan — [2]Department of Mechanical and Electrical Systems Engineering, Faculty of Engineering, Kyoto University of Advanced Science, Kyoto, Japan

Mg alloys with long-period stacking, which have a unique structure with synchronized concentration modulation and structural modulation are attracting attention for their high strength. Various studies are currently being conducted to understand their high mechanical properties and plastic deformation behaviors. We investigated the tensile and compressive dependence of the stacking fault energy (SFE) by using first-principles calculations for the Mg-Y-Zn system, which is a typical LPSO-Mg alloy. As with hcp-Mg, the change in SFE due to tensile and compressive loading was greater on the basal plane than on the prismatic

plane. This work was supported by JST, CREST Grant Number JPMJCR2094, Japan.

MM 28.4 Thu 11:00 H23

Understanding crystal defects mechanisms with atomistic simulations and knowledge engineering — •Abril Azocar Guzman, Guojing Huang, and Stefan Sandfeld — Institute for Advanced Simulations, Materials Data Science and Informatics (IAS-9), Forschungszentrum Jülich GmbH, Aachen, Germany

Crystallographic defects play a key role for determining the physical properties of materials. Computational methods, such as density functional theory and molecular dynamics, have been widely used to investigate these defects and their mechanisms at the atomic scale. However, the application of these methods require increasingly complex workflows. To enable workflow and data reusability, as well as meaningful interpretation, it is crucial to ensure well-described (meta)data at each step of the workflow, from atomic structure to computed material properties. Our aim is to facilitate data-driven approaches in materials science by establishing semantic standards for representing material structures, including defects, simulation workflows, and calculated properties. Using this framework, datasets of crystal defects simulations can be generated in the form of a materials knowledge graph. We showcase the application for the study of hydrogen segregation at grain boundaries in iron and nickel, quantifying the influence of the local atomic environment on the energetics of the system. The resulting knowledge graph incorporates structure-property relationships and serves as a tool to understand defect mechanisms at the atomic scale. Additionally, it provides a robust data foundation for exploring the potential of emerging methods in the field of knowledge engineering.

MM 28.5 Thu 11:15 H23

Effect of Cold Work on the Microstructure and Properties of Hierarchical Nanoporous Metals — •Weiche Chang[1] and Shan Shi[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany,

Nanoporous metals with bicontinuous porous network, high specific surface area, and low density have shown promising applications as light-weight structural materials and high-performance functional materials in actuators, sensors, and various energy devices. Recently, monolithic hierarchical nanoporous gold (HNPG) has been tailor-made via a two-step dealloying method and has shown improved mechanical properties and much lower density than non-hierarchical nanoporous gold. The effects of ligament size and structural hierarchy on the strength of HNPG have also been well studied via macro- or micro-compression approaches. In this work, we further explore the role of cold working treatments before and after second step dealloying on the mechanical properties of HNPG using micropillar compression tests. Furthermore, HNPG with a controllable degree of anisotropy and a much wider range of solid fractions are obtained.

MM 29: Liquid and Amorphous Materials

Time: Thursday 12:00–12:45 Location: H10

MM 29.1 Thu 12:00 H10

Molecular Feuds and Fragment Tales: Exploring Cyanobiphenyl Liquid Crystals with Cryo Atom Probe Tomography — •Kuan Meng, Kang'an Wang, Sebastian Eich, and Guido Schmitz — Stuttgart University,Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

Liquid crystals exhibit the fascinating duality of liquid-like fluidity and solid-like long-range order, requiring nanoscale characterization techniques with high spatial resolution and chemical sensitivity. Atom probe tomography (APT) uniquely meets these requirements, offering unprecedented insights into the behavior of anisotropic organic molecules. This talk bridges liquid crystal science and APT by exploring cyanobiphenyl systems (5CB, 8CB, and 8OCB).

We investigated the field evaporation behaviors of these molecules, observing remarkable stability under high electric fields. Molecular signals dominated (90% for 5CB and 8CB, 70% for 8OCB), with fragmentation patterns influenced by oxygen atoms. The fragments were classified as alkyl chains, single phenyl derivatives, cyanobiphenyl residues, and cyano-hydrogen substitution pairs. Spatially, both molecular and fragment signals correlate strongly with laser orientation: fragmentation decreases from illuminated to shadowed regions, reflecting cleavage behavior under thermal gradient-induced field variations. Additionally, APT revealed the uniform mixing of 5CB and 8CB across various ratios, as well as the lattice plane of the crystal structure of pure 8CB. In the crystalline regions, we will discuss how the molecules field evaporate at specific angles relative to their intrinsic orientations.

MM 29.2 Thu 12:15 H10

Peptide Analysis at Atomic Resolution with Atom Probe Tomography — •Sakshi Sinha and Guido Schmitz — Department of Materials Physics, Institute of Material Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Atom Probe Tomography (APT) promise decisive advancements in nanoscale characterization of biomolecules, since it offers in principle single atom sensitivity in the study of organic molecular structures. In our experiments, we test the analysis of carnosine (β-alanylhistidine), in aqueous solution since water provides a natural biological environment. The investigated dipeptide is for example essential for brain and muscle function. By combining cryogenic sample preparation with advanced laser-pulsing techniques, APT enables three-dimensional mapping of carnosine's atomic composition and the distribution of various molecule fragments in the water matrix. Remarkably, the concentration of the solution controls the detected fragmentation behavior in the full range from single atoms to the full peptide molecule. So, the measurement conditions can be optimized to preferentially address the questions regarding the local stoichiometry or the different subunits of the molecule.

MM 29.3 Thu 12:30 H10

Fe self-diffusion in Fe-Al-Si melts - A combined ab initio molecular dynamics and experimental study — •Katharina Dammer[1], Fan Yang[1], Elke Sondermann[1], Florian Kargl[1], Andreas Meyer[1,2], and Noel Jakse[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut Laue-Langevin (ILL), 38042 Grenoble, France — [3]Université Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

Understanding the structural, dynamic and thermophysical properties of binary and ternary Al-Fe-Si alloys in the liquid and supercooled state before solidification is crucial to ensure the desired microstructure and therefore ideal product properties. With an increasing iron content in the alloy, the liquidus temperature increases and exceeds 1000°C for most ternary Al-Si-Fe alloys. At these high temperatures, experiments are more delicate to perform, making it challenging to obtain information on transport coefficients and (partial) structure factors.

We present a combined first principle-based molecular dynamics (AIMD) simulations and experimental study of Al-Fe melts. Measurements were performed using quasi elastic neutron scatting (QENS) to obtain the self-diffusion coefficients of Fe at different Al-Fe compositions as a function of temperature. We intend to achieve in the future an improved simulation scheme using machine learning that realistically covers a larger range of the phase diagram, which cannot be easily assessed with experiments.

MM 30: Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: H23

MM 30.1 Thu 11:45 H23

Untersuchungen des Bruchverhaltens im Bereich der Ultra-Langzeitfestigkeit von Federstählen — •Jörg Gollnick — THM, FB ME, Wiesenstr. 14, 35390 Gießen

In einer hochfrequenten resonanten Anwendung als Spiegel für Laserscanner werden Federstähle des Typs Ck101 im Grenzbereich belastet. Im Rahmen eines Forschungsvorhabens wurden die spezifischen Möglichkeiten untersucht, die Lebensdauer dieser Bauteile zu steigern. Bislang wurden nur unzureichende Lebensdauern erreicht.

Bemerkenswert war die Ausprägung des Versagensverhaltens, dass in Zusammenhang mit der Fertigungstechnologie einem Sprödbruch unter Mode III nach den bruchmechanischen Ansätzen gemäß Griffith entspricht. Aus der Erklärung der Schädigungen wurden weitere Möglichkeiten untersucht, die Lebensdauer nicht nur zu steigern sondern weiterhin die nach Paris-Erdogan zu erwartende

Dauerfestigkeit genau zu bestimmen.

Mit hohen Frequenzen im Bereich bis zu 10000kHz werden Bauteile bis zu 10 Milliarden Schwingungen im Grenzbereich betrieben. Eine mehrstufige Auswertung nach dem Treppenstufenverfahren zeigt, dass eine Auswertung in diesem Segment nicht nur möglich ist, sondern als geeignete Strategie angesehen werden darf, die Erkenntnisse der Ultra-Langzeitfestigkeit diesbezüglich zu erweitern.

Weitergehende Versuche werden vorgestellt.

Falls gewünscht kann der Vortrag und Beitrag gerne auch auf englisch abgefasst werden.

MM 30.2 Thu 12:00 H23

Searching for ferroelectric porous metal organic frameworks using machine-learning and Monte-Carlo-simulations — •Thomas Bergler[1,2], Harald Oberhofer[1,2], and Dirk Volkmer[3] — [1]University of Bayreuth, Germany — [2]Bavarian Center for Battery Technologies — [3]University of Augsburg, Germany

Metal organic frameworks (MOFs) have so far found a number of successful applications, among them as storage for gasses and filter for gas mixtures. So far these mostly incorporated them as passive materials, but recent research points the way towards a more active role, possibly through the external manipulation of the materials' internal properties. One recent example for such a property is the susceptibility of the lattice parameters of a number of MOFs towards electric fields. Inspired by this, the aim of our project is to further investigate this behavior and potentially design ferroelectric MOFs. Using a hierarchy of Monte-Carlo-simulations aided by Machine-Learning (ML) we sample the design space MOFs augmented by rotatable polar groups. In succession, we first sample a huge space of rotors in a simplified point-dipole model. A selection of thus uncovered MOF geometries is then investigated with a specially parameterized atomistic model to confirm earlier predictions. Using this data, an ML model is trained to predict the dielectric properties of such polar rotor-augmented MOFs. The best candidates extracted with this procedure are finally evaluated with density functional theory. MOF geometries surviving this funnel-like approach can finally be checked experimentally for a variety of applications, ranging from data-storage to gas nano-funnelling.

MM 30.3 Thu 12:15 H23

Atomic Scale Insights into A-site Deficient Perovskite Catalysts: $La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ — •Roham Talei Jeid — Institute for Material Physics, University of Stuttgart, Deutschland

This study investigates the atomic-scale properties of the A-site-deficient perovskite catalyst $La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ (La07FM), emphasizing the role of iron oxide (FeO) in redox reactions. Advanced techniques, including scanning transmission electron microscopy (STEM), energy-dispersive X-ray spectroscopy (EDXS), and a custom Python-based strain mapping tool linked to chemical analysis reveal nanoscale La deficiencies and Fe enrichments at grain boundaries as key for catalytic activity. Post-catalysis studies identify Fe-rich, FeO-like nanoparticles at strained, defective grain boundaries, underscoring the impact of A-site deficiencies on performance in NOx denitrification (DeNOx). These findings highlight how A-site deficiencies and Fe-rich nanostructures enhance catalytic efficiency, offering broader insights into electrochemistry and heterogeneous catalysis.

MM 30.4 Thu 12:30 H23

Use of LiMn2O4 for switching applications in silicon waveguide circuits — •Vinit Agarwalla[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Insitut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237, Düsseldorf

Lithium ion intercalation and deintercalation play an important role in determining the storage performance of cathode materials for lithium ion batteries. However, intercalation of ions also regularly modifies electron structure and optical properties of the materials. This study explores the possibility of exploiting the optical properties of the cathode material LiMn2O4 (LMO) for optical switching applications in silicon waveguide circuits. For this, LMO is coated as a cladding around Si waveguides suitable for the 1550 nm wavelength of optical telecommunication. To stabilize the interface a thin intermediate Si oxide film is tested as an optical transparent reaction barrier. Our TEM images and the EDX mapping show that the Si does not react with LMO for oxide layer thickness as low as 10 nm. Previous work has explored the change in resonance wavelength of reflectance spectra with lithiation/ delithiation in the visible region[1]. In extension, we have measured FTIR reflectance spectra in the near IR region. They show a fairly continuous spectrum between visible and IR region with reflectance going to 100 % and a gradual shift in resonance wavelength in the IR region with Li intercalation. The optical response on light transmission along the wave guides has been determined in dependence on the degree of lithiation.

[1]. DOI:10.1002/adom.201701362

MM 30.5 Thu 12:45 H23

Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art — •Andrea Fantin, Anna Maria Manzoni, Reza Darvishi Kamachali, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding the intricate atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties for diverse applications. This contribution tries to provide a brief overview of the state-of-the-art experimental techniques employed to probe local lattice distortions and chemical short-range order in HEAs, with specific focus on X-ray absorption spectroscopy and total scattering. The main problem to overcome in multi-component alloys is the intrinsic reduced scattering contrast between nearest neighbors in the periodic table, which limits the amount of information that can be extracted from the data. This statement remains valid when employing transmission electron microscopy, as well. Specific examples such as the Al-Co-Cr-Cu-Fe-Ni fcc system [Small Science 4(2), 2300225 (2024); Nature Communications 15(1), 7815 (2024)] and the MoNbTaW bcc system [Materials Research Letters 12(5), 346-354 (2024)] will be outlined. It comes clear that rather than specific techniques, it is only the combination of several experiments, supported by simulations and multi-technique simultaneous structural refinements, that can help in disentangling the different contributions to performances of each element within the alloy solid solution, with strength and weaknesses depending on the specific experimental measurements.

MM 31: Data-driven Materials Science: Big Data and Worksflows

Materials Properties and more

Time: Thursday 15:00–18:00 Location: H10

MM 31.1 Thu 15:00 H10

Thermodynamic stability of the materials in the Materials Cloud three-dimensional crystals database (MC3D) — •Timo Reents[1,2], Marnik Bercx[1], and Giovanni Pizzi[1,2] — [1]Laboratory for Materials Simulations (LMS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institut (PSI), CH-5232 Villigen PSI, Switzerland — [2]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

High-throughput studies based on ab initio methods such as Density Functional Theory (DFT) enable the analysis of physical properties across a broad chemical space. Here, we present the Materials Cloud three-dimensional crystals database (MC3D), a DFT optimized and curated structural database of experimentally known inorganic crystals. All calculations are managed and driven by the AiiDA [1, 2] workflow engine, allowing to browse the full provenance graph and to share the results in the Materials Cloud [3]. We introduce the protocols behind MC3D, the new frontend, and we then focus on the thermodynamic stability. To improve the agreement between the theoretical and experimental thermodynamic stability, we apply empirical [4] and machine-learning [5] based corrections, and improve upon them, discussing the agreement with experimental data on stability.

[1] Huber, S.P. et al., Sci Data, 2020, 7, 300.
[2] Uhrin, M. et al., Comp. Mat. Sci., 2021, 187, 110086.
[3] Talirz, L. et al., Sci Data 7, 299 (2020).
[4] Stevanović, V. et al., Phys. Rev. B, 2012, 85, 115104.
[5] Gong, S. et al., JACS Au, 2022, 2, 1964-1977.

MM 31.2 Thu 15:15 H10

high-throughput computation and machine learning modeling of magnetic moments and Mössbauer spectroscopy for Fe-based intermetallics — •Bo Zhao, Xiankang Tang, and Hongbin Zhang — Institute of Materials Science, Technische Universität Darmstadt, Otto-Berndt-Str. 3, 64287 Darmstadt, Germany

Understanding the relationship between the local crystalline environment and magnetic properties is a fundamental challenge in condensed matter physics and materials science. This study explores this relationship in Fe-based intermetallic compounds, focusing on the magnetic moments and Mössbauer parameters of iron atoms, including the isomer shift, electric field gradient, and magnetic hyperfine field. High-throughput calculations and machine learning techniques are employed to predict magnetic properties based on local atomic structures, using smooth overlap of atomic positions (SOAP) as local descriptors. The results first reveal the sparsity of relevant materials in the Materials Project database. Lever-

aging high-throughput, system-specific data, the study demonstrates strong correlations between local atomic environments and magnetic properties, achieved through machine learning models. Furthermore, the limitations of symmetry-invariant descriptors in predicting tensor-like properties, such as the electric field gradient, are highlighted. By incorporating a graph-based equivariant autoencoder, the model achieves improved predictions by effectively capturing the symmetry of local environments.

MM 31.3 Thu 15:30 H10

Advanced Machine Learning of ^{17}O NMR in Non-Magnetic Oxides: High-Throughput Calculation, Prototype Compound Analysis, and Transfer Learning — •Zhiyuan Li, Bo Zhao, Hongbin Zhang, and Yixuan Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt Germany

The study of ^{17}O NMR spectroscopy is crucial for understanding the local structure of oxides, where the naturally occurring NMR-active oxygen isotope, ^{17}O, provides unique insights into local environments due to its large chemical shift range and quadrupolar nature. In this work, we present a high-throughput workflow integrating AiiDa and CASTEP to calculate the NMR parameters of over 7100 compounds from the Materials Pro ject database, followed by utilizing machine learning models to predict ^{17}O NMR parameters. Furthermore, taking $BaTiO_3$ as an example, we identify prototypical ABO_3 crystal structures, construct $BaTiO_3$ analogs via substitution, perform ab initio molecular dynamics simulations to generate 3000 perturbated structures, and evaluate the NMR parameters. The results of our machine learning modeling with such additional dataset reveal that incorporating perturbated structures enhances the accuracy of the machine learning model. Moreover, by leveraging transfer learning, using previously trained model from our high-throughput dataset, the predictivity for the newly generated $BaTiO_3$ analogs can be further improved.

MM 31.4 Thu 15:45 H10

Advancing chemical shielding predictions in organic solids — •Matthias Kellner and Michele Ceriotti — École Polytech- nique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In this presentation, we showcase our recent advancements in machine learning for predicting chemical shieldings in organic solids. Leveraging symmetry-adapted machine learning models, our updated infrastructure facilitates the accurate prediction of chemical shielding anisotropy and enables structure optimization driven by chemical shielding gradients. We will highlight how integrating machine learning potentials with property prediction models provides unique insights into atomistic processes, offering a powerful framework for exploring the complex behavior of organic materials.

MM 31.5 Thu 16:00 H10

Active learning workflow for mixed-halide perovskite stability and electronic band-structure — •Tim Bechtel[1,2], Santiago Rigamonti[1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Germany — [2]Max Planck Institute for Solid-State Research, Stuttgart, Germany

Mixed-halide perovskites are promising materials for stable and efficient light harvesting and emission applications, and their composition can be tailored to match relevant regions of the light spectrum [1]. Theoretical predictions from first-principles calculations can provide insight into stability, ground-state properties, and electronic structure [2,3]. Comparison with experimental results for "real" materials is, however, challenging. For example, the consideration of chemical (dis)order requires huge supercells, which is computationally out of reach with state-of-the-art methodology. For the family of $CsPb(Cl_xBr_yI_{1-x-y})_3$ compounds, we bridge this gap with an active learning workflow. It is based on a fine-tuned machine learning interatomic potential [4] that interpolates between already seen compositions, and actively explores new composition ranges. This approach allows for data-efficient predictions of stability through finite-temperature phase diagrams and optical properties for a wide range of compositions.

[1] H. Näsström, PhD Thesis, https://doi.org/10.18452/24939
[2] F. Pan, *et al.*; https://doi.org/10.1021/acs.chemmater.4c00571
[3] J. Laakso, *et al.*; https://doi.org/10.1103/PhysRevMaterials.6.113801
[4] I. Batatia, *et al.*; https://doi.org/10.48550/arXiv.2401.00096

15 min. break

MM 31.6 Thu 16:30 H10

Towards Multi-Fidelity Machine Learning Using Robust Density Functional Tight Binding Models — •Mengnan Cui[1,2], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of Bayreuth, Physical Chemistry V: Theory and Machine Learning

Machine learning has revolutionized the atomistic simulation of molecules and materials, offering unparalleled computational speed with high accuracy. However, its performance depends heavily on the quality and quantity of training data, presenting challenges due to the scarcity of high-fidelity datasets (beyond semilocal DFT). This study investigates transfer learning (TL) across multiple fidelities for molecules and solids, examining the role of fidelity levels and configuration/chemical space overlap in pre-training and fine-tuning. This reveals negative transfer driven by noise from low-fidelity methods like DFTB, which can significantly impact fine-tuned models. Despite this, multi-fidelity approaches consistently outperform single-fidelity learning and, in some cases, even surpass TL based on foundation models by leveraging an optimal overlap of pre-training and fine-tuning chemical spaces.

MM 31.7 Thu 16:45 H10

Enhancing FAIR Data Management with Automated Visualization of Calculations — •N. Daelman[1], E. Boydas[1], B. Mohr[1], J.M. Pizarro[1], T. Bereau[2], C. Draxl[1], L.M. Ghiringhelli[3], M. Girard[4], D. Usvyat[5], R. Valenti[6], S. Botti[7], and J.F. Rudzinski[1] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]Dept. of Mater. Sci. and Eng., FAU Erlangen — [4]Max Planck Inst. for Poly. Res., Mainz — [5]Inst. für Chem., HU Berlin — [6]Inst. für Theor. Phys., GU Frankfurt/M — [7]RC-FEMS, Ruhr Uni. Bochum

In contrast to data science packages, first-degree data post-processing tends to lock people into silos built around a particular simulation software. NOMAD [nomad-lab.eu][1] is an open-source and community-driven data infrastructure that breaks open these silos by extracting scientific data from over 60 code packages into a code-agnostic schema within a research data management (RDM) ecosystem [2]. This talk showcases NOMAD*s new visualization features at various levels of RDM. At the level of individual calculations, NOMAD provides now more detailed electronic structure visualizations and fast, dynamic rendering of heavy files. Automated visualization does not imply, however, a lack of customizability. NOMAD provides support for tailored figures and larger-scale specialization via an accessible plugin-based system. At the level of research projects, NOMAD allows for quick monitoring of the data coverage via a fully customizable dashboard.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 31.8 Thu 17:00 H10

NOMAD CAMELS: An Open-Source Solution for Creating FAIR Data from Experiments — •Alexander Fuchs[1,2], Johannes Lehmeyer[1,2], Michael Krieger[1,2], and Heiko Weber[1,2] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]FAIRmat Consortium

NOMAD CAMELS is a configurable open-source measurement software. It is suited to control experiments and records fully self-describing experimental data. It has its origins in the field of experimental physics where a wide variety of measurement instruments are used in frequently changing experimental setups and measurement protocols. CAMELS provides a graphical user interface (GUI) which allows the user to configure experiments without the need of programming skills or deep understanding of instrument communication. CAMELS translates user-defined measurement protocols into stand-alone executable Python code for full transparency of the actual measurement sequences. Metadata inflow from Electronic Lab Notebooks (ELNs) and data output into such is well supported for a seamless workflow. CAMELS is designed with a focus on full recording of data and metadata aligned with the NeXus ontology. When shared with others, data produced with CAMELS allow full understanding of the measurement and the resulting data in accordance with the FAIR principles.

MM 31.9 Thu 17:15 H10

Databases of Fermi surfaces and de Haas-van Alphen oscillation frequencies from first principles simulations — •Nataliya Paulish[1], Junfeng Qiao[2], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Fermi surface (FS) of a metal separates occupied from unoccupied electronic states. Knowing its shape is crucial to understanding the electronic properties of the material. Accurate simulation of the FS requires a very dense sampling of the Brillouin zone, and thus direct density functional theory (DFT) calculations are limited by their computational cost. To overcome this difficulty, we use interpolation from a basis of spatially localized projectability disentangled Wannier functions (PDWFs) - a recently developed algorithm for automated Wannierization [1]. Using this algorithm, FSs were generated for over 7'000 inorganic metals. We also computed de Haas-van Alphen frequencies associated with each FS, enabling direct comparison of our simulations with experiments. The procedure is fully automated using the AiiDA workflow engine [2]. Our database will be published openly online and browsable on the Materials Cloud MC3D section (https://mc3d.materialscloud.org).

[1] J. Qiao, G. Pizzi, N. Marzari, npj Comput Mater 9, 208 (2023)
[2] S. P. Huber et al., Scientific data 7, 1 (2020)

MM 31.10 Thu 17:30 H10

A systematic benchmark of G_0W_0 calculations — •Marc Thieme, Max Grossmann, Malte Grunert, and Erich Runge — Technische Universität Ilmenau, Ilmenau, Germany

Accurate and efficient ab initio electronic structure calculations of semiconductors and insulators are a prerequisite for building large, high-quality databases for machine learning (ML). However, the "optimal" choice (speed vs. accuracy) of the approximations used, i.e. the exchange-correlation (XC) functional for density functional theory (DFT) calculations or a particular many-body perturbation theory, remains unclear. A systematic benchmark of band gaps of solids using several different DFT XC functionals by Borlido et al [1,2] showed that hybrid functionals perform exceptionally well and seem to be the functionals of choice. The present study addresses the question of whether G_0W_0 calculations provide a sufficient increase in accuracy to justify their increased computational cost compared to simpler DFT calculations with hybrid functionals. We calculate the band gaps for about 300 materials using the G_0W_0 method starting from LDA/PBE DFT calculations. The deviations between G_0W_0 and experimental band gaps are systematically compared with those of the best hybrid functionals

[1] Borlido et al., J. Chem. Theory Comput. 15, 9 (2019)
[2] Borlido et al., npj Comput. Mater. 6, 96 (2020)

MM 31.11 Thu 17:45 H10

Machine Learning-Assisted Design of Magnetic Materials: Predicting Properties for not purely ternary $Nd_2Fe_{14}B$ — •Manuel Enns, Daniel Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

$Nd_2Fe_{14}B$-based hard-magnetic materials are widely used for strong permanent magnets. Their re-use and recycling after the end of the magnet's life cycle opens the question of the degradation of the magnetic properties due to the incorporation of unintentional impurity elements originating from the recycling procedures. In this talk, we present a data-mining and machine-learning (ML) approach using kernel-based learning methods to predict the influence of impurity atoms in $Nd_2Fe_{14}B$-based materials. The magnetic-property data used for training and testing the ML model were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. We demonstrate that our ML approach can accurately predict the saturation magnetization, the uniaxial anisotropy constant, and the formation energy for $Nd_2Fe_{14}B$ with impurities added by recycling.

MM 32: Transport in Materials: Diffusion, Charge or Heat Conduction

Battery Materials, Effects of Defects

Time: Thursday 15:00–17:45 Location: H22

MM 32.1 Thu 15:00 H22

Kinetic analysis of lithium transport in silicon anode using operando optical microscopy — •Shihao Wei, Monica Mead, Yug Joshi, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Germany

The performance of silicon(Si) anodes in lithium(Li)-ion batteries is significantly influenced by the kinetics of Li insertion and migration, particularly at the phase boundaries formed during cycling. Traditional techniques, such as EIS, SIMS, and NMR, are limited in providing detailed kinetic information at internal phase boundaries. This study proposes a novel approach to measure Li migration across phase boundaries in Si-based anodes. First, reflectance spectroscopy is employed to examine the optical response of Si thin films sputtered onto copper current collectors at various charge states, revealing reversible electrochromic behavior and the effect of Li content on spectral characteristics. Based on this, operando optical microscopy is developed to track the lithiation front, by using SU-8 photoresist as a patterning tool. The lithiation process is predominantly governed by diffusion-controlled parabolic growth, with minimal evidence of interface-controlled linear growth. Interestingly, applying the same method during delithiation, a significant slow-down of delithiation front appears. In addition, temperature-dependent diffusion behaviors are explored, quantified with an Arrhenius-like model. By altering the geometry of the photoresist patterns, the transport dynamics are analyzed under two distinct scenarios: a 1D semi-infinite planar configuration and a 2D finite circular configuration.

MM 32.2 Thu 15:15 H22

Crossing Boundaries? Probing Ion Conduction across Interfaces in Solid Electrolytes using Computational NMR Spectroscopy — •Tabea Huss[1], Federico Civaia[1], Simone Köcher[2,1], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH

Grain boundaries are critical, yet poorly understood factors affecting ion transport in solid-state electrolytes. The spin-alignment echo (SAE) nuclear magnetic resonance (NMR) experiment is a versatile tool to study the manifold transport processes of quadrupolar ions in these solid state materials. However, assigning the measured decay coefficients to physical transport phenomena often proves to be challenging. We have previously demonstrated that we can replicate the SAE experiment for bulk materials using a multi-scale machine learning framework.[1] This framework simulates both the atomic structure and dynamics of solid-state systems, along with generating solid state NMR observables. Our approach has already allowed us to predict electric field gradients over molecular dynamics trajectories and use them to compute decay constants that align with ion hopping times in bulk lithium thiophosphates. In this work, we extend our methodology to explore ion transport in grain boundary structures of the solid-state electrolyte $Li_{10}GeP_2S_{12}$. We extract SAE time constants and differentiate among various decay processes, advancing another step towards direct comparability with experimental results.

[1] A. F. Harper *et al.*, Faraday Discuss., (2024).

MM 32.3 Thu 15:30 H22

Theoretical Investigation of Electron Transport in the $LiMnPO_4$ Battery Material — •Franz Winkler[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technologies

Developing better batteries and thus battery materials is a crucial step in humanity's urgent energy transition. Thereby, theory can play an important role in characterizing and understanding the properties of the involved materials. In this contribution we present our work on $LiMnPO_4$ which exhibits some desirable properties such as a high energy density and a high potential and thus operating voltage. However, its adoption is hampered by a bad electronic conductivity.

Using electronic density functional theory (DFT), we compute the parameters of conductivity for both band- and polaronic hopping transport, to identify possible bottlenecks and thus possible future improvements of the material. For this we consider both the paramagnetic and antiferromagnetic configuration of $LiMnPO_4$. Due to the well known failures of plain semi-local DFT to represent both localized polaronic configurations and complex spin structures, we thereby use Hubbard-corrected DFT for the bulk of our calculations and range-separated hybrid DFT as a reference. Improvements suggested by our theoretical results can then help experimental collaborators to establish synthetic routes towards more efficient battery materials.

MM 32.4 Thu 15:45 H22

Lithium transport in Lithium Manganese Oxide as a function of temperature, concentration and grain size measured by operando optical microscopy — •Monica Mead[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf

Common methods for the determination of diffusion coefficients in electrode materials require critical interpretation, as their formal derivations rely on restrictive assumptions (e.g. galvanostatic/potentiostatic intermittent titration technique (G/PITT), electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV)). Alternatively, an optical method for studying ion transport in battery electrodes through operando microscopy can be applied. Here, the measurement of diffusion coefficients is done on thin films in lateral diffusion geometry and is based on an optical response upon ion intercalation. This allows measuring the diffusion coefficient as a function of temperature, concentration and grain size. In this work, diffusion of Li ions in Lithium Manganese Oxide (LMO) is studied by operando microscopy. The temperature dependence of the diffusion coefficient, providing the activation energy via the Arrhenius relation, and the diffusion coefficients for the bulk/grain boundaries of LMO can be determined. Additionally, it is possible to find the concentration dependence by an inverse Boltzmann-Matano method on concentration profiles derived from the intensity profiles along the diffusion direction.

MM 32.5 Thu 16:00 H22

Charge Transport Simulation in the High State-Of-Charge using Kinetic Monte Carlo — •Roya Ebrahimi Viand, Chiara Panosetti, Christoph Scheurer, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

Understanding charge transport in solids is crucial for improving energy storage systems such as lithium-ion batteries. The diffusion of particles in solid materials typically involves rare transitions between low-energy sites, making kinetic Monte Carlo (kMC) an effective tool for studying the long-time dynamics. To address the computational challenges posed by long-range Coulomb interactions, we utilize fast rules for updating the process rates at each kMC step. We investigate ion transport on an isotropic rectangular lattice as well as in lithium graphite structures at high states of charge. We find that small changes in the ion

concentration can significantly influence ion mobility, depending on temperature and dielectric response. This happens near stoichiometric concentrations, where the ions freeze in a Coulomb superlattice where effective motion is energetically uphill. Introducing defects or excess ions then opens effective pathways for diffusion. Finally, we discuss the possibility of multiple quasi-stationary states manifesting in different mobilities under the same applied conditions and concentrations.

15 min. break

MM 32.6 Thu 16:30 H22

Electrical characterization of the gate length dependence in graphene field-effect transistors — •Daniel Nickel[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP - Leibnitz Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

Integrating graphene into silicon complementary metal-oxide semiconductor technology for electronic and optoelectronic applications holds great promise but faces challenges such as limited graphene mobility. This work addresses this limitation by using graphene field-effect transistors (GFETs) to analyze the influence of fabrication parameters on the electrical properties of graphene and to investigate the gate length dependence of sheet mobilities at T = 300 K. The GFET devices are fabricated with a wolfram back-gate on a 200 mm SiO_2/Si wafer, transferring chemical vapor deposition-grown graphene, patterning it, and forming graphene channel contacts with Pd/Au and Ni. The Dirac point is well detected in electrical measurements, indicating the transition between p- and n-type conduction. Graphene mobility is evaluated using the transconductance method and total resistance fit, revealing peak mobilities of μ_p = 715 cm^2/Vs for the p-branch and μ_n = 986 cm^2/Vs for the n-branch, with dependencies on channel length and contact metals used. Funding was provided by the EU's Horizon 2020 research and innovation program under the Graphene Flagship grant agreement no. 101189797.

MM 32.7 Thu 16:45 H22

Structural and electronic impact of defective sites and their effects on the thermoelectric properties of scandium nitride thin films — •Luigi Cigarini, Urszula Danuta Wdowik, and Dominik Legut — IT4Innovations, VŠB Technical University of Ostrava, 17. listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

The Landauer model provides a theoretical tool to understand the electronic transport mechanisms that deeply govern at the atomic scale the thermoelectric conversion of interesting materials. Transition metals nitrides are currently studied for potential applications in energy conversion. Modeling the effects on electronic transport that result from the electronic and structural modifications produced by oxygen impurities and spatial vacancies in scandium nitride (ScN), we propose a theoretical interpretation for new experimental results revealing a strong dependence of the thermoelectric properties of ScN thin films on procedural changes during their fabrication. We find that the thermoelectric properties of ScN are actually decisively determined by the structural and electronic factors caused by the presence of these defects or impurities. Evaluating to what extent these material's overall properties are influenced by these features necessarily requires a theoretical approach. This is particularly true as the presence of oxygen, which proves to be a decisive factor, is extremely difficult to control in standard fabrication processes and experimental conditions. The results presented in this contribution demonstrate the potential of this theoretical approach in studying the thermoelectric properties of these materials uncovering future strategies for improvement.

MM 32.8 Thu 17:00 H22

Helium Interaction with Atomic Level Defects in TungstenStudied by Positron Annihilation Spectroscopy — •Vassily Vadimovitch Burwitz[1,2], Annemarie Kärcher[1,3], Maik Butterling[4], Eric Hirschmann[4], Emma Huntley[2], Adrian Langrehr[1,2], Maciej Oskar Liedke[4], Lucian Mathes[1,2], Thomas Schwarz-Selinger[3], Christoph Springl[1,2], Monia Vadrucci[5,6], Andreas Wagner[4], and Christoph Hugenschmidt[2] — [1]TU München, School of Natural Sciences, Physikdepartment — [2]TU München, MLZ — [3]MPI für Plasmaphysik, Garching — [4]HZDR, Institute of Radiation Physics — [5]ENEA, Development of Particle Accelerators and Medical Applications, Frascati (RM), Italy — [6]Italian Space Agency, Science and Innovation Directorate, Rome

Understanding the type and evolution of lattice defects in tungsten (W) is of interest in nuclear fusion materials research. We therefore investigated W(111) mono-crystals by positron annihilation Doppler-broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS). Both complementary methods are sensitive tools for the examination of the defect type and concentration. The literature currently lacks conclusive experimental work regarding the influence of He decoration of vacancies on PAS. We therefore irradiated samples by 4.5 MeV electrons to different damage levels in order to specifically produce mono-vacancies in W. We will present DBS and PALS measurements, both performed with a slow positron beam, before and after plasma loading with 50 eV He ions. The implantation energy is chosen low enough to prevent displacement damage.

MM 32.9 Thu 17:15 H22

Formation energies and charge transition levels of charged point defects in Hematite — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

Hematite (Fe_2O_3), an iron oxide fundamental to the process of iron ore reduction, exhibits rich defect physics and off-stoichiometric features, as iron can occur as either Fe^{3+} and Fe^{2+}. Charged point defects and the associated Fe^{2+}/Fe^{3+} transitions play an important role in phenomena such as thermodynamic stability, phase transitions between iron oxides, and electronic structure modulation. In order to correctly account for these effects in the prediction of defect equilibria, phase diagrams, diffusion, and related properties, a robust framework for understanding defect thermodynamics and constructing a comprehensive defect model at the ab initio level is essential. Here, we employ DFT+U as an efficient tool for studying strongly correlated systems. In view of the delocalization error of standard functionals, DFT+U is crucial to investigate Fe^{2+} ions as distinct species. Moreover, it systematically opens the band gap of the bulk iron oxides. Since Hubbard U parameter has a direct influence on the band structure and Fe-related defect states in the band gap, we investigate the impact of U values on the computed formation energies of vacancies and interstitials. Our results show that the defect formation energies have a surprisingly weak dependence on U, thus allowing reliable predictions. We analyze the electronic structures of the defects in detail to uncover the underlying physical mechanisms.

MM 32.10 Thu 17:30 H22

Contribution of damped collective modes to thermopower in the strange metal phase of cuprates — •Giovanni Mirarchi[1], Sergio Caprara[2,3], Carlo Di Castro[2], Götz Seibold[4], and Marco Grilli[2,3] — [1]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Dipartimento di Fisica, Sapienza Università di Roma, P. le Aldo Moro 5, 00185 Roma, Italy — [3]ISC-CNR, Unità di Roma Sapienza, P. le Aldo Moro 5, 00185 Roma, Italy — [4]Institut für Physik, BTU Cottbus-Senftenberg - PBox 101344, D-03013 Cottbus, Germany

The strange-metal behavior, which is still an unsolved problem in condensed matter physics, is typically signaled by anomalies in thermodynamic and transport properties, including the famous linear-in-temperature resistivity [1]. The best-known case of strange-metal behavior in literature is that of high-temperature superconducting cuprates, whose strange-metal phase seems to always be accompanied by some kind of dynamical charge order [2]. Based on the experimental evidence of damped short-ranged charge density collective modes in the strange-metal phase of cuprates [3], we propose a scenario in which these collective modes can affect the phenomenology of this phase by interacting with electrons and by directly contributing to thermodynamics and transport [4]. In this talk, the concept of heat current in the presence of damping is discussed and used to describe the Seebeck effect in cuprates through a mechanism analogous to phonon drag. [1] Nat. Phys. 15, 142-147 (2019). [2] Science 337, 821 (2012). [3] Science 365, 906-910 (2019). [4] Commun. Phys. 5, 10 (2022).

MM 33: Invited Talk: P. Sonnweber-Ribic

Time: Friday 9:30–10:00 Location: H10

Invited Talk MM 33.1 Fri 9:30 H10

Fatigue in steels: Micromechanical modelling of cyclic damage — •Petra Sonnweber-Ribic[1], Alexandra Stark[1], and Christian Elsässer[2] — [1]Robert Bosch GmbH, Renningen — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg

Fatigue is a common phenomenon in engineering structures and can lead to unexpected failures, especially in critical components such as aircrafts, trains, and automotive parts. Understanding the mechanisms behind fatigue is crucial for ensuring the safety and reliability of these structures. A specific challenge of fatigue lies in the difficulty of external detection, as the initial stages of fatigue

damage manifest as highly localized processes within specific microstructural domains.

The micromechanical modelling offers a method for predicting fatigue properties and achieving a more profound comprehension of damage and relevant micromechanical parameters. Initially, this is based on the representation of the underlying microstructure of the material and the description of local plastic deformation using the crystal plasticity method. This approach has been successfully employed in industrial environment to assess the role of different metallographic phases in relation to local cyclic damage, among other applications.

Subsequently, this methodology can be enhanced by integrating a hydrogen diffusion approach and advanced damage models to consider the influence of hydrogen on fatigue damage mechanisms. The relevance of different influencing factors is analyzed based on selected examples.

MM 34: Development of Calculation Methods

Atomic Structure, Quantum Effects

Time: Friday 10:15–12:15 Location: H10

MM 34.1 Fri 10:15 H10

Enhancing 3D Volume Reconstruction in Atom Probe Tomography through Curvature-Based Tip Shape Analysis — Sebastian Eich and •Guido Schmitz — Department for Materials Physics, Institute for Materials Science, University of Stuttgart

Atom Probe Tomography (APT) provides chemical analysis of nanometric volumes with single-atom sensitivity in 3D. Traditionally, reconstruction assumes a hemispherical tip shape, which can lead to significant distortions, especially due to local magnification effects.

Instead of relying on in-situ correlative microscopy, we propose a numerical method to extract the emitter shape from the event density statistics on the 2D detector plane. This method is based on the fundamental relationship between event density and the local Gaussian curvature of the tip surface, with no mathematical restrictions other than convexity. By knowing the curvature and assuming suitable boundary conditions, the surface profile can be uniquely reconstructed, bypassing the need for a hemispherical assumption.

The method is implemented as an easy-to-use Python module, which will be demonstrated using various simulated and experimental datasets involving complex tip shapes. This approach significantly reduces the local magnification effects at material interfaces with contrasting evaporation thresholds and is expected to improve the accuracy of atom probe reconstructions.

MM 34.2 Fri 10:30 H10

Sum frequency generation from real-time simulation in 2D crystals — •Mike Nico Pionteck[1], Myrta Grüning[2,3], Simone Sanna[1], and Claudio Attaccalite[3,4] — [1]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany — [2]School of Mathematics and Physics, Queen's University Belfast, United Kingdom — [3]European Theoretical Spectroscopy Facilities (ETSF) — [4]CNRS/Aix-Marseille Université, Centre Interdisciplinaire de Nanoscience de Marseille UMR 7325 Campus de Luminy, France

Sum and difference frequency generation (SFG, DFG) are powerful experimental techniques which involve the interaction of two laser with frequency ω_1 and ω_2, generating an output beam with frequency $\omega = \omega_1 \pm \omega_2$ as second-order nonlinear response. These techniques are widely used to study 2D materials, providing complementary insights to those obtained from infrared and Raman spectroscopy.

We present an implementation of SFG and DFG within the Yambo code [1], based on real-time time-dependent adiabatic GW (TD-aGW). To account for local field effects and electron-hole interactions, our approach reduces to the Bethe-Salpeter equation (BSE) in the linear limit regime. We demonstrate this framework by calculating SFG and DFG signatures in h-BN and MoS_2. Furthermore, the method enables the extraction of higher-order response functions (e.g. TPA). This work establishes a first-principles approach to nonlinear optics, enabling investigations of optical responses of bulk materials with high versatility.

[1] D. Sangalli *et al.*, J. Phys. Condens. Matter **31**, 325902 (2019).

MM 34.3 Fri 10:45 H10

Ab initio calculations of longitudinal electrical conductivity using a Wannier-based coherent potential approximation — •Shota Namerikawa and Takashi Koretsune — Department of Physics, Tohoku University, Sendai, Japan

We present a longitudinal electrical conductivity calculation method for disordered alloys applicable from a wide range of density functional theory (DFT) codes based on the first-principles Wannier-based coherent potential approximation (Wannier-CPA). For evaluation of electrical conductivity, we employ two complementary methods; the Kubo-Greenwood formula and numerical analytic continuation of the current-current correlation function. We apply the developed method to Ag-Pd alloys and find that the results obtained by the Wannier-CPA reasonably reproduce previous studies by the well-established CPA implementation based on the Korringa-Kohn-Rostoker Green*s function method (KKR-CPA).

MM 34.4 Fri 11:00 H10

Ab-initio-based analysis of phonon contributions to negative thermal expansion of *a*-tin — •Petr Čípek[1,2], Jana Pavlů[2], Martin Friák[1], and Alena Michalcová[3] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Rep. — [2]Dept. Chem., Masaryk Uni., Brno, Czech Rep. — [3]Dept. Met. Corr. Eng., Uni. Chem. Technol. Prague, Czech Rep.

We applied quantum-mechanical calculations to investigate tin's thermodynamic and dynamic stability in its various allotropic forms. Focusing specifically on the *a*-Sn, our results showed a negative thermal expansion within the temperature range from T = 0 K to T = 45 K. No similar phenomenon appears in spectra of other allotropic modifications of tin. That means that the origin of this behaviour is connected to the diamond structure of alpha tin. We investigated the behaviour of the Grüneisen constant of *a*-tin in reciprocal space to explain the causes of this phenomenon. There are interesting temperature-dependent contributions of individual phonon modes from different k-points in the reciprocal space. In particular, these contributions are negative at all studied temperatures for the k-points around k-point X (0, 0, 0.5) and positive around k-point Γ (0, 0, 0). Negative thermal expansion of *a*-Sn at low temperatures is thus related to the behaviour of phonons around k-points X, M and N.

MM 34.5 Fri 11:15 H10

Bayesian Uncertainty Estimates for Spin-Component-Scaled Second-Order Møller-Plesset Perturbation Theory — •Elisabeth Keller and Johannes Margraf — Universität Bayreuth, Bayreuth, Germany

Spin-component-scaled second-order Møller-Plesset perturbation theory (SCS-MP2) improves upon MP2 by separately scaling the same-spin and opposite-spin MP2 contributions, achieving near coupled cluster (CCSD(T)) accuracy in some applications. However, the optimal scaling parameters vary by target domain, limiting the transferability of any given SCS-MP2 parameterization. To address this limitation, we employ a Bayesian multilevel linear regression model to obtain a robust parameterization for SCS-MP2, termed BSCS-MP2, predicting various energetic properties, including total, atomization, reaction, and non-covalent interaction energies. Additionally, the Bayesian model provides credible intervals to quantify the uncertainty of the BSCS-MP2 energy predictions. We evaluate how these uncertainty estimates adjust to data quality and model complexity, and assess their robustness for out-of-sample inference.

15 min. break

MM 34.6 Fri 11:45 H10

pyTTN, an open source toolbox for Quantum Dynamics simulations using Tree Tensor Network states — Lachlan Lindoy, •Daniel Rodrigo-Albert, Yannic Rath, and Ivan Rungger — National Physical Laboratory, Teddington, TW11 0LW, United Kingdom

The simulation of large-scale dissipative quantum systems is a significant challenge arising in several areas of physics and chemistry. In this talk we will discuss pyTTN, our recently developed software package for simulating dynamical properties of open quantum systems. This package makes use of Tree Tensor Network (or equivalently, Multi-Layer Multi-Configuration Time-Dependent Hartree) based representations of the state vector, and features both single- and multi-set ansätze, as well as adaptive bond dimension through subspace expansion techniques. The software has been designed with a focus on performance and ease of setup of new models and wavefunction topologies, including simple preparation of zero- and finite-temperature calculations with general bosonic, fermionic, and spin Hamiltonians. We will demonstrate the capabilities of the package with both unitary dynamics and non-unitary pseudomode-based approaches for the simulation of Anderson impurity models.

MM 34.7 Fri 12:00 H10

Spectral properties from an efficient analytical representation of the GW self-energy within a multipole approximation — •Dario Alejandro Leon[1], Kristian Berland[1], and Claudia Cardoso[2] — [1]Norwegian University of Life Sciences, As, Norway — [2]S3 Centre, Istituto Nanoscienze, CNR, Modena, Italy

We propose an efficient analytical representation of the frequency-dependent GW self-energy via a multipole approximation (MPA-Σ). Similar to the earlier developed multipole approach for the screening interaction W (MPA-W) [Phys. Rev. B 104, 115157 (2021)], the multipole-Padé model for the self-energy is interpolated from a small set of values evaluated numerically in the complex frequency plane. As for MPA-W , we show that an appropriate choice of the frequency sampling is paramount to guarantee computational efficiency and high level of accuracy in the description of the self-energy. Crucially, MPA-Σ enables a multipole representation for the interacting Green's function G (MPA-G), providing straightforward evaluation of all the spectral properties. Combining the MPA-W and MPA-Σ schemes considerably reduces the cost of full-frequency self-energy calculations, especially when targeting spectral band structures in a wide energy range. We validate the MPA-Σ approach in bulk Si, Na and Cu, monolayer MoS2, the NaCl ion-pair and the F2 molecule, as prototypical semiconducting and metallic materials of different dimensionality. Moreover, toy MPA-Σ models with one and two poles and their corresponding MPA-G solutions, are used to examine the quasiparticle picture in different situations.

MM 35: Transport in Materials: Diffusion, Charge or Heat Conduction

Diffusion

Time: Friday 10:15–11:45 Location: H22

MM 35.1 Fri 10:15 H22

Influence of second phase precipitation on bulk diffusion of Ni in the CoFeMnNiV high-entropy alloy — •Aditya Burla[1], Mohan Muralikrishna Garlapati[1], Aditya Srinivasan Tirunilai[2], Guillaume Laplanche[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster, Germany — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum, Germany

High-entropy alloys (HEAs), or multi-principal element alloys represent a new class of metallic materials that offer tremendous opportunities for advancing materials science due to their vast compositional space and exceptional properties. While tracer diffusion and sigma phase precipitation kinetics in the Co-Cr-Fe-Mn-Ni system have been widely studied, the interaction between the two has received limited attention. The present work focuses on an equiatomic CoFeMnNiV HEA, in which Vanadium is known to have a strong tendency to stabilize the sigma phase. Therefore, this element promotes its precipitation in the CoFeMnNiV alloy, particularly at temperatures below ~1080°C, even after short anneal times of just 1 h in the fully recrystallized state. In this study, bulk diffusion of Ni is investigated using the radiotracer technique. A strong impact of sigma phase precipitation on the self-diffusion kinetics was discovered and analyzed. The obtained tracer diffusivities follow an Arrhenius-type relationship when estimated in the stable microstructures, whereas concurrent precipitation enhances the tracer diffusion rates.

MM 35.2 Fri 10:30 H22

Investigation of lateral hydrogen diffusion in polycrystalline molybdenum trioxide thin films — •Tim K. Hecker, Martin Becker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Molybdenum trioxide thin films were prepared by RF sputter deposition exploring a wide range of growth parameters. To characterise the thin films, electrochemical, Raman, and XRD experiments were conducted. In order to gain a deeper understanding of the diffusion of hydrogen in these thin films, the samples were microstructured with a PMMA film in a way that restricts the contact surface with the electrolyte to a narrow stripe-like gap. This enables the lateral diffusion of hydrogen beneath the PMMA film to be studied using a transmission experiment, making use of the electrochromic properties of molybdenum trioxide. This increases the accessible spatial and temporal scale by several orders of magnitude, significantly improving the spatial and temporal resolution of the in-situ transmission measurement. Spatially resolved transmission measurements in the wavelength range of 633±55 nm demonstrate that the investigated diffusion is dependent on the hydrogen concentration. The results are also supported by a spatially and temporally resolved diffusion simulation. Furthermore, the measurement method presented here is universally applicable to electrochromic thin film samples.

MM 35.3 Fri 10:45 H22

Diffusion and activation energies of hydrogen and its isotopes in boron structure — •Bianca Solomonea[1,2], Calin Pantis-Simut[2,3], Mihaela Cosinschi[2,3], Paul Dinca[1], Corneliu Porosnicu[1], and George Nemnes[2,3] — [1]National Institute for Laser, Plasma and Radiation Physics (INFLPR), Atomiştilor Street 409, 077125 Măgurele, Ilfov, Romania — [2]Faculty of Physics, Univer- sity of Bucharest, Atomistilor 405, Magurele-Ilfov 077125, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineer- ing, Reactorului 30, Magurele-Ilfov 077125, Romania

The retention and release of hydrogen isotopes in plasma-facing materials (PFM) is a critical concern for the ITER project. The decision to construct the Tokamak reactor as a fully tungsten-based machine presents challenges regarding plasma ignition and stability, particularly due to impurities in the working gases. Boronization is applied to retain impurities by forming covalent bonds with oxygen and nitrogen. This study uses ab initio calculations via Density Functional Theory (DFT), molecular dynamics (MD), and the nudged elastic band (NEB) method in the SIESTA code to examine boron structures in crystalline and amorphous forms. Activation energies for trapping, detrapping, and diffusion processes are determined. Given the difficulty of defining hydrogen-isotope diffusion in boron structures, and its importance for retention and desorption in redeposited or co-deposited layers of the PFM, we focus on identifying the potential diffusion trajectories of hydrogen within the boron structure. This includes mapping a potential landscape and locating local minima and saddle points.

MM 35.4 Fri 11:00 H22

Diffusion behavior of Li ions in crystalline and amorphous Li-Zr-O and Li-Nb-O phases — •Daniel Mutter[1], Diego A. Pantano[2], Christian Elsässer[1], and Daniel F. Urban[1] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]TotalEnergies OneTech, 2 place Jean Millier, 92400 Courbevoie, France

Li containing transition metal oxides are known as good ionic conductors. Performing classical molecular dynamics simulations with a Morse potential model based on the Bond Valence method, the diffusion behavior of Li ions is investigated in crystalline and amorphous phases with the stoichiometries Li_2ZrO_3 and $LiNbO_3$. The diffusivities are obtained from a statistical Arrhenius analysis of mean square displacement curves at different temperatures. The crystalline phase of Li_2ZrO_3 exhibits two well-defined migration mechanisms: vacancy-mediated migration is dominant below and a collective site exchange of Li ions above a crossover region between about 1700 and 1800 K. The latter mechanism, which is related to the formation of Frenkel pair defects and subsequent rotation of Li-Li pairs, also prevails in the amorphous phases with a strongly reduced activation energy. This is explained by a smaller equilibrium separation of Li ions in the amorphous phase than in the crystal structure. The demonstrated methodology and the discussed results shed light on a hitherto rarely described diffusion mechanism in ionic metal-oxide materials relevant for ion-battery applications.

MM 35.5 Fri 11:15 H22

Ag bulk and grain boundary diffusion in AlCoCrFeNi2.1 compositionally complex alloy — •Heng Zhang, Mohan Muralikrishna Garlapati, Sergiy V Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Munster, Wilhelm-Klemm-Str. 10

Bulk and grain boundary diffusion of Ag in a eutectic Al-Co-Cr-Fe-Ni multi-principal element system is measured using the radiotracer technique and applying the 110Ag radioisotope. An equilibrium microstructure was produced by rotary forging and annealing of cast and homogenized initial casting ingot material. Ag diffusion is measured in the temperature interval from 673K to 1373K accounting for volume (at high temperatures) and short-circuit (at moderate and low temperatures) diffusion contributions. In the present case, interphase boundaries can potentially contribute in addition to grain boundaries to the short-circuit diffusion. The grain- and interphase-boundary diffusion experiments were performed in the B-type kinetic regime based on Harrison's classification. The results are analyzed with respect to constituent phases (FCC and B2) and different interface types. The contribution of interphase boundary diffusion is analyzed in detail.

MM 35.6 Fri 11:30 H22

Mechano-chemical coupling induced by Co grain boundary diffusion in SIGMA5(310) Cu bicrystals — •Esakkiraja Neelamegan[1], Anoosheh Akbari[1], Hui Ding[2], Harald Rösner[1], Daniel Gaertner[1], Christian Liebscher[2,3], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster-48149 Germany — [2]Max-Planck-Institut für Sustainable Materials, Düsseldorf, Germany — [3]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundary diffusion of 57Co in pure copper SIGMA-5(310)[001] bicrystals is investigated using the radiotracer technique. Experiments are conducted under both the type-B and type-C kinetics regimes, as classified by Harrison. By varying the amount of applied 57Co tracer solution, characteristic changes in

the shape of the penetration profiles are observed and attributed to Co segregation induced changes of the grain boundary structure. The structural changes due to the Co addition are examined by scanning transmission electron microscopy. The elastic strains near the grain boundary are measured using nano-beam diffractions with a nanometer resolution. The Co-induced variations of the GB structure provide an intriguing picture, particularly when considering their influence on the diffusion behaviour in the presence of deliberately introduced solute atoms.

MM 36: Mechanical Properties

Nanomaterials and Alloys

Time: Friday 10:15–13:00 Location: H23

MM 36.1 Fri 10:15 H23

STEM investigation of early precipitation reactions in Al-Cu alloys — •Johannes Berlin and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Due to their excellent strength-to-weight ratio, heat-treatable Al-Cu alloys have been widely used since their invention. Although the occurring precipitates in naturally aging aluminium alloys are well known, the very early stages of formation mechanisms still are a topic of ongoing research. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history and effects of microalloying, on early-stage precipitate formation and transformation in Al. Due to their strong binding potential to quenched in vacancies even a few hundred ppm of trace elements such as tin and indium can alter the natural aging process drastically. Even after prolonged natural ageing, a slight increase in temperature can lead to drastic changes in precipitation size and densitiy inthese materials. This proves a long-lasting supersaturation of the material with vacancies. Additionally, these results are compared to the measurements of hardness, DSC and electrical resistance.

MM 36.2 Fri 10:30 H23

Surface structure and reactivity of Aluminium alloys studied by DFT — •Zhengqing Wei[1], Inna V. Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[3], Maik Gude[3], Julia Hufenbach[4,5], and Sibylle Gemming[1,6] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]ILK, TU Dresden, Germany — [4]IFW Dresden, Germany — [5]Inst. Materials Science, TU-BA Freiberg, Germany — [6]MAIN Center, TU Chemnitz, Germany.

Classically, the mechanical properties of alloys are attributed to the action of stress fields around defect sites and to their combined influence on the overall elastic moduli. The present study employs first-principles modeling to include also changes of the electronic structure and investigate the bonding, stability, and reactivity changes around impurities in the bulk and at surfaces. We focus on Al alloys with low amounts of substitutional Mg, Zr, and Si atoms. The results indicate that the electron density changes mostly within the first coordination sphere around the impurity, the bond lengths vary locally within few percent, and there exists a thermodynamic driving force for most elements to diffuse to or near surfaces or interfaces. Stable 2D surface alloy compositions in part differ from the bulk phase and exhibit an element-specific reactivity with air and polymer coatings. Modeling the adsorption of oxygen, nitrogen and the PEEK polymer from first principles gives access to modified local potentials for the classical modeling of large-scale surface and interface areas (tu-dresden.de/ing/forschung/Graduiertenkollegs/grk2868#intro).

MM 36.3 Fri 10:45 H23

Active learning-based interatomic potential for investigating mechanical properties of Al-Mg-Zr alloys — •Lukas Volkmer, Leonardo M. Sandonas, Gianaurelio Cuniberti, and Markus Kästner — TU Dresden

The unique properties of aluminum-based alloys, such as low density, high specific strength, and excellent resistance to oxidation and corrosion, enable the design of advanced metamaterials. In this work, we theoretically investigate the effect of alloying aluminum with magnesium and zirconium on its thermodynamic and mechanical properties. Since exploring the vast chemical compound space of these alloys through Density Functional Theory (DFT) calculations is computationally prohibitive, we developed a scalable and transferable machine learning interatomic potential (MLIP) capable of accurately calculating diverse properties of Al-Mg-Zr alloys. The MLIP was trained using an active learning technique based on ab initio molecular dynamics simulations, Bayesian statistics, and kernel ridge regression. This methodology ensures that the MLIP captures the effects of alloying concentration and atomic configurations up to the solubility limit, providing access to highly accurate physicochemical properties of a wide range of Al-based alloys at a reasonable computational cost. We expect this approach to enable efficient phase space exploration, offering a robust tool for designing advanced Al-based alloys with optimized properties.

MM 36.4 Fri 11:00 H23

Phase identification by Raman Spectroscopy on pre-oxidized AISI 316L-MgO composite produced by Spark Plasma Sintering — •Julia Richter[1], Mahnaz Mehdizadehlima[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, D-09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner-Straße 5, D-09599 Freiberg

Re-usage, recycling and upcycling of MgO-C refractories as they are widely used in the steel industry are crucial for resource efficiency. Our upcycling concept is aimed at steel-MgO composite anodes for application in the extraction of aluminum by fused-salt electrolysis. The composite anode material is produced by Spark Plasma Sintering based on 60 vol.% AISI 316L steel powder and 40 vol.% MgO. In this stage of development, the raw material is fused fresh MgO instead of recyclate as a proof of concept. Pre-oxidation treatment of the developed composite is intended to enhance the material's corrosion resistance in the aggressive environment of molten cryolite during application. In order to gain a better understanding of the oxidation behavior at different temperatures, phase identification is required. For this purpose, Raman spectroscopy as a sensitive, non-destructive, non-contact method is employed complementary to other investigative techniques; e.g., Scanning Electron Microscopy.

MM 36.5 Fri 11:15 H23

Atomic Cluster Expansion for Ag-Au-Pd alloys — •Yanyan Liang, Matous Mrovec, Yury Lysoroskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germay

Ternary alloys of Ag-Au-Pd are of technological importance in catalysis and electrical applications. However, the system lacks reliable and efficient interatomic potentials capable of accurately describing structural and thermodynamic properties, particularly for investigating complex segregation and ordering phenomena in bulk systems and nanoclusters. In this work, we present an atomic cluster expansion (ACE) model parameterized for the Ag-Au-Pd system with quantum-level accuracy. We demonstrate that the ACE model provides an accurate description of fundamental properties, including structural stability and thermodynamics, not only for the elemental metals but also for their binary and ternary compounds. Furthermore, we highlight the wide applicability of the ACE model for large-scale atomistic simulations, enabling predictive modeling of complex phenomena.

15 min. break

MM 36.6 Fri 11:45 H23

Scalable fabrication and mechanical behavior of hierarchical nanoscale network nickel — •Ulrike Dette[1,2], Lukas Lührs[2], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of mechanically robust two-level hierarchical nanoporous gold by two-step electrochemical dealloying has enabled the demonstration of enhanced mechanical properties and reduced density attributed to the structural hierarchy in the nanoscale network materials. This work aims to develop a new method for the scalable fabrication of low-cost hierarchical nanoscale network metals. Here, two- and three-level hierarchical network (HN) Ni samples are successfully prepared from Ni foams by a novel and simple alloying-dealloying method. Bulk three-level HN Ni samples are characterized by three well-defined strut/ligament sizes (160 μm, <10 μm and <10 nm) and a low density down to 0.06. In addition, we systematically perform mechanical studies on both two- and three-level HN Ni via macroscopic compression tests. We propose general scaling equations between mechanical properties and relative density for HN materials.

MM 36.7 Fri 12:00 H23

Transferable machine learning interatomic potential for Au nanoparticles — •Jovana Vlahović, Cem Sevik, and Milorad V. Milošević — University of Antwerp, Groenenborgerlaan 171, Antwerp, Belgium

Effective molecular dynamics and Monte Carlo simulations fundamentally depend on the accuracy of interatomic potentials, which define the potential energy surface as a function of atomic positions. This precision is essential for metallic nanoparticles (NPs), whose small size and diverse morphologies demand robust modelling. While classical empirical potentials offer computational efficiency,

they often lack the necessary accuracy and density functional theory (DFT) calculations, though highly accurate, are computationally prohibitive for NPs with thousands of atoms. This work introduces a machine learning-based interatomic potential for Au NPs, trained on a compact dataset of bulk structures, surface slabs and NPs containing up to 55 atoms. Our training dataset includes a diverse set of atomic configurations with corresponding properties obtained from ab initio molecular dynamics calculations, which we use to train a Gaussian Approximation Potential (GAP) via Gaussian Process Regression. Parameter optimization was performed to maximize model accuracy, and LAMMPS validation tests demonstrated GAP performance against DFT benchmarks. In addition, transferability tests on larger NPs of various shapes reveal our GAP's robustness beyond the training set. Comparisons with an existing GAP model and the universal MACE potential underscore our model's improved accuracy and generalizability for Au NPs.

MM 36.8 Fri 12:15 H23

Scaling behavior of Poisson's ratio in hierarchical nanoporous materials — •Haonan Sun[1,2], Lukas Lührs[2], Wei-che Chang[3], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of crack-free monolithic hierarchical nested network nanoporous gold allows the investigation of the benefits of hierarchy in the aspect of mechanical properties at the nanoscale. It has been demonstrated that hierarchical nanoporous gold (HNPG) can achieve a substantially reduced solid fraction and enhanced specific stiffness and strength compared with non-hierarchical nanoporous gold. However, the role of hierarchical structure on Poisson's ratio has not been investigated yet. In this work, mm-sized HNPG samples are made out of an Ag93Au7 master alloy by a dealloying-coarsening-dealloying method. We then explore the elastic and plastic Poisson*s ratios of HNPG by using digital image correlation during compression tests. Remarkably, a scaling law of the elastic Poisson's ratio in hierarchical nanoporous materials with respect to the solid volume fraction is proposed and excellently supported by our experiments. This work enriches the understanding on the relationship between mechanical properties and microstructure in hierarchical network materials at the nanometer scale.

MM 36.9 Fri 12:30 H23

Frenkel pair energetics in disordered solid solutions and implications for alkali feldspar diffusivity — •Alexander Gorfer, Rainer Abart, and Christoph Dellago — University of Vienna, Vienna, Austria

Predicting defect concentrations from the density of states (DOS) of formation energies in disordered materials has recently been formulated for vacancies in high entropy alloys. That methodology however does not translate to disordered ionic crystals as charged defects need to be paired up to ensure charge neutrality. Here, we present a general expression to predict the defect concentrations of Frenkel pairs in disordered ionic crystals out of the DOS of formation energies of both positively and negatively charged defects. To demonstrate its applicability we use a recently developed machine learning force field to calculate the DOS of formation energies for different states of (dis)ordering in alkali feldspar (Na, K)$AlSi_3O_8$, an abundant mineral in the Earth's crust. Applying our expression to these DOS reveals a significant increase in the concentration of point defects in disordered ionic crystals as pairs of low formation energy defect states between the positively and negatively charged DOS can be identified. Implications for the diffusivity that controls the exsolution of alkali feldspars which is an important phenomenon in the formation of magmatic and metamorphic rocks are discussed.

MM 36.10 Fri 12:45 H23

Ferromagnetism at ambient temperature in Cantor and nanocomposite high-entropy alloys induced by severe plastic deformation — •Shabnam Taheriniya, Harald Rösner, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

In this study, single phase Cantor (CoCrFeMnNi) and nanocomposite high-entropy alloys (HEAs) (CoCrFeMnNi and HfNbTaTiZr) were processed using high-pressure torsion (HPT), subjecting the samples to a constant pressure of 9 GPa either as a single disk or stacked disks, with the top anvil rotating at 1 rpm at ambient temperature for up to 15 revolutions. Vibrating sample magnetometry (VSM) confirmed that HPT processing induces the development of ferromagnetic properties. The distribution and orientation of magnetic domains post-deformation were examined in detail using differential phase contrast scanning transmission electron microscopy (DPC STEM), analytical TEM and atom probe tomography (APT) analysis. Our study demonstrates that HPT processing of HEAs induces a transition from paramagnetic to ferromagnetic states at ambient conditions. This deformation-induced ferromagnetism can be explained by the cocktail effect in HEAs, where the formation of ferromagnetic particles is linked to deformation-induced element-selective atomic migration and local enrichment of ferromagnetic elements.

MM 37: Functional and Complex Materials

Time: Friday 12:00–12:45 Location: H22

MM 37.1 Fri 12:00 H22

Unveiling Material Dynamics with Machine-Learned Interatomic Potentials — •Ferenc Tasnadi, Bobur Mukhamedov, Amanda Ehn, Florian Trybel, and Igor A. Abrikosov — IFM Linköping University

Machine-learned interatomic potentials (MLIPs) have revolutionized our ability to understand the properties of materials with complex dynamical processes. In this work, we present an active learning MLIP strategy to: (i) investigate the elasticity of alloys near dynamical instability [1] and (ii) explore dynamical bond disorder in high-pressure synthesized PN2 [2]. bcc-Ti-based alloys have wide industrial applicability, ranging from low-modulus biomedical implants to high-strength GUM metals. The low-temperature dynamical instability of bcc-Ti can be tailored through the addition of bcc stabilizers (Nb, Ta, Zr, V), resulting in anomalous mechanical properties such as elinvar behavior or high anisotropy with low modulus in Ti-Nb-Zr and Ti-Zr-Sn alloys. Pnictogen compounds (Group 15 elements) exhibit fascinating chemistry due to the variety of bonding configurations, as demonstrated in the recently studied P-N system [2]. Long-timescale MLIP-driven simulations reveal that N-N distances connecting the P-N octahedra vary dynamically between single-bonded and non-bonding configurations. The results are compared with experimental observations. If time permits, we will demonstrate how MLIP-driven molecular dynamics simulations can offer deeper insights into materials exhibiting Peierls instability. [1] New J. Phys. 22 113005 (2020); J. Vac. Sci. Technol. A 42, 013412 (2024). [2] Chem. Eur. J. 2022, 28, e202201998.

MM 37.2 Fri 12:15 H22

Decoding Molecular Ion Dissociation Effects in Atom Probe Tomography of Iron Oxides — •Shyam Katnagallu[1], SeHo Kim[1], Shalini Bhatt[1], Daniel K Schreiber[2], Jörg Neugebauer[1], Baptiste Gault[1], and Christoph Freysoldt[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Energy and Environment Directorate, PNNL, Richland, USA.

To mitigate CO2 emissions, we require efficient carbon-free reduction processes for iron ores. Atom probe tomography (APT) can elucidate the gradual reduction of FexO at the nanometer length scale, but it is hindered by compositional bias. We investigated the changes in the measured composition of FeO, Fe2O3, and Fe3O4 across a range of analysis conditions. However, APT of ionic or covalently bonded materials often results in molecular ions. The metastability of these molecular ions, under an intense electrostatic field, makes them vulnerable to dissociation. These processes can significantly impact the analytical performance of APT. For instance, neutral molecules formed through dissociation may not be detected or may have a time-of-flight no longer associated with their actual mass, leading to their loss from the analysis. To predict possible dissociation reactions of molecular ions, we employed density-functional theory that considered the spin states of the molecules. The energetically favoured reactions were traced onto multi-hit correlation histograms to validate their existence within APT data. These detected reactions were carefully analysed to assess the impact of neutrals resulting from dissociation reactions on the performance of APT for analysing iron oxides.

MM 37.3 Fri 12:30 H22

Entropy Decoupling in Vacancy Formation of BCC High-Entropy Alloys — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

The temperature-dependent vacancy formation energies in MoTaNbW systems have been calculated using a machine-learning-based interatomic potential that accurately captures the simultaneous effects of configurational and vibrational entropies, along with their coupling. Our results indicate that at elevated temperatures, careful treatment of the chemical potential is essential. We computed the distributions of vacancy formation energies up to the melting point, explicitly accounting for anharmonic vibrational effects. The findings demonstrate that, in this system, the local atomic environment around a vacancy exerts minimal influence on the vibrational entropy contributions.

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Overview of Invited Talks and Sessions

(Lecture halls H1, H2, H4, H6, H8, H11, H24, and H25; Poster P2 and P3)

Invited Talks

O 7.4	Mon	11:15–11:45	H11	**Nanoimaging the electronic, plasmonic, and phononic structure and dynamics of 2D materials** — •Sarah King
O 8.1	Mon	10:30–11:00	H24	**Chiral reactions at surfaces elucidated by machine learning and enhanced sampling** — Raymond Amador, Enrico Trizio, Peilin Kang, Umberto Raucci, Hannah Bertschi, Marcella Iannuzzi, Jacob Wright, Roland Widmer, Oliver Gröning, Michele Parrinello, •Daniele Passerone
O 10.1	Mon	15:00–15:30	H2	**Probing coherent optical emission processes with ultrafast scanning electron microscopy** — •Albert Polman
O 10.5	Mon	16:15–16:45	H2	**Ultrafast exciton dynamics in momentum space** — Alexander Neef, Tommaso Pincelli, Lawson Lloyd, Shuo Dong, Samuel Beaulieu, Tania Mukherjee, Sebastian Hammer, Malte Selig, Dominik Christiansen, Andreas Knorr, Martin Wolf, Jens Pflaum, Laurenz Rettig, •Ralph Ernstorfer
O 15.1	Mon	15:00–15:30	H24	**Kondo and Yu-Shiba-Rusinov resonances: transport and coupling** — •Laëtitia Farinacci, Gelavizh Ahmadi, Gaël Reecht, Benjamin W. Heinrich, Contanstin Czekelius, Felix von Oppen, Katharina J. Franke
O 15.2	Mon	15:30–16:00	H24	**Electron delocalization in a 2D Mott insulator** — •Amadeo L. Vazquez de Parga, Cosme G. Ayani, Michele Pisarra, Iván M. Ibarburu, Clara Rebanal, Manuela Garnica, Fabián Calleja, Fernando Martín
O 15.3	Mon	16:00–16:30	H24	**Kondo or no Kondo, that is the question** — •Alexander Weismann, Neda Noei, Niklas Ide, Richard Berndt
O 15.4	Mon	16:30–17:00	H24	**Evidence for spinarons in Co atoms on noble metal (111) surfaces** — •Artem Odobesko
O 15.5	Mon	17:00–17:30	H24	**Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures** — •Samir Lounis
O 26.1	Tue	10:30–11:00	H2	**Attosecond Electron Microscopy** — •Peter Baum
O 27.7	Tue	12:00–12:30	H4	**Ultrafast electrochemistry beyond the RC time constant** — •Yujin Tong
O 30.5	Tue	11:30–12:00	H11	**Resonant molecular transitions in femtosecond second harmonic generation spectroscopy of Fe-porphyrin/Cu(001)** — •Andrea Eschenlohr, Rui Shi, Jinghao Chen, Ping Zhou, Uwe Bovensiepen, Wolfgang Hübner, Georg Lefkidis
O 31.3	Tue	11:00–11:30	H24	**Single molecule machines on surface** — •Francesca Moresco
O 57.3	Wed	11:00–11:30	H2	**Floquet engineering in black phosphorus** — •Changhua Bao, Shaohua Zhou, Benshu Fan, Michael Schüler, Teng Xiao, Hui Zhou, Zhiyuan Sun, Peizhe Tang, Sheng Meng, Wenhui Duan, Shuyun Zhou
O 61.3	Wed	11:00–11:30	H11	**Polaritons in two-dimensional materials and hybrids probed by electron beams** — •Nahid Talebi
O 62.5	Wed	11:30–12:00	H24	**On-Surface Synthesis with Hydrogen Atoms** — •Szymon Godlewski
O 64.1	Wed	15:00–15:30	H2	**Topological spin structures in two-dimensional van der Waals magnets and heterostructures** — •Stefan Heinze
O 64.2	Wed	15:30–16:00	H2	**Ferromagnetic Order in 2D Layers of Transition Metal Dichlorides** — Andrea Aguirre, Andres Pinar, Diego Soler, Carmen Gonzalez-Orellana, Jon Ortuzar, Oleksandr Stesovych, Celia Rogero, Jose Ignacio Pascual, Pavel Jelinek, Maxim Ilyn, •Martina Corso
O 64.3	Wed	16:00–16:30	H2	**Tailoring spin lattice in van der Waals monolayer crystals** — •Ying-Shuang Fu
O 64.4	Wed	16:30–17:00	H2	**Spin excitations in 2D heterostructures from realistic fermionic models** — •António Costa

O 66.1	Wed	15:00–15:30	H8	**Unveiling the crucial role of kinetic modeling of gas flows in vacuum and fusion technologies** — •Christos Tantos, Thomas Giegerich
O 66.2	Wed	15:30–16:00	H8	**Advances in traceable vacuum and outgassing rate measurements** — •Matthias Bernien, Annas Bin Ali, Thomas Bock, Tom Rubin, Janez Setina, Perrin Waldock, Kirk Madison, Karl Jousten
O 68.9	Wed	17:00–17:30	H24	**On-Surface Synthesis of Porphyrins and BN-Substituted Carbon Scaffolds** — •Willi Auwärter
O 91.1	Thu	15:00–15:30	H24	**Infrared Nanoscopy and Tomography of Intracellular Structures** — Joachim Heberle, Katerina Kanevche, •Emmanuel Pfitzner, David Burr, Janina Drauschke, Andreas Elsaesser, Jacek Kozuch
O 91.2	Thu	15:30–16:00	H24	**Coherent Raman Imaging** — •Michael Schmitt, Juergen Popp
O 91.3	Thu	16:00–16:30	H24	**Sum Frequency Generation Microscopy of Electrochemical Interfaces** — •Steven Baldelli
O 100.1	Fri	10:30–11:00	H24	**Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things** — •Steven Lee
O 100.2	Fri	11:00–11:30	H24	**MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research** — •Andreas Römpp

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff, Matthias Florian, Frank Jahnke
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger, Julian Wiercinski, Moritz Cygorek

Invited Talks of the joint Symposium Pushing the Boundaries of Fair Data Practices for Condensed Matter Insights: From Workflows to Machine Learning (SYFD)

See SYFD for the full program of the symposium.

SYFD 1.1	Wed	9:30–10:00	H1	**Pushing the Boundaries of Fair Data Practices for Condensed Matter Insight** — •Astrid Schneidwind
SYFD 1.2	Wed	10:00–10:30	H1	**Establishing Workflows of Experimental Solar Cell Data into NOMAD** — Edgar Nandayapa, Paolo Graniero, Jose Marquez, Michael Götte, •Eva Unger
SYFD 1.3	Wed	10:30–11:00	H1	**Building up the EOSC Federation** — •Ute Gunsenheimer
SYFD 1.4	Wed	11:15–11:45	H1	**Data-Driven Materials Science for Energy-Sustainable Applications** — •Jacqueline Cole
SYFD 1.5	Wed	11:45–12:15	H1	**Machine Learning and FAIR Data in X-ray Surface Science** — •Stefan Kowarik

Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

O 1.1–1.4	Sun	16:00–18:00	H3	**Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)**
O 2.1–2.3	Sun	16:00–18:15	H10	**Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)**
O 3.1–3.1	Mon	9:30–10:15	H24	**Overview Talk Kerstin Volz**
O 4.1–4.10	Mon	10:30–13:00	H4	**Solid-Liquid Interfaces: Structure**
O 5.1–5.10	Mon	10:30–13:00	H6	**Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale I**
O 6.1–6.9	Mon	10:30–12:45	H8	**Oxides and Insulator Surfaces: Structure, Epitaxy and Growth**
O 7.1–7.8	Mon	10:30–12:45	H11	**Focus Session Ultrafast Electron Microscopy at the Space-Time Limit I**
O 8.1–8.9	Mon	10:30–13:00	H24	**Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation I**
O 9.1–9.8	Mon	10:30–12:30	H25	**Surface Reactions**
O 10.1–10.9	Mon	15:00–17:45	H2	**Focus Session Ultrafast Electron Microscopy at the Space-Time Limit II**
O 11.1–11.12	Mon	15:00–18:00	H4	**Electronic Structure of Surfaces: Spectroscopy, Surface States I**
O 12.1–12.11	Mon	15:00–17:45	H6	**Nanostructures at Surfaces I**
O 13.1–13.10	Mon	15:00–17:30	H8	**Organic Molecules on Inorganic Substrates: Adsorption and Growth**

O 14.1–14.12	Mon	15:00–18:00	H11	**2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
O 15.1–15.8	Mon	15:00–18:15	H24	**Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)**
O 16.1–16.12	Mon	15:00–18:00	H25	**Scanning Probe Techniques: Method Development**
O 17.1–17.12	Mon	18:00–20:00	P2	**Poster Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation**
O 18.1–18.7	Mon	18:00–20:00	P2	**Poster Focus Session Ultrafast Electron Microscopy at the Space-Time Limit**
O 19.1–19.2	Mon	18:00–20:00	P2	**Poster Surface Magnetism**
O 20.1–20.11	Mon	18:00–20:00	P2	**Poster Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale**
O 21.1–21.8	Mon	18:00–20:00	P2	**Poster Heterogeneous Catalysis**
O 22.1–22.6	Mon	18:00–20:00	P2	**Poster Surface Reactions**
O 23.1–23.21	Mon	18:00–20:00	P2	**Poster Ultrafast Electron Dynamics**
O 24.1–24.11	Mon	18:00–20:00	P2	**Poster Scanning Probe Techniques: Method Development**
O 25.1–25.1	Tue	9:30–10:15	H24	**Overview Talk Jörg Kröger**
O 26.1–26.9	Tue	10:30–13:00	H2	**Focus Session Ultrafast Electron Microscopy at the Space-Time Limit III**
O 27.1–27.9	Tue	10:30–13:00	H4	**Solid-Liquid Interfaces: Reactions and Electrochemistry I**
O 28.1–28.7	Tue	10:30–12:15	H6	**Graphene: Electronic Structure and Excitations (joint session O/HL)**
O 29.1–29.10	Tue	10:30–13:00	H8	**2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)**
O 30.1–30.8	Tue	10:30–12:45	H11	**Surface Magnetism**
O 31.1–31.9	Tue	10:30–13:00	H24	**Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II**
O 32.1–32.9	Tue	10:30–12:45	H25	**Heterogeneous Catalysis I**
O 33.1–33.21	Tue	13:30–15:30	P3	**Poster Graphene: Electronic Structure and Excitations**
O 34.1–34.6	Tue	13:30–15:30	P3	**Poster Solid-Liquid Interfaces: Reactions and Electrochemistry**
O 35.1–35.4	Tue	13:30–15:30	P3	**Poster Solid-Liquid Interfaces: Structure**
O 36.1–36.8	Tue	13:30–15:30	P3	**Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)**
O 37.1–37.5	Tue	13:30–15:30	P3	**Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)**
O 38.1–38.5	Tue	13:30–15:30	P3	**Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)**
O 39.1–39.6	Tue	14:00–15:30	H4	**Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules I**
O 40.1–40.6	Tue	14:00–15:30	H6	**Surface Dynamics**
O 41.1–41.5	Tue	14:00–15:15	H8	**Heterogeneous Catalysis II**
O 42.1–42.6	Tue	14:00–15:30	H11	**Electron-driven Processes**
O 43.1–43.7	Tue	14:00–15:45	H24	**Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale II**
O 44.1–44.3	Tue	18:00–20:00	P2	**Poster Oxides and Insulator Surfaces: Structure, Epitaxy and Growth**
O 45.1–45.18	Tue	18:00–20:00	P2	**Poster Spins on Surfaces at the Atomic Scale**
O 46.1–46.13	Tue	18:00–20:00	P2	**Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties**
O 47.1–47.5	Tue	18:00–20:00	P2	**Poster Electron-driven Processes**
O 48.1–48.4	Tue	18:00–20:00	P2	**Poster Surface Dynamics**
O 49.1–49.11	Tue	18:00–20:00	P2	**Poster Nanostructures at Surfaces**
O 50.1–50.9	Tue	18:00–20:00	P2	**Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth**
O 51.1–51.5	Tue	18:00–20:00	P2	**Poster Electronic Structure of Surfaces: Spectroscopy, Surface States**
O 52.1–52.5	Tue	18:00–20:00	P2	**New Methods: Experiment**
O 53.1–53.2	Tue	18:00–20:00	P2	**Poster Electronic Structure Theory**
O 54.1–54.1	Tue	18:00–20:00	P2	**Poster New Methods: Theory**
O 55.1–55.3	Tue	18:00–20:00	P2	**Poster Topology and Symmetry-protected Materials**
O 56.1–56.1	Wed	9:30–10:15	H24	**Overview Talk Pavel Jelinek**
O 57.1–57.9	Wed	10:30–13:00	H2	**Ultrafast Electron Dynamics I**
O 58.1–58.10	Wed	10:30–13:00	H4	**Solid-Liquid Interfaces: Reactions and Electrochemistry II**
O 59.1–59.10	Wed	10:30–13:00	H6	**Spins on Surfaces at the Atomic Scale I**
O 60.1–60.9	Wed	10:30–12:45	H8	**Plasmonics and Nanooptics: Fabrication, Characterization and Applications I**
O 61.1–61.8	Wed	10:30–12:45	H11	**2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)**
O 62.1–62.9	Wed	10:30–13:00	H24	**Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation III**
O 63.1–63.8	Wed	10:30–12:30	H25	**Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules II**
O 64.1–64.8	Wed	15:00–18:00	H2	**Focus Session Atomic Scale Investigation of Magnetic 2D Materials**
O 65.1–65.11	Wed	15:00–17:45	H6	**Solid-Liquid Interfaces: Reactions and Electrochemistry III**
O 66.1–66.10	Wed	15:00–18:00	H8	**Vacuum Science Technology: Theory and Applications**
O 67.1–67.11	Wed	15:00–17:45	H11	**Ultrafast Electron Dynamics II**
O 68.1–68.10	Wed	15:00–17:45	H24	**Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation IV**

O 69.1–69.10	Wed	15:00–17:30	H25	**Nanostructures at Surfaces II**
O 70.1–70.1	Wed	18:00–20:00	P2	**Poster Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules**
O 71.1–71.5	Wed	18:00–20:00	P2	**Poster Plasmonics and Nanooptics: Fabrication, Characterization and Applications**
O 72.1–72.13	Wed	18:00–20:00	P2	**Poster Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy**
O 73.1–73.10	Wed	18:00–20:00	P2	**Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules**
O 74.1–74.7	Wed	18:00–20:00	P2	**Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth**
O 75.1–75.1	Wed	18:00–20:00	P2	**Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)**
O 76.1–76.3	Wed	18:00–20:00	P2	**Poster Focus Session Atomic Scale Investigation of Magnetic 2D Materials**
O 77.1–77.3	Wed	18:00–20:00	P2	**Poster Vacuum Science Technology: Theory and Applications**
O 78.1–78.1	Thu	9:30–10:15	H24	**Overview Talk Manish Garg**
O 79.1–79.8	Thu	10:30–12:30	H2	**Ultrafast Electron Dynamics III**
O 80.1–80.8	Thu	10:30–12:30	H4	**Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I**
O 81.1–81.8	Thu	10:30–12:30	H6	**Heterogeneous Catalysis III**
O 82.1–82.8	Thu	10:30–12:30	H8	**Plasmonics and Nanooptics: Fabrication, Characterization and Applications II**
O 83.1–83.8	Thu	10:30–12:30	H11	**2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)**
O 84.1–84.5	Thu	10:30–13:00	H24	**Gerhard Ertl Young Investigator Award Competition**
O 85.1–85.9	Thu	10:30–12:45	H25	**New Methods: Theory**
O 86.1–86.10	Thu	15:00–17:30	H2	**Electronic Structure of Surfaces: Spectroscopy, Surface States II**
O 87.1–87.10	Thu	15:00–17:30	H4	**Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy I**
O 88.1–88.11	Thu	15:00–17:45	H6	**2D Materials: Stacking and Heterostructures (joint session O/HL)**
O 89.1–89.11	Thu	15:00–17:45	H8	**Metal and Semiconductor Substrates: Structure, Epitaxy and Growth**
O 90.1–90.10	Thu	15:00–17:30	H11	**Spins on Surfaces at the Atomic Scale II**
O 91.1–91.7	Thu	15:00–17:30	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)**
O 92.1–92.13	Thu	15:00–18:15	H25	**Electronic Structure Theory**
O 93	Thu	19:00–19:30	H1	**Members' Assembly**
O 94	Thu	19:30–20:30	H1	**Post Deadline Session**
O 95.1–95.1	Fri	9:30–10:15	H24	**Overview Talk Kai Rossnagel**
O 96.1–96.10	Fri	10:30–13:00	H4	**Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy II**
O 97.1–97.8	Fri	10:30–12:30	H6	**Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties II**
O 98.1–98.8	Fri	10:30–12:30	H8	**Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules**
O 99.1–99.10	Fri	10:30–13:00	H11	**Ultrafast Electron Dynamics IV**
O 100.1–100.7	Fri	10:30–12:45	H24	**Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)**
O 101.1–101.7	Fri	10:30–12:15	H25	**Topology and Symmetry-protected Materials (joint session O/TT)**
O 102.1–102.1	Fri	13:15–14:00	H1	**Closing Talk Andreas Heinrich**

Members' Assembly of the Surface Science Division

Thursday 19:00–19:30 H1

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

O 1: Tutorial: How to Use NOMAD's Workflow Utilities to Improve Data Management and Facilitate Discovery in Materials Science (joint session O/TUT)

NOMAD (nomad-lab.eu) [1] is an open-source, community-driven data infrastructure, that supports automated (meta)data extraction from a wide range of simulations, including ab initio and advanced many-body calculations as well as molecular dynamics simulations. NOMAD allows users to store both standardized and custom complex simulation workflows, which not only streamlines data provenance and analysis but also facilitates the curation of AI-ready datasets. This tutorial will focus on recently developed workflow functionalities and utilities within the NOMAD infrastructure. These advances enable high-throughput interfacing with the NOMAD repository, opening improved discovery pipelines by leveraging the benefits of NOMAD's comprehensive and FAIR-compliant data management system [2].

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

Time: Sunday 16:00–18:00 Location: H3

Tutorial O 1.1 Sun 16:00 H3

FAIR-data management with the NOMAD infrastructure: Core functionalities — •Joseph F. Rudzinski — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this first part of the tutorial series, an overview of the NOMAD infrastructure will be provided. Attendees will learn how NOMAD processes raw data and stores it within a generalized data structure, and the corresponding GUI features that allow users to comfortably browse data. An example scenario will also be set up for use throughout the remainder of the tutorial series: *A researcher with a variety of data obtained within a project workflow would like to upload this data to NOMAD in order to link it to their manuscript while exposing the details of their (meta)data and retaining the scientifically relevant connections between the individual project tasks.*

Tutorial O 1.2 Sun 16:30 H3

Using NOMAD's API for project management — •Nathan Daelman — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, you will learn how to interface with NOMAD programmatically using a Python module built to simplify the API (application programming interface). Functionalities for uploading data, editing metadata of uploads, creating datasets with multiple uploads, and publishing data will be covered. Attendees will use these functionalities to manage a portion of the data from the example project workflow, in particular, the subset of data that is automatically recognized and processed by one of NOMAD's existing parsers. *(For attendees without any Python experience, an alternative route to upload via the GUI will also be demonstrated!)*

Tutorial O 1.3 Sun 17:00 H3

Creating custom entries in NOMAD using yaml schema and ELN integration — •Andrea Albino — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this part of the tutorial series, attendees will learn how to create custom entries to store data that is not already supported by one of NOMAD's parsers. The basics of writing a schema, using NOMAD's ELN (electronic lab notebook) integration, and how to create simple plots of your data to visualize in the GUI will be covered. Attendees will then use this knowledge to manage the remainder of the data from the example project workflow, which is not automatically recognized by NOMAD.

Tutorial O 1.4 Sun 17:30 H3

Creating custom workflow entries in NOMAD to link multiple uploads — •Bernadette Mohr — Physics Department and CSMB Adlershof, Humboldt-Universität zu Berlin, Germany

In this last part of the tutorial series, attendees will complete the example project workflow storage by creating a custom workflow entry in NOMAD that connects all the uploaded tasks. The basics of the schema for defining custom workflows will be covered, followed by a demonstration of the straightforward creation of the required workflow file using the same workflow utility Python module as in the first part of the tutorial series. Finally, attendees will navigate NOMAD's interactive workflow graph visualizations to investigate the uploaded data, and learn how to obtain a DOI for their workflow.

O 2: Tutorial: Do it Yourself Guide for Simulating Complex Magnetism: From Theoretical Foundations to Hands-on Spin-dynamics (joint session O/TUT)

This tutorial is designed for students, early-career researchers, and anyone interested in the foundational principles and practical methods for simulating magnetic materials. The journey begins with an introduction to the fundamentals of spin lattice Hamiltonians and their various forms, including a detailed discussion of their derivation (Lecture 1). Next, we explore state-of-the-art techniques for extracting magnetic exchange interactions from first-principles calculations through an engaging overview (Lecture 2). The final session (Lecture 3) delves into atomistic spin-dynamics simulations using the SPIRIT code, a versatile tool compatible with both smartphones and laptops. Throughout, we will emphasize the theoretical framework underpinning these approaches. The participants will have the freedom to explore a large range of phenomena, such as domain walls, skyrmions, and their dynamics under applied currents or torques.

Time: Sunday 16:00–18:15 Location: H10

Tutorial O 2.1 Sun 16:00 H10

Derivation of the spin-lattice Hamiltonian: Heisenberg, beyond Heisenberg, DMI, nematic exchange — •Hiroshi Katsumoto — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52428 Jülich, Germany

Magnetization textures, such as domain walls, skyrmions, or hopfions, are very active areas of condensed matter physics. These magnetic textures are usually explained based on the Heisenberg and the relativistic Dzyaloshinskii-Moriya interaction (DMI). Comparisons with experiments have shown that, in many cases, these interactions are insufficient, and a whole range (sometimes called a zoo) of higher-order symmetric and antisymmetric interactions have been proposed. In this tutorial, based on four elemental ingredients: Coulomb interaction, indistinguishability of electrons, spin, and spin-orbit interaction (SOI),

I present a framework for systematically constructing exact spin-lattice models containing all spin Hamiltonians, including higher-order terms dependent on spin quantum numbers and lattice size. Examples of spin Hamiltonians for spin-1/2 and spin-1 systems up to four lattice sites are discussed. The tutorial also explores higher-order relativistic exchange interactions derived from SOI. I consider perturbations up to the 2nd order of SOI and organize (anti)symmetric interactions. Finally, the classicalization of quantum spin relevant to magnetism in solids is discussed, culminating in a spin-lattice model that provides a theoretical framework for extracting material-dependent exchange interactions via numerical calculations and enables the modeling of magnetic textures. – DFG supports the work through SPP-2137 Skyrmionics.

Tutorial O 2.2 Sun 16:45 H10

Computing magnetic exchange interactions using DFT — •Manuel dos Santos Dias — Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom

Magnetic materials are an unending source of fascinating physical behaviour which have fundamental appeal but also important technological applications. In order to understand, quantify and predict the properties of magnetic materials, we need information about the magnetic exchange interactions (introduced in the preceding tutorial), which control how the different magnetic atoms interact with each other and respond to external stimuli. This tutorial will give an overview on first-principles approaches to the calculation of magnetic exchange interactions using density functional theory (DFT). First I will outline how the properties of magnetic materials can be computed with and what capabilities are offered by different DFT codes. Next I will discuss how to map DFT calculations to spin models and when such a mapping is expected to work, followed by a discussion of the two main approaches to compute magnetic exchange interactions: the infinitesimal rotation method and the spin cluster expansion. Lastly, I will explain how to obtain simple information from the computed magnetic exchange interactions, such as the magnetic ground state and the spin wave spectrum, and how to connect to atomistic spin dynamics (for instance using the Spirit code covered in the next tutorial), Monte Carlo and micromagnetic simulations.

Tutorial O 2.3 Sun 17:30 H10

Hands-on atomistic spin-dynamics simulations with Spirit — •Thorben Pürling[1,2] and Moritz Sallermann[1,2,3] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, D-52425 Jülich — [2]Physics Department, RWTH-Aachen University, D-52062 Aachen — [3]University of Iceland

Atomistic spin-dynamics is a powerful, fascinating and educational simulation approach to studying the stability and dynamics of mesoscopic spin-textures such as skyrmions on the basis of atomistic spin-models. It can be used as digital twin to experiments.In this tutorial, participants will be introduced to the atomistic spin model and learn interactively how to perform atomistic spin simulations using the Spirit code [1]. We will cover common computational methods employed in atomistic spin simulations, emphasizing their practical application through the Spirit software framework [2]. The majority of the session will be dedicated to engaging exercises, where participants will work through example problems using Jupyter notebooks that interface directly with Spirit. Participants are encouraged to come with basic knowledge of Python and bring their charged laptops to fully engage in the tutorial. We provide a website [3] to keep you updated such that you arrive at the tutorial prepared for a hands-on experience.

We acknowledge funding from the ERC grant 856538 (project "3D MAGIC").

[1] Gideon P. Müller *et al.*, 10.5281/zenodo.7746551 (2024)
[2] https://spirit-code.github.io
[3] https://spirit-code.github.io/dpg-regensburg2025

O 3: Overview Talk Kerstin Volz

Time: Monday 9:30–10:15 Location: H24

Topical Talk O 3.1 Mon 9:30 H24

Insights in real and electronic structure of interfaces by electron microscopy — •Kerstin Volz — Philipps-Universität Marburg, Center for Quantum Materials and Sustainable Technology (mar.quest) and Department of Physics, Hans Meerwein Str., 35032 Marburg, Germany

Internal interfaces between materials are decisive for the functionality of many devices. Hence, an understanding of the atomic as well as electronic structure across interfaces is essential. Electron microscopy can give insights into these properties from Angstrom to several micrometer length scales. With examples from semiconductors, batteries and 2D materials I will show, how Scanning Transmission Electron Microscopy (STEM) can be used to gain the desired information. Thereby, a focus will be on state of the art and quantitative techniques like 4-dimensional STEM, where real as well as momentum space are mapped to derive information on composition, but also on electric fields. These properties will be correlated to fundamental excitations of the charge carrier system at interfaces, e.g., excitons, probed by monochromated Electron Energy Loss Spectroscopy (EELS).

O 4: Solid-Liquid Interfaces: Structure

Time: Monday 10:30–13:00 Location: H4

O 4.1 Mon 10:30 H4

The Impact of the Gold Interface on the Structure and Properties of Aqueous Sodium Citrate Solution — •Elspeth Smith and Marialore Sulpizi — Ruhr-Universität Bochum, Bochum, Germany

Gold nanoparticles (AuNPs) are used widely, with many commercial applications due to their being well suited for catalysis. Owing to the method of production/stabilisation, AuNPs are often suspended in a solution of aqueous sodium citrate, a system with complicated interplays which we seek to elucidate in this work.

Through the use of a previously developed polarisable gold model we have performed all atom classical molecular dynamics simulations of a variety of systems and concentrations of sodium citrate solution, employing the SPC/E water model and a CHARMM based citrate model, with and without a gold interface. In order to better understand the dual effect of both the gold interface and sodium citrate on the water's structure, we employ a number of widely used order parameters for water. As the structure of water in close proximity to AuNPs is difficult to observe experimentally and has possibly large applications for their use in catalysis, we hope to obtain a better understanding of this elusive phenomenon.

O 4.2 Mon 10:45 H4

Rationalizing the "Anomalous" Electrochemical Stark Shift of CO at Pt(111) Through Vibrational Spectroscopy and Density-Functional Theory Calculations — •Elias Diesen[1], Mehmet Ugur Coskun[2], Sergio Díaz-Coello[2], Vanessa J. Bukas[1], Julia Kunze-Liebhäuser[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Department of Physical Chemistry, University of Innsbruck, Austria

We employ infrared reflection absorption spectroscopy (IRRAS) and first-principles density-functional theory (DFT) to revisit the reported "anomalous" negative Stark shift of the CO stretch frequency at Pt(111) in aqueous electrolyte [1]. Our measurements confirm the existence of a potential region with negative Stark shift around 0.5 V vs. RHE at sufficiently high CO concentration in the electrolyte. As these are exactly the same conditions for the occurrence of a phase transition from a (2×2)–3CO to a $(\sqrt{19} \times \sqrt{19})$R23.4°–13CO adsorbate structure [2], we explicitly compute the Stark shift for these two phases using DFT. Neither phase exhibits a negative Stark shift, but the absolute stretch frequencies of atop CO in the two structures are slightly shifted with respect to each other. Remeasuring IRRAS with high resolution indeed reveals a doublet character of the absorption band in the potential region corresponding to the negative Stark shift. Separate fits of the two components then yield positive Stark shifts in quantitative agreement with the calculated values.

[1] Stamenkovic et al., J. Phys. Chem. B 109, 678 (2005); [2] Wei et al., J. Phys. Chem. C 125, 3066 (2021)

O 4.3 Mon 11:00 H4

Adatom Dynamics at Water/Pt(111) Interface from Ab Initio Free Energy Analysis — •Sung Sakong[1], Jonas Lindner[2], Ulrich Ross[3], Michael Seibt[3], Christian Jooss[2], and Axel Gross[1] — [1]Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany — [2]Institute of Materials Physics, University of Göttingen, 37077 Göttingen, Germany — [3]4th Institute of Physics Solids and Nanostructures, University of Göttingen, 37077, Göttingen, Germany

Recent electron diffraction experiments investigated the local structures of the water/Pt(111) interface, a selected model system for investigating the structural properties of the electric double layer (EDL). The reconstructed phase signals of the diffraction data yield the time average of the interface structures with Angstrom resolution and observe the static Pt lattice and dynamic particles above the lattice. Since the time-averaged signals from experiments are often

challenging to relate to the corresponding atomic structures of dynamic particles, we probe the interface structure by including Pt adatoms using the ab initio molecular dynamics (AIMD) method. The free energy of Pt adatoms is analyzed by including the vibrational entropy calculated from the AIMD trajectories using the two-phase thermodynamics method. While the dynamics of water molecules are captured within the AIMD trajectories, the relatively slow Pt adatom dynamics are estimated by a free energy analysis, Blue Moon ensemble sampling. By comparing the Water/Pt(111) and Vacuum/Pt(111) models, we will discuss the role of surrounding water molecules and try to relate the model EDL configurations to the experimental findings.

O 4.4 Mon 11:15 H4

Effect of the damping function in dispersion corrected density functional theory on properties of liquid water — •Knut Nikolas Lausch[1,2], Redouan El Haouari[1,2], Daniel Trzewik[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Accounting for non-local dispersion interactions is essential to achieve chemical accuracy when applying approximate density functional theory (DFT) to large molecular or condensed systems. A popular approach is to add a damped correction potential, based on the London formula, after convergence. Damping is required to avoid the diverging short-range behavior of the London formula and double counting of interactions treated locally by the exchange-correlation (xc) functional. Often two forms of damping, known as zero- and Becke-Johnson-damping, are employed and it is generally assumed that the choice has only a minor impact on performance even though the resulting correction potentials differ quite dramatically. Here, we demonstrate that the choice of damping function can have a major impact on properties obtained from molecular dynamics simulations of liquid water suggesting that the significance of damping in dispersion corrected DFT needs to be reevaluated.

O 4.5 Mon 11:30 H4

Elucidating the double layer structure of protic ionic liquid electrolytes for next-generation fuel cells — •Christian Rodenbücher, Yingzhen Chen, Federico Parisi, Piotr M. Kowalski, and Carsten Korte — Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-3 & IET-4), 52425 Jülich, Germany

Polymer electrolyte membrane fuel cells (PEMFCs) are the backbone of a future hydrogen-based renewable energy system. Increasing their operation temperature to 100–160 °C would allow for a simpler water management and the use of waste heat. In this temperature range, conventional proton conducting polymers such as Nafion are not applicable, since they rely on the presence of water. Hence, we study immidazolium-based protic ionic liquids, which provide a high thermal and chemical stability and a high proton conductivity. We present experimental investigations using impedance spectroscopy, infrared spectroscopy, and atomic force microscopy combined with atomistic simulations by molecular dynamics and density functional theory. Our results reveal that depending on the electrode charge, a dense layered structure of alternating anion and cation layers is formed. Upon the addition of water, which is naturally produced during fuel cell operation, the structuring becomes distorted resulting in the accumulation of water at the interface and the increase of the onset potential of the oxygen reduction reaction. Our findings illustrate that the kinetics of the fuel cell reactions is influenced not only by bulk properties of the electrolyte but also by the adsorption at the electrode, which may be tuned by designing ionic liquids with bespoke properties.

O 4.6 Mon 11:45 H4

Polarizable model of graphite and its applications to nanotechnology — Krishan Kanhaiya[1], Hendrik Heinz[2], and •Marialore Sulpizi[3] — [1]Ruhr-Universität Bochum — [2]University of Colorado Boulder — [3]Ruhr-Universität Bochum

Graphitic materials are of significant importance in the research and industrial community due to their tunable electrical conductivity, band gap, thermal property and high strength to mass ratio. They are used in battery or fuel cells as electrodes, refractory material, lubricant, aerospace, water purification, and biosensing etc.. We present a realistic, all-atom polarizable model of graphite with flexible dummy electrons to model the polarizable nature of electron cloud, similar to the approach which was used to describe image charge effects for ions approaching metal surfaces. The models predict density, lattice parameters, surface energy, hydration energy, water contact angle and elastic constants within 1%, 1%, 5%, 5%, 5% and ~15 % respectively as per the Interface Force Field protocol. Additionally, the model also reproduces experimental and DFT data on binding energies and profiles for cations , anions and neutral molecules (water, amino acids, and organic molecules). We further discuss friction coefficient across the graphene surface and nanotubes in order to model flow characteristics of water over such surfaces . An accurate description of such systems is key to design improved functional materials and devices for water desalination and blue energy (electric energy from salinity gradient in two different electrolyte solutions).

O 4.7 Mon 12:00 H4

Elucidating the interaction of small organic pollutants at ice surfaces with sum-frequency generation spectroscopy — •Gurivi reddy Yettapu[1,2], Luca B. Manning[2], and Jenee D. Cyran[2] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Boise State University, Boise, USA

Small organic pollutants interacting with ice and water surfaces in the troposphere are relevant for atmospheric compositional changes.[1] Their interactions with hexagonal basal-plane oriented single crystalline ice have been scarcely revealed.[2] Methanol and acetone are two smallest organic molecules that interact differently with single crystalline ice surfaces. Herein, we probed their direct interaction on ice and water interfaces with surface-specific, mode selective sum-frequency generation spectroscopy. Our results show significant difference in the frequency of H-bonding O-H oscillators of water molecules present at the ice interface.[3] The distinct behavior of the adsorption of these molecules could explain their relevant atmospheric compositions. [1] F. Dominé and P. B. Shepson, Science, 297, 1506-1510 (2002). [2] J. D. Cyran et al., Angew. Chem. Int. Ed., 58, 3620-3624 (2019). [3] G. R. Yettapu et al., Faraday Discussions, just accepted (2024).

O 4.8 Mon 12:15 H4

Exploring Charged Aqueous Interfaces with Depth-Resolved SFG/DFG Vibrational Spectroscopy — •Sarabjeet Kaur, Álvaro Díaz Duque, Alexander Fellows, Martin Wolf, and Martin Thämer — Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society

Charged aqueous interfaces are crucial in biological, atmospheric, and chemical processes, where surface electric fields influence ion distributions and interfacial dynamics. Water mediates these interactions, with effects spanning nanometers. The Gouy-Chapman (GC) model and variants describe ion distributions but oversimplify water as a continuous medium, neglecting molecular-level behaviors like impact of structure, orientation, and hydrogen-bonding dynamics. This omission leaves important aspects of interfacial phenomena unexamined. We address these gaps using depth-resolved vibrational spectroscopy combining phase-resolved sum- and difference-frequency generation (SFG and DFG). This technique reveals depth-dependent water responses and connects electric potential anisotropy with molecular reorientation. Our findings identify two distinct interfacial layers, challenging the single-layer GC model. Spectral analysis shows structural differences between the compact and diffuse layers. Additionally, concentration-dependent studies highlight discrepancies between the observed decay length of orientational anisotropy and the predicted Debye length. These results underscore the limitations of the GC variant model and continuum solvent approaches in capturing water's molecular-level behavior at charged interfaces.

O 4.9 Mon 12:30 H4

Resolving the water structure at iron-oxide/water interface — •Harsharan Kaur[1], Moritz Zelenka[1,2], and Ellen Backus[1,2] — [1]University of Vienna, Faculty of Chemistry, Institute of Physical Chemistry, Währinger Str. 42, 1090 Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Among different iron-oxide polymorphs, Fe3O4 is utilized as a catalyst for industrial-gas shift and photocatalytic water splitting reactions, where it often encounters water. [1] Fe3O4 surface is known to protonate and deprotonate on contact with pH-variant aqueous media. [1] However, less is known about the interfacial species and their molecular orientation under ambient condition. Herein, we explore these attributes at the magnetite-water interface as function of solution pH with macroscopic amount of water. Magnetite films of ~50 nm thick were prepared using magnetron sputtering and were found to sustain Fe3O4 phase combined with FeO or γ-Fe2O3 state. The interface was examined with SFG vibrational spectroscopy. Due to its selection rule, a vibrational spectrum of only the interfacial species is obtained in case of centrosymmetric bulk materials like Fe3O4 and water. We observed a pH-dependent variation in the H-bonding strength of the interfacial water molecules and the presence of Fe-OH groups at alkaline pH. Besides, the water orientation varies with pH. By comparing the results for Fe3O4 to Fe2O3, a detailed molecular picture of interfacial water at these relevant iron oxides will be presented. [1]. Z. Bielan, S. Dudziak, A. Kubiak, E. Kowalska, Appl. Sci. 11 (2021) 10160.

O 4.10 Mon 12:45 H4

Structural and dynamical properties of the Solvated Electron From Ab Initio Molecular Dynamics Simulations — •Anna Karolyna Macieira Silva Gomes and Marialore Sulpizi — Ruhr-University Bochum, Bochum, Germany

The solvated electron is a critical species in plasma/liquid and plasma/solid/liquid interfaces, serving as the primary reducing agent generated at plasma electrodes in contact with liquids. Recently, experimental studies have revealed differences in the properties of solvated electrons formed via plasma compared to other methods, such as water radiolysis. It has been proposed that the unique conditions at plasma interfaces, including electric fields, may alter the electron's solvation properties.

Despite extensive investigations into solvated electrons, their behavior in the presence of electric fields remains unexplored. This project employs atomistic molecular dynamics simulations to explore the influence of electric fields on the structure and dynamics of solvated electrons in aqueous solutions. Ab Initio Molecular Dynamics (AIMD), utilizing hybrid functionals, have been shown to offer a accurate approach to modeling the electronic properties of this system, while remaining computationally feasible for capturing relevant time and length scales.

O 5: Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale I

Time: Monday 10:30–13:00 Location: H6

O 5.1 Mon 10:30 H6

Simulated tip-enhanced Raman scattering fingerprints of doped triangulenes — •Orlando Silveira[1,2], Markus Junttila[1], Shawulienu Kezilebieke[2,3], and Adam Foster[1,4] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Department of Physics, Nanoscience Center, University of Jyvaskyla, Jyvaskyla, Finland — [3]Department of Chemistry, University of Jyvaskyla, Jyvaskyla, Finland — [4]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa, Japan

Triangulenes are organic molecules promising for future applications in spintronics technologies, and fine tunning their electronic and magnetic properties will only extend the potential applications. A reliable possibility for such control is doping the triangulenes with different atoms such as nitrogen and boron. Usually, the reaction yield of triangulenes is quite small, and it is prohibitive to use techniques with high cross section such as Raman to chemically characterize the triangulenes. In the other hand, scanning probe microscopy (SPM) techniques have been successfully used for their structural characterization. In this work, we propose that the tip-enhanced Raman scattering (TERS) can be used for simultaneous chemical and structural characterization of the triangulenes. Our work offers a new perspective to study the triangulenes, as their vibrational properties have not yet been fully investigated, and the same simulation protocol used here can be applied to any other type of molecule.

O 5.2 Mon 10:45 H6

Plasmon-induced reaction in hydrogen-bonded molecular networks studied by laser-coupled STM — •Youngwook Park, Adnan Hammud, Martin Wolf, and Akitoshi Shiotari — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Hydrogen-bonded molecular networks are widely found in natural systems and play an important role in the development of functional molecular assemblies. Understanding chemical reactions within these networks requires molecular-level spatial resolution, which is challenging for photochemical studies. In this talk, we present a plasmon-induced reaction in 2D hydrogen-bonded assemblies, studied with a laser-coupled scanning tunneling microscope (STM). We investigated triphenylene-2,6,10-tricarboxylic acid forming a honeycomb network on Au(111) through hydrogen bonds. Our findings showed that photo-induced deformation of the network was localized to a few molecules beneath the Ag tip under visible laser illumination. In contrast, a PtIr tip, which lacks plasmonic activity in the visible range, failed to trigger the reaction. By varying the laser wavelength, we identified that non-thermal (hot) electrons generated by plasmons mediate the reaction. This was confirmed by initiating the reaction with non-thermal electrons from the STM tip without laser irradiation. Our results highlight the potential of plasmonic STM tips for precise control over molecular network structure and reactivity.

O 5.3 Mon 11:00 H6

Motion of molecular motors on ultra-thin NaCl islands on Cu(111) — •Monika Schied[1,2], Grant J. Simpson[1], Ken Kolar[1], Dongdong Liu[3], James M. Tour[3], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]CNR-IOM, Italy — [3]Rice University, USA

Molecular motors are designed to overcome nature's random motion by converting external energy into controlled, uni-directional rotation. Studying them on a solid surface can be advantageous, as it offers confinement in two dimensions, making it easier to observe the directionality of their motion. In previous studies on metallic surfaces, indeed uni-directional rotation has been observed [1]. However, the activation of the motor functionality is likely suppressed due to the hybridisation of the molecular orbitals with the electron bath of the metal. In order to preserve the inherent electronic structure of the free molecule, we studied Feringa-type motors adsorbed on ultra-thin NaCl layers on Cu(111), which electronically decouples them from the metal substrate, while still permitting measurements with the low-temperature scanning tunnelling microscope (LT-STM). We excited the molecules with UV light, which – in contrast to voltage pulses – acts remotely without altering the local potential energy landscape with the STM tip. In this way, we could induce the motion of individual molecules.

[1] M. Schied et.al., ACS Nano 2023, 17, 4, 3958-3965

O 5.4 Mon 11:15 H6

Triggering chemical reactions in single molecules with ultrashort THz pulses — •Niklas Friedrich, Carmen Roelcke, Tzu-Chao Hung, Yaroslav Gerasimenko, Rupert Huber, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

In lightwave-driven scanning tunnelling microscopy (LW-STM), the electric-field transient of ultrashort laser pulses focused into the junction of a tunnelling microscope acts as a bias-voltage transient and thereby controls tunnelling on ultrashort timescales. This allows unravelling the dynamics of quantum systems in pump-probe experiments with atomic spatial and femtosecond temporal resolution [1].

Here, we show that LW-STM can be used to trigger chemical reactions on ultrashort timescales. We study free-base naphthalocyanine molecules (H2Nc) on 2ML NaCl on Cu(111). In DC-biased experiments, this system switches between different tautomers upon injection of high-energy tunnelling electrons [2]. We find that the same reaction is facilitated by ultrashort voltage transients in LW-STM for transients far exceeding the voltage of the lowest unoccupied molecular orbital. Furthermore, even a stepwise deprotonation of the molecule is activated by the ultrashort laser pulses when increasing the voltage transient beyond a threshold value.

[1] Roelcke et al. Nat. Photon. 18, 595-602 (2024) [2] Liljeroth et al. Science 317, 1203-1206 (2007)

O 5.5 Mon 11:30 H6

Spatial coherent phonon spectroscopy on 2H-$MoTe_2$ using THz-STM — •Vibhuti Rai, Junyoung Sim, Florian Faaber, Sergey Trishin, Nils Bogdanoff, Tom Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

Scanning tunneling microscopy (STM) offers subnanometer spatial resolution. However, it lacks the temporal resolution required to investigate the dynamics of various elementary excitations such as phonons. By integrating STM with a pump-probe scheme that utilizes two terahertz (THz) pulses acting as transient bias voltages, subpicosecond time resolution can be achieved [1,2]. Here, we demonstrate that our custom-built THz setup, combined with an STM operating at 5K in an ultra-high vacuum, can be used to excite and detect lattice vibrations on the surface of 2H-$MoTe_2$. The time-resolved spectrum shows a long-lasting oscillatory signal that is sensitive to surface defects [3,4]. Fourier analysis reveals the presence of two prominent excitation modes. We correlate the excited modes with coherent phonons. The spatial variation of such coherent phonon spectroscopy further reveals that one of the two excited modes are enhanced by the surface defects.

[1] Cocker, et al. Nat. Photon. 7, 620-625 (2013)
[2] Yoshida et al. ACS Photonics 6, 6, 1356-1364 (2019)
[3] Liu et al. Sci. Adv. 8, eabq5682 (2022)
[4] Roelcke et al. Nat. Photon. 18, 595-602 (2024)

O 5.6 Mon 11:45 H6

Charge Transfer in Lightwave-Driven Scanning Tunneling Microscopy — •Nils Krane, Jonas Allerbeck, Laric Bobzien, S. Eve Ammerman, and Bruno Schuler — Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Lightwave-driven STM is a promising technique for exploring ultrafast charge-state dynamics at nanoscale. The tip electrode of the STM provides spatial resolution at the single-atom level, while single-cycle lightwave pulses supply an ultrafast voltage source at GHz to multi-THz frequencies that injects charge carriers to the system. In contrast to optical far-field measurements, the STM tip interacts with the investigated system also between the pulses where the applied voltage is low. This allows for ultrafast back tunneling of electrons from an excited charge state via discharging to the tip electrode, resulting in zero net current. Equal magnitude of forward and backward tunneling hence quenches the time-integrated charge rectification and imposes a major challenge on investigating ultrafast nanoscale charge dynamics. In this talk, I discuss the consequences of back tunneling for lightwave-driven STM and time-domain pump-probe techniques, at the example of picosecond charge-state lifetimes related to selenium vacancies in WSe_2 studied with THz-STM. I outline pathways to overcome this challenge by utilizing effects such as the Franck-Condon blockade or spin multiplicity for the promotion of unidirectional charge transport. A theoretical model

based on the master equation, accurately reproduces the time-dependent tunneling processes observed in the experiments.

O 5.7 Mon 12:00 H6

Ultrafast Coulomb blockade in an atomic-scale quantum dot — Jonas Allerbeck[1], •Laric Bobzien[1], Nils Krane[1], S. Eve Ammerman[1], Daniel E. Cintron Figueroa[2], Joshua Robinson[2,3], and Bruno Schuler[1] — [1]Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]Department of Chemistry, The Pennsylvania State University, University Park, 16802, PA, USA — [3]Department of Physics and Department of Materials Science and Engineering, The Pennsylvania State University, University Park, 16802, PA, USA.

Controlling electron dynamics at optical clock rates is a fundamental challenge in lightwave-driven nanoelectronics. At the example of individual selenium vacancies (Vac_{Se}) in few-layer tungsten diselenide (WSe_2), which are prototypical atomic-scale quantum dots with localized defect states, I present ultrafast charge transfer in the time domain using lightwave-driven scanning tunneling microscopy (LW-STM). Layer-dependent decoupling of Vac_{Se} in WSe_2 varies the average charge-state lifetime of defect states from 1.2 ps (1L) to 3 ns (4L), showing an unexpected sub-exponential. Picosecond terahertz (THz) source pulses, focused onto the picocavity of the STM, control and read the charge state of individual Vac_{Se} quantum dots. THz pump-THz probe time-domain sampling of the defect charge population captures atomic-scale snapshots of the transient Coulomb blockade, a signature of charge transport via quantized defect states. These results open new avenues for exploring charge dynamics and lightwave-driven electronics at the space-time limit.

O 5.8 Mon 12:15 H6

THz Pulse induced Luminescence in a Scanning Tunneling Microscope — •Kurt Lichtenberg, Johannes Schust, Felix Huber, Ines Hartkopf, Susanne Baumann, and Sebastian Loth — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Light-matter interaction at the atomic scale lies at the heart of many processes in nature and technology, ranging from light harvesting to quantum communication applications. But experimental tools to access the respective dynamics at this scale with sufficient time resolution are rare.

Here we show a proof-of-concept combination of the ultrafast time resolution of THz scanning tunneling microscopy (THz STM) with tunneling-induced light emission at the atomic scale (Scanning Tunneling Luminescence).

We use intense sub-cycle THz pulses to excite plasmons in the tunnel junction consisting of a gold tip and a bare silver sample. We find that THz-induced voltage transients ignite luminescence in ultrashort time intervals within a fraction of a single period of the THz pulse that was used for the excitation. These ultrafast luminescence bursts can be used to sample the waveform of a second THz pulse with femtosecond time resolution.

This work contributes to a new line of methodology, that can probe the rich dynamics of light emission from single atoms and molecules.

O 5.9 Mon 12:30 H6

Ultrafast manipulation of charge-density wave order with THz-STM — Shaoxiang Sheng[1,2], Kurt Lichtenberg[1], Susanne Baumann[1], and •Sebastian Loth[1,3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany

Charge-density wave (CDW) materials present unique opportunities for exploring the interplay between structural distortions and the collective dynamics of complex electronic phases at the atomic scale. We use terahertz spectroscopy in the scanning tunneling microscope (THz-STM) to investigate charge-order dynamics in the prototypical CDW materials 2H-$NbSe_2$ and 1T-TaS_2. By employing tip-enhanced terahertz electric fields, we directly excite phase dynamics of the charge order and probe their local electronic response by terahertz-induced electron tunneling. Our measurements show that the incommensurate CDW of $NbSe_2$ features slow phase dynamics in the proximity of defects [1], whereas the commensurate CDW of TaS_2 exhibits fast reconfigurations within individual domains. The presented spatially resolved dynamics of CDWs demonstrate how atomically localized THz excitation can be leveraged to manipulate electronic states with femtosecond temporal precision, offering insights into the fundamental mechanisms of electronic or structural phase transitions in different materials.

[1] S. Sheng, et al., Nat. Phys. 20, 1603 (2024).

O 5.10 Mon 12:45 H6

Tracking phonon-induced electronic dynamics on atomic scale with ultrafast tunnelling spectroscopy — Carmen Roelcke, Lukas Kastner, Maximilian Graml, Jan Wilhelm, Jascha Repp, Rupert Huber, and •Yaroslav Gerasimenko — Department of Physics and Regensburg Centre for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg, Germany

Atomic-defect-based quantum systems in monolayers and moiré heterostructures of 2D materials have attracted huge interest for their qubit and single-photon emission functionalities, but directly observing the interplay of their electronic structure with elementary excitations remained a long-held dream.

We directly resolve in space, time and energy how spin-orbit-split bound states of an individual Se vacancy – an atomic single-photon emitter – evolve under coherent lattice vibrations in moiré-distorted WSe_2 using lightwave-driven scanning tunnelling spectroscopy [1]. We selectively launch a drum phonon mode with a THz pulse coupled to the tip and take ultrafast snapshots of electronic spectrum on atomic scales faster than a vibration period. Such ultrafast tunnelling spectra reaching ~300 fs temporal resolution reveal transient energy shifts of the lower vacancy state by up to 40 meV, depending on the amplitude and phase of the coherent lattice vibration. We discuss how THz fields can couple via the Coulomb interactions to the drum mode, and how the interplay of Se-W bonds distortion and image charge renormalization affect the energy levels of the vacancy.

[1] C. Roelcke et al., Nat. Photon. 18, 595-602 (2024)

O 6: Oxides and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Monday 10:30–12:45 Location: H8

O 6.1 Mon 10:30 H8

Characterizing Approximants of Oxide Quasicrystals with a Novel Geometric Approach — •Martin Haller, Sebastian Schenk, Stefan Förster, and and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Oxide quasicrystals (OQCs) are aperiodic 2D oxide films exhibiting dodecagonal symmetry, which are grown on hexagonal metal substrates. This dodecagonal symmetry arises from a square-triangle-rhombus tiling, derived from Ba, Sr, or Eu hosted within a Ti-O network [1]. Approximants are periodic structures composed of the same tiling elements, thus exhibiting a close structural relationship to the OQC. Variations in stoichiometry lead to the emergence of different approximant structures, ranging from simple tilings with a triangle:square:rhombus frequency ratio of 4:2:0 to more complex configurations such as the 60:22:8 approximant [2]. In this presentation, we will introduce newly discovered approximant phases identified in the Sr-Ti-O/Pd(111) and Eu-Ti-O/Pd(111) systems through STM and LEED. Specifically, we will discuss two hexagonal approximants with tiling frequency ratios of 20:3:6 and 8:0:3, as well as an oblique 10:3:2 approximant. Additionally, we will apply a novel geometric approach for characterizing the tilings derived from STM data [3]. This innovative method provides a measure in a 4D hyperspace for classifying the relationship of approximants to the parent OQC.

[1] Schenk et al., Nature Communications, 13, 7542 (2022)
[2] Wührl et al., Phys. Rev. B, 107, 195414 (2023)
[3] Imperor-Clerc et al., Phys. Rev. B, 110, 144106 (2024)

O 6.2 Mon 10:45 H8

Chromium Oxide Thin Films on Pt(111): An STM and DFT Excursion through the Phase Diagram — •Ghada Missaoui[1], Piotr Igor Wemhoff[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Formation of chromium oxide thin films on Pt(111) was investigated by electron diffraction and low-temperature scanning tunneling microscopy. Depending on the nominal Cr coverage and the oxygen-chemical potential used for preparation, two oxide phases were identified. A $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase emerges at sub-monolayer Cr exposure and O-rich oxidation conditions, while a (2x2) phase develops at higher coverage and after a vacuum-annealing step. For both phases, the atomic nature of cationic and anionic sub-lattices and the chemical composition were determined in detail. Guided by this experimental input, a global structure optimization was performed by genetic algorithms and key configurations were refined by density functional theory calculations afterwards. For the $(\sqrt{3} \times \sqrt{3})R30^\circ$ phase, good agreement was revealed for a Cr_3O_6 trilayer, comprising a mixture of Cr^{3+} and Cr^{4+} ions in the central cationic plane. The (2x2) phase matches well a Cr_6O_{11} film, in which an O-Cr-O trilayer is capped by a Cr_2O_3 honeycomb plane. The identified configurations not only reproduce structure and symmetry deduced from experiment but also have the most favorable energetics at the employed oxygen chemical potential.

O 6.3 Mon 11:00 H8

Ferroelectric perovskite oxides: from bulk to surface polarization — •Dominik Wrana[1], Llorenç Albons[2], Marta Macyk[1], Andrzej Jasicki[1], Aji Alexander[2], Jesus Redondo[2], Igor Sokolovic[3], Pavel Kocan[2], Konrad Szajna[1], Martin Setvin[2], and Franciszek Krok[1] — [1]Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czechia — [3]Institute of Applied Physics, TU Wien, Vienna, Austria

In leveraging the spontaneous polarization of ferroelectrics for photo-, pyro-, and piezocatalysis, it is essential to develop a comprehensive model of ferroelectricity's impact on perovskite surfaces.

Here we investigate oxide perovskites, which are known to exhibit record-high efficiencies toward water spitting. Careful analysis of ferroelectricity exhibited on surfaces of single crystals of as-cleaved ferroelectric $BaTiO_3(001)$ and $KNbO_3(001)$ compared to quantum paraelectric $KTaO_3(001)$ reveals phenomena at both single-atom and macroscales. Polarization optical and scanning electron (SEM) microscopy data provides the spatial information of 90° ferroelectric domains, which typically have a width of 5-20 μm and length of up to hundreds of um. Actual domain structure and their directionality are provided by piezoresponse force microscopy (PFM) imaging, which also provides the correlation of surface reactivity with polarization.

qPlus ncAFM is used to demonstrate a reversible ferroelectric polarization of (1x1) surfaces at the nanoscale, by application of different tip-sample bias voltages.

O 6.4 Mon 11:15 H8

The influence of strain-induced ferroelectricity on the fracture of oxide perovskites — •Christian Ritterhoff and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

The cleaving of bulk crystals using mechanical force is a common procedure to obtain well-defined surfaces under UHV conditions. While this method avoids chemical changes in the surface composition due to etching and annealing procedures, the strain necessary for cleavage can induce ferroelectric phase transitions during the fracture process whose influence is still visible on the as-cleaved surface, as shown, for example, by Sokolović *et al.* [1] for mechanically cleaved $SrTiO_3$.

Here, we present density-functional theory calculations to discuss the influence of increasing strain on the magnitude of possible ferroelectric distortions and the development of a spontaneous polarization for three prototype perovskite oxides: cubic $SrTiO_3$, ferroelectric $BaTiO_3$, and polar $KTaO_3$. First, we estimate the critical strain for mechanical cleavage in fracture Mode 1 and Mode 2. Subsequently, we calculate the polarization of the material at the point of fracture and discuss the implication on surface charges and the formation of surface defects.

[1] I. Sokolović, M. Schmid, U. Diebold, M. Setvín, Phys. Rev. Mater. **3** (2019) 034407

O 6.5 Mon 11:30 H8

Segregation Effects in 2D Mixed Oxide Nano-Islands: Edge Structure and Composition in Mixed V-Fe Oxide Monolayers — Ying Wang[1], Piotr Igor Wemhoff[1], Ghada Missaoui[1], •Niklas Nilius[1], Jacek Goniakowski[2], and Claudine Noguera[2] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Low-coordinated atoms residing at the edges of oxide nanostructures play an important role in heterogenous catalysis. Their local configuration is however hardly available, especially for ternary materials with variable stoichiometry. In this study, low-temperature STM is employed to analyze the edge configurations of V-Fe-O honeycomb islands grown on Pt(111) as a function of film composition. The islands are delimited by zigzag and armchair edges, the latter with a tendency to reconstruct into sequences of four, five, six and seven-membered rings. STM spectroscopy is used to identify the chemical nature of the edge atoms. The thermodynamic forces for V or Fe segregation to the edges, both oxygen and cation terminated, are analyzed by DFT calculations. In an oxidizing environment, formation of vanadyl-terminated (VO-) edges is energetically favorable, while Fe atoms segregate towards the edges at O-poor conditions. The observed behavior is explained by the higher oxygen affinity of V versus Fe edge cations, and reflected in the higher stability of terminal vanadyl compared to ferryl groups. Our findings indicate a new pathway to tailor the chemical composition and catalytic reactivity of oxide edges via cationic mixing.

O 6.6 Mon 11:45 H8

Mapping the Energy-Angle-Landscape in lab-based X-ray photoelectron spectroscopy for Depth Profiling of Oxide Layers — •Martin Wortmann[1,4], Beatrice Bednarz[2], Olga Kuschel[2,3], Klaus Viertel[4], Negin Beryani Nezafat[5], Jan Schmalhorst[1], Gabi Schierning[5], Joachim Wollschläger[3], Andreas Hütten[1], and Timo Kuschel[1,2] — [1]Bielefeld University, Bielefeld, Germany — [2]Johannes Gutenberg University Mainz, Mainz, Germany — [3]University of Osnabrück, Osnabrück, Germany — [4]Bielefeld University of Applied Sciences, Bielefeld, Germany — [5]University of Duisburg-Essen, Duisburg, Germany

Many metals are reactive to atmospheric oxygen, forming stable nanometer-thin oxide layers by spontaneous self-passivation. Such native oxide layers are commonly analyzed by X-ray photoelectron spectroscopy (XPS). We previously introduced a method to calculate depth profiles from single fixed-angle spectra by fitting all emission peaks instead of just one, thus resembling energy-resolved XPS without the need for a synchrotron [1]. Here, we combine this approach with angular-dependent measurements, fitting the measured intensity ratios of oxide and metal as a function of energy (i.e. inelastic mean free path) and angle. This method not only improves the accuracy of earlier models and peak fittings but also paves the way for a more holistic understanding of the XPS spectrum.

[1] Wortmann et al., Small Methods 8(3), 2300944 (2024)

O 6.7 Mon 12:00 H8

The polar spinel $MgAl_2O_4$ (001) surface is stabilized by an aluminum-rich reconstruction — •David Kugler[1], Andrea Conti[1], Johanna I. Hütner[1], Soumyajit Rajak[2], Matthias Meier[1], Nan Jiang[2], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], Gareth S. Parkinson[1], and Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Department of Chemistry, University of Illinois Chicago, USA

The atomic-scale surface structure of spinel oxides is key to understanding their catalytic properties. Magnesium aluminate ($MgAl_2O_4$, spinel), which gave this class of materials its name, is a wide-gap insulator and poses considerable challenges for experimental surface structure determination. Noncontact atomic force microscopy (nc-AFM) with a qPlus sensor and a well-defined tip apex allowed us to directly resolve the surface structure with atomic resolution and chemical sensitivity. The $MgAl_2O_4(001)$ surface adopts a $c(2\times4)$ reconstruction accompanied by an increase of the Al/Mg ratio, as detected by x-ray photoelectron spectroscopy (XPS). The reconstructed surface is enriched in aluminum and contains ordered pairs of octahedrally coordinated magnesium atoms replacing their tetrahedral bulk sites. This charge redistribution within the reconstructed surface layer stabilizes the otherwise polar $MgAl_2O_4(001)$ termination. The proposed surface reconstruction is similar to those observed on other spinel oxides, such as $Fe_3O_4(001)$ and $Mn_3O_4(001)$, suggesting a universal mechanism for compensating the polarity of spinel (001) surfaces.

O 6.8 Mon 12:15 H8

Elucidating the Growth Mechanism of 2D GaS on Sapphire in a Multitechnique Approach — •Stefan R. Kachel[1,2], Robin Günkel[2], Leonard Neuhaus[1], Oliver Massmeyer[2], Lukas Erlemeier[1], Kassandra Zoltner[1], Florian Münster[1], Carsten von Hänisch[1], Kerstin Volz[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Germany — [2]Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Germany

The utilization of 2D layers of GaS with its ultraviolet bandgap holds promise for applications in solar-blind photodiodes and LEDs. However, the growth of these 2D layers remains a significant challenge, driving considerable interest in understanding the growth mechanism underlying the metal-organic chemical vapor deposition (MOCVD) process. This study investigates the growth of 2D GaS using conventional precursors as well as a newly synthesized single-source precursor (SSP) on sapphire in a multitechnique approach. Scanning transmission electron microscopy (STEM) reveals that the formation of a closed Ga layer on the sapphire surface is a prerequisite for GaS growth. This finding is supported by temperature-programmed desorption (TPD) experiments showing intact desorption of the S-precursor, while the Ga-precursor decomposes partially even at low temperatures, leaving Ga residues on the surface, as confirmed by X-ray photoelectron spectroscopy (XPS). The new SSP enables the deposition of thin mixed layers of Ga and S on sapphire. Refining such single-source precursors could provide a pathway toward efficient growth of 2D GaS.

O 6.9 Mon 12:30 H8

Surface Reconstructions Govern Ice Nucleation on Silver Iodide – A Noncontact-AFM Investigation — •Johanna I. Hütner[1], Andrea Conti[1], David Kugler[1], Franziska Sabath[3], Florian Mittendorfer[1], Michael Schmid[1], Angelika Kühnle[2], Ulrike Diebold[1], and Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, 1040, Austria — [2]Department of Chemistry, Bielefeld University, Bielefeld, 33615, Germany — [3]Max Planck Institute for Polymer Research, Mainz, 55128, Germany

Silver iodide (AgI) is used as a cloud seeding material due to its ability to nucleate ice efficiently, which is explained by the good lattice match between AgI and hexagonal ice. However, AgI consists of stacked planes of positively charged Ag^+ alternating with negatively charged I^-. Cleaving a AgI crystal along the (0001) plane thus exposes Ag^+ and I^- terminated surfaces. Both terminations are polar and inherently unstable.

We present atomically resolved noncontact atomic force microscopy (NC-AFM) images that show how AgI(0001) surfaces compensate for this non-zero electric dipole perpendicular to the surface. Both Ag and I terminated surfaces

form reconstructions, whose structure affects their ice nucleating abilities. NC-AFM images of UHV-cleaved surfaces exposed to water vapor reveal that ice forms an epitaxial layer only on the Ag terminated surface, whereas on the I termination ice forms three-dimensional clusters.

These atomic-level observations could enhance our understanding of ice formation processes in the atmosphere.

O 7: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit I

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Monday 10:30–12:45 Location: H11

O 7.1 Mon 10:30 H11

Ultrafast Low-Energy Electron Microscopy — •Johannes Otto[1,2,3], Leon Brauns[1,2], Benjamin Schröder[1,2], and Claus Ropers[1,2,3] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Max Planck School of Photonics

Low-Energy Electron Microscopy (LEEM) allows for imaging the first atomic layers of a surface with nanometer resolution by reflecting a low-energy electron beam [1]. This contribution reports on the first implementation and initial results of Ultrafast LEEM. We replaced the electron source of a conventional instrument with a laser-triggered tip-shaped photoemitter enabling imaging with nanometer spatial and picosecond temporal resolution [2]. We show first real-space dynamics including a thermally-induced intensity suppression (transient Debye-Waller effect) and strain-wave propagation. Additionally, we report on stimulated inelastic electron-light scattering (IELS) at beam energies below 100 eV, as recently proposed theoretically [3]. The demonstrated capabilities of the instrument open up new possibilities to investigate a wide range of dynamical phenomena at surfaces.

[1] W. Telieps and E. Bauer, Surface Science 162, 163 (1985).
[2] A. Feist et al., Ultramicroscopy 176, 63 (2017).
[3] A. P. Synanidis et al., Sci. Adv. 10, eadp4096 (2024).

O 7.2 Mon 10:45 H11

Ultrafast Electron Dynamics in Surface Plasmon Polariton Nanofoci — •Pascal Dreher, Alexander Neuhaus, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

Surface plasmon polaritons (SPPs) are collective wave-like excitations of the electron system of a metal surface that hold great potential for enhancing light-based energy conversion processes. Such enhancement is based on the efficient generation of highly-excited hot electrons via the decay of SPPs on a femtosecond timescale. To understand the corresponding microscopic dynamics, it is essential to gain a direct view into the plasmonically-generated hot electron distributions and to distinguish them from optically-generated hot electrons.

We achieve these goals by combining topologically-robust SPP nanofoci with time- and angle-resolved photoelectron spectroscopy in a photoemission microscope. This approach allows us to investigate the ultrafast non-equilibrium electron dynamics driven by SPPs on the native length-, momentum-, time-, and energy scales. We observe plasmonically-driven above-threshold electron emission, and ponderomotive shifts of the electron emission spectra provide us with a direct measure of the local SPP field strength. For different exemplary metal surfaces with distinct surface band structures we gain a direct view into the hot electron distributions generated via the coherent and incoherent decay of SPPs.

O 7.3 Mon 11:00 H11

Mechanisms and Dynamics of Electron Emission from Graphitic Surfaces: Insights from Correlated and Time-Resolved Spectroscopies — •Alessandra Bellissimo[1], Florian Simperl[1], Felix Blödorn[1], Wolfgang S.M. Werner[1], Gyula Halasi[2], László Óvári[2], Csaba Vass[2], Nikolett Oláh[2], Zoltán Filus[2], Tímea Grósz[2], Chinmoy Biswas[2], Balázs Major[2], Imre Seres[2], Aref Imani[1], Paolo A. Carpeggiani[1], Maosheng Hao[1], and Florian Libisch[1] — [1]TU WIEN, Vienna, Austria — [2]ELI-ALPS, Szeged, Hungary

The electron emission behaviour of graphitic surfaces was investigated using advanced spectroscopic methods alongside static & time-resolved Photo-Electron Emission Microscopy (PEEM). At TU WIEN, electron-pair coincidence spectroscopy on pyrolytic graphite detected *correlated* electron pairs from single scattering events, directly linking energy-loss processes to the secondary electron (SE) spectrum. The $(\pi + \sigma)$-plasmon was resolved in terms of the involved interband transitions revealing strong final-state resonances in the SE spectrum. Static photoemission from graphite(0001) was studied using PEEM at the NanoESCA end station at ELI-ALPS, employing extreme ultraviolet linearly polarised photons generated via High-Harmonic Generation in Argon. The k-space-resolved photoelectron (PE) signal associated to the above-mentioned final-state resonances in the SE-spectrum reflects the symmetry of the conduction bands involved in the PE-emission process. Attosecond time- and k-space-resolved RABBITT measurements provided insights into PE-emission dynamics across the Brillouin zone.

Invited Talk O 7.4 Mon 11:15 H11

Nanoimaging the electronic, plasmonic, and phononic structure and dynamics of 2D materials — •Sarah King — University of Chicago, Chicago, IL, United States

Heterogeneity plays a critical role in chemistry and physics, from the role of defect states in the carrier dynamics of semiconductors to interfaces and surfaces in catalysis. However, our ability to visualize nano-scale domains and properties in materials and their effect on material dynamics has been hampered by the simple challenge of our inability to meet the necessary nanometer and femtosecond timescales. I will discuss recent efforts by my group to determine the interplay of heterogeneity and morphology on the intrinsic optoelectronic and thermoelectric properties of materials. Using polarization-dependent photoemission electron microscopy (PD-PEEM) we have imaged the spatially dependent optical selection rules of black phosphorus, distinguishing edge-specific modes, and antiferroelectric domains of β'-In2Se3, with spatial resolution as good as 25 nm. Through ultrafast transmission electron microscopy, we've been able to determine how the bond anisotropy and structural morphology of few-layer black phosphorus impacts phonon dynamics. Ultimately my group seeks to identify ways to modify the impact of structural heterogeneity in materials and rationally design energy efficient interfaces on the nanoscale.

O 7.5 Mon 11:45 H11

Time-resolved momentum microscopy with fs-XUV photons at high repetition rates with flexible energy and time resolution — •Karl Schiller[1], Lasse Sternemann[1], Matija Stupar[1], Alan Omar[2], Martin Hoffmann[2], Jonah Nitschke[1], Valentin Mischke[1], David Janas[1], Stefano Ponzoni[1,3], Giovanni Zamborlini[1,4], Clara Saraceno[2], and Mirko Cinchetti[1] — [1]TU Dortmund University, Dortmund, Germany — [2]Ruhr University Bochum, Germany — [3]Ecole Polytechnique, Paris, France — [4]Karl-Franzens-University Graz, Austria

We present a versatile setup for time-resolved ARPES that combines an energy-filtered momentum microscope with a custom-designed high-harmonic generation (HHG) photon source [1]. The HHG source is powered by a commercial

multi-100 kHz Yb-based ultrafast laser system delivering femtosecond pulses in the extreme ultraviolet range. A nonlinear pulse compression stage, utilizing spectral broadening in a Herriott-type bulk multi-pass cell, enables flexible control of the driving pulse duration. This adaptability allows two distinct operational modes, optimized for either energy or time resolution, making the setup highly suitable for ultrafast photoelectron microscopy at the space-time limit. We demonstrate the system's capabilities by tracking conduction band dynamics in the valleys of a bulk WS_2 crystal. Using uncompressed laser pulses, we achieve an energy resolution better than (107 ± 2) meV. Compressed pulses, in contrast, yield a time resolution of (48.8 ± 17) fs.

[1] Optica Open Preprint 115282 (2024)

O 7.6 Mon 12:00 H11

Dark field photoelectron momentum microscopy of electric field gated 2D semiconductors — •Jan Philipp Bange[1], Bent van Wingerden[1], Jonas Pöhls[1], Wiebke Bennecke[1], Paul Werner[1], David Schmitt[1], AbdulAziz AlMutairi[3], Daniel Steil[1], R. Thomas Weitz[1], G. S. Matthijs Jansen[1], Stephan Hofmann[3], Giuseppe Meneghini[2], Samuel Brem[2], Ermin Malic[2], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Philipps-Universität Marburg, Germany — [3]University of Cambridge, U.K.

A possibility to tune many-body interactions in two-dimensional semiconductors is in-situ electric field gating, which allows precise and reversible control of the filling of states in a moiré potential. In combination with ARPES for static band structure measurements, this approach has been shown to be a powerful experimental probe [1]. However, the study of excited states in gated 2D material structures, such as interlayer excitons [2] and trions, has so far remained elusive.

Here we combine time-resolved momentum microscopy with dark field imaging techniques to gain access to many-body interactions on femtosecond time and nanometer lengthscales [3]. We use this method to study electric field gated homobilayer WSe_2 and report the ultrafast formation of quasiparticles as a function of applied gate voltage.

[1] Nguyen *et al.*, Nature **572**, 220 (2019).
[2] Bange *et al.*, Science Advances **10**, eadi1323 (2024).
[3] Schmitt *et al.*, Nature Photonics, in press, arXiv.2305.18908.

O 7.7 Mon 12:15 H11

Plasmonic spin meron pair: Spatio-temporal topology revealed by time resolved polarimetric photo-emission microscopy — Pascal Dreher[1], •Alexander Neuhaus[1], David Janoschka[1], Alexandra Roedl[1], Tim Meiler[2], Bettina Frank[2], Timothy J. Davis[1,2,3], Harald Giessen[2], and Frank Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [3]School of Physics, University of Melbourne, Parkville Victoria 3010, Australia

We have developed a novel method, polarimetric photo-emission electron microscopy (polarimetric PEEM), which combines an optical pump-probe polarimetry with photo-emission electron microscopy. This method enables the accurate generation and measurement of surface plasmon polariton fields at deep sub-wavelength spatial resolution and sub-cycle temporal resolution. Using polarimetric PEEM, we extend the study of electromagnetic fields on surfaces to a spin quasi-particle with the topology of a meron pair and analyze its topology by calculating the Chern number. We find the Chern number to be C=1 and constant over time, demonstrating the stability of the plasmonic meron pair on a femtosecond time scale. Additionally, we show that the in-plane vectors of the three-dimensional field are constrained by the embedding topology of the space as dictated by the Poincare-Hopf theorem.

O 7.8 Mon 12:30 H11

Momentum microscopy with attosecond time resolution at ELI ALPS to map the full Brillouin zone — Gyula Halasi[1], Csaba Vass[1], Nikolett Oláh[1], Zoltán Filus[1], Tímea Grósz[1], Chinmoy Biswas[1], Tamás Csizmadia[1], Lénárd Gulyás Oldal[1], Balázs Major[1], Péter Jójárt[1], Felix Blödorn[2], Florian Simperl[2], Aref Imani[2], Paolo Carpeggiani[2], Péter Dombi[1], Wolfgang S.M. Werner[2], Alessandra Bellissimo[2], and •László Óvári[1] — [1]ELI ALPS, Szeged, Hungary — [2]Vienna University of Technology, Austria

Time-resolved photoemission is a highly efficient tool for unraveling surface electron dynamics. The coupling of a photoemission electron microscope (PEEM) with an imaging hemispherical analyzer in our NanoESCA end station allows for the combination of spectroscopy and microscopy in real or momentum space. The NanoESCA end station is attached to a high harmonic generation (HHG) beamline, hence time-resolved momentum microscopy studies can be performed in a pump-probe scheme. To illustrate the performance of our user-ready system, the first results obtained by the RABBITT (Reconstruction of Attosecond Beating By Interference of Two-photon Transitions) scheme are presented. In this experiment, a graphite(0001) single crystal was studied, and RABBITT oscillations have been identified throughout the whole Brillouin zone, with attosecond precision, in the form of a time-resolved momentum space movie.

O 8: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation I

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Monday 10:30–13:00 Location: H24

Invited Talk O 8.1 Mon 10:30 H24

Chiral reactions at surfaces elucidated by machine learning and enhanced sampling — Raymond Amador[1], Enrico Trizio[2], Peilin Kang[2], Umberto Raucci[2], Hannah Bertschi[1], Marcella Iannuzzi[3], Jacob Wright[1], Roland Widmer[1], Oliver Gröning[1], Michele Parrinello[2], and •Daniele Passerone[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Italian Institute of Technology, Genova, Italy — [3]Department of Chemistry, University of Zurich, Switzerland

Experiments performed at the surface of the chiral intermetallic compound PdGa unleash a fascinating surface chemistry phenomenology including regioselectivity and enantioselectivity, in which the energetics is dominated by mid-range dispersive molecular interactions with the substrate. The corresponding modelling of chiral and prochiral adsorption and reactions requires both a high level of electronic structure theory and an appropriate statistical sampling of the reactants, transition state and products ensemble. We show that machine learning potentials based on DFT molecular dynamics trajectories and recently introduced enhanced sampling techniques allow to describe both the thermodynamics and the kinetics of reactions investigated in the laboratories next-door,

such as an Orito-like reaction catalysed by PdGa. Moreover, we study a chirality switching of a bianthracene molecule by applying a method introduced by some of us, based on the committor function and the variational principle that it obeys: its minimum uses a self-consistent procedure that starts from information limited to the initial and final states and reveals the transition state ensemble.

O 8.2 Mon 11:00 H24

On-surface molecular recognition driven by chalcogen bonding — •Luca Camilli — University of Rome Tor Vergata

The manipulation of organic architectures on surfaces through supramolecular interactions has been achieved by using, for example, H- and halogen-bonding. Chalcogen bonding interactions (ChBIs), which belongs to the same category, have not. The interest in ChBIs relies on its orbital mixing nature that provides semiconducting properties to the assemblies.[1] Here, we combine scanning tunnelling microscopy measurements and quantum chemistry calculations to present the first example of ChBI-driven molecular self-assembly on metal surfaces.[2] We show that pyrene-based modules bearing chalcogenazole pyridine moieties undergo self-assembly into dimers through double Ch***N interactions on Au(111) and Ag(110). Synchrotron-based spectroscopy techniques are used to gain more insights into the chemistry of the ChBI and to reveal its fingerprint [unpublished data]. Finally, experimental scanning tunnelling spectroscopy and its simulations based on the framework of density functional theory are used to investigate the electronic properties of the self-assembled systems [unpublished data]. This study sheds light on a promising avenue for future research in the bottom-up engineering of two-dimensional monolayered supramolecular chalcogenide-type materials, as we delve into the novel role of ChBIs in surface-based molecular recognition.

References 1. D. Romito et al. Angew. Chem. Int. Ed. 2022, 61 (38), e202202137. 2. L. Camilli, et al. JACS Au 4, 2115 (2024)

O 8.3 Mon 11:15 H24

Self-assembly, electronic structure, and switching of norbornadiene derivative photoswitches — •Shreya Garg[1], Vishakya Jayalatharachchi[1], Pedro Ferreira[2], Roberto Robles[3], Sajjan Mohammad[1], Shivani Singh[1], Nicolás Lorente[3,4], Kasper Moth-Poulsen[2], Meike Stöhr[1,5], and Sabine Maier[1] — [1]Department of Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany — [2]Polytechnic University of Catalonia, Catalonia, Spain — [3]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [4]Donostia International Physics Center (DIPC), San Sebastian — [5]University of Applied Sciences of the Grisons, Switzerland

Molecular photoswitches such as norbornadiene (NBD) derivatives are promising energy storage compounds due to their ability to switch to the metastable quadricyclane (QC) isomer with long half-lives and high-energy storage density. However, the NBD/QC derivative photoswitches remain largely unexplored on the surface. Here, we discuss the self-assembly, electronic structure, and switching of carboxylic acid- functionalized NBD derivative on the Au(111) surface using scanning tunneling microscopy complemented by density functional theory calculations. To explore the impact of the molecule-surface interactions, we also studied them on graphene, which acts as a decoupling layer. We observed distinct hydrogen-bonding motifs between the NBD derivatives on the two surfaces. Our study highlights differences in the electronic properties between the Au(111) and graphene surface, providing insights into optimizing their switching performance on surfaces.

O 8.4 Mon 11:30 H24

Kinetics of the on-surface reactions of 3,3"-dibromo-p-terphenyl on Cu(111): Cis-trans isomerization as rate limiting step towards the final configurations — •Mohit Jain[1], Tamam Bohamud[1], Daniel Kohrs[2], Nathaniel Ukah[2], Hermann A. Wegner[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Institut für Organische Chemie and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

The kinetics of the on-surface synthesis reactions of 3,3"-dibromo-p-terphenyl were investigated at fixed surface temperature of 300 K. The initially adsorbed molecules linked through C-Cu-C bonds were found in configurations consisting of long, chain-like and few shorter ring-like structures. With the progression of the reaction through time at 300 K, the configurations showed a shift from long chains and closed structures to 3-molecule ring structures. These structures then slowly aligned to form surface-wide phases of 3-molecule closed-ring structures.

The lateral surface mobility of the molecules was observed to be high at 300 K along with the frequent cleavage and re-formation of the C-Cu-C bond; nevertheless the actual transformation of chain structures towards complete ring structures was detected at a much longer timescale. By quantitative analysis, the trans-to-cis isomerization of the molecules which is necessary for closed-ring formation, was found to be the rate limiting step. To further consolidate the results, experiments with different substitution patterns of the p-terphenyl molecules were performed.

O 8.5 Mon 11:45 H24

Stability and Reactivity of Fe-DCA 2D Metal-Organic Framework on Graphene — •Zdeněk Jakub[1], Dominik Hrůza[1], Taduáš Lesovský[1], Ayesha Jabeen[1], Jakub Planer[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Purkyňova 123, Brno 61200, Czechia — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno 61200, Czechia

2D Metal-Organic Frameworks (2D MOFs) are promising materials for applications in catalysis, sensing or spintronics. 2D MOFs based on 9,10-dicyanoanthracene (DCA) linker molecules are particularly intriguing due to their recently demonstrated magnetic and topological properties. Here, we study the reactivity of Fe-DCA supported on a weakly-interacting substrate, graphene/Ir(111). Using Scanning Tunneling Microscopy (STM), X-Ray Photoemission Spectroscopy (XPS) and Low-Energy Electron Microscopy/Diffraction (LEEM/LEED) we test how the Fe-DCA responds to exposure to CO, O_2, and thermal annealing. Our data indicate that CO readily adsorbs at room temperature, and the 2D MOF remains stable. In contrast, adsorption of O_2 causes structural collapse of the 2D MOF, leaching the Fe cations from the Fe-DCA islands and leaving patches of self-assembled DCA on the surface. Thermally, the Fe-DCA structure decomposes upon annealing above 100 °C. Overall, our work addresses the limits of thermal and chemical stability of metal-DCA systems; such knowledge is relevant for any potential application of these materials.

O 8.6 Mon 12:00 H24

Tuning the properties of 2D Metal-Organic Frameworks by doping of the support — •Ayesha Jabeen[1], Zdeněk Jakub[1], Dominik Hrůza[1], Lenka Černá[1], Pavel Procházka[1], Jakub Planer[1], and Jan Čechal[1,2] — [1]CEITEC-Central European Institute of Technology, Brno University of Technology, Purkyňova 123, Brno 61200, Czech Republic — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno 61200,Czech Republic

2D metal-organic frameworks (MOFs) are extensively studied due to their tailorable properties, which make them promising for applications in catalysis, energy storage and sensing. Here, we show how the properties of 2D MOFs can be further tuned by varying the energy-level alignment with the supporting surface. We demonstrate this on the case of Ni-TCNQ 2D MOF, that we synthesized atop graphene/Ir(111) with different doping levels. The graphene doping is achieved by intercalation of heteroatoms at the graphene/Ir(111) interface; namely oxygen (for p-doping) and dysprosium (for n-doping). The changes in the support*s Fermi level position are clearly identified by photoemission techniques (XPS/UPS/ARPES). The Ni-TCNQ 2D MOFs supported on differently doped graphene show distinct properties, as evidenced by STM, XPS and LEEM/LEED. Most notably, XPS suggests that the charge state of the embedded Ni atoms can be controlled, as we observe two distinct components of Ni core levels, whose ratio depends on the support′s doping level. These findings highlight the potential of support doping for tailoring the properties of designer 2D MOFs.

O 8.7 Mon 12:15 H24

Theoretical Investigation of Dibromopyrene and Iodotriphenylene on Sodium Chloride Coated Copper Substrate — •Florian Pfeiffer[1], Julian Ernst[1], André Schirmeisen[2], Daniel Ebeling[2], and Simone Sanna[1] — [1]Institute for Theoretical Physics, Justus Liebig University Giessen, Germany — [2]Institute for Applied Physics, Justus Liebig University Giessen, Germany

Organic 2D materials are of great interest for various applications in molecular electronics. Increasingly sophisticated methods of on-surface manipulation via probe tips extend the scope of possible structure modifications to tune the (electronic) properties of such nanostructures.

Halogenated organic precursors such as DBP and IT are the building blocks for the assembly of more complex structures. A sodium chloride bilayer helps to electronically decouple the metallic Cu(111) substrate from adsorbates, increasing mobility and thus simplifying manipulation.

The Vienna Ab initio Simulation Package [1] implementation of density functional theory was used to calculate potential energy surfaces and nudged elastic bands for modelling adsorption behaviour and diffusion pathways, respectively. Comparability with experimental results [2] was achieved by simulation of scanning tunneling and atomic force microscopy using the Probe-Particle Model [3].

[1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993)
[2] Q. Zhong et al., Nat. Chem. 13, 1133 (2021)
[3] P. Hapala et al., Phys. Rev. B 90, 085421 (2014)

O 8.8 Mon 12:30 H24

On-Surface Design of Highly-Ordered Two-Dimensional Networks Stabilized by Nonmetal Atoms — •Alisson Ceccatto[1,3], Gustavo Campi[2], Vanessa Carreño[1], Eidsa Ferreira[1], Natalie J. Waleska-Wellnhofer[3], Eva Marie Freiberger[3], Simon Jaekel[3], Duncan John Mowbray[2], Christian Papp[3,4], Hans-Peter Steinrück[3], and Abner de Siervo[1] — [1]Geb Wataghin Physics Institute - University of Campinas - Campinas/Brazil —

[2]School of Physical Sciences and Nanotechnology, Yachay Tech University, 100119 Urcuquí, Ecuador — [3]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [4]Angewandte Physikalische Chemie, FU Berlin, Arnimallee 22, 14195 Berlin, Germany

Supramolecular nanoarchitectures have been widely explored to precisely design low-dimensional materials at atomic and molecular levels. Herein, by combining STM measurements and DFT calculations, we report the 2D self-assembled of 1,3,5-tris[4-(pyridin-4-yl)-[1,1-biphenyl])benzene (TPyPPB) molecules on Ag(111) in the presence of Cl adatoms. The adsorption of the TPyPPB molecules on the clean Ag(111) surface forms a porous SAM stabilized by hydrogen bonds. Such packing can be explored as a host-guest material for atom/molecular confinement. However, in the presence of Cl adatoms, the molecular arrangement changes dramatically. The molecular assembly changes its geometry, forming a non-porous SAM stabilized by unconventional H–Cl–H bonds.

O 8.9 Mon 12:45 H24

On-surface synthesis of drone-shaped oligomers via carbenes — •Yunjun Cao[1], Joel Mieres-Perez[2], Julien Frederic Rowen[3], Akshay Hemant Raut[3], Paul Schweer[1], Wolfram Sander[3], Elsa Sanchez-Garcia[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Lehrstuhl Physikalische Chemie I, NC 5/72, Ruhr-Universität Bochum, 44801, Bochum — [3]Organic Chemistry II, Ruhr-Universität Bochum, D-44801 Bochum, Germany

The development of on-surface synthesis strategies opens opportunities to fabricate sophisticated nanostructures with tailored geometries, symmetries, and other properties. Here, we demonstrate that carbenes can be used as building blocks for fabricating highly branched oligomers with different symmetries on a Ag(111) surface. We synthesize highly symmetric drone-shaped oligomers, which are formed via C=C coupling of two carbenes to create a core, followed by C-H activation of the core with additional carbenes to create branches. Less symmetric drone-shaped oligomers are formed through the cyclodehydrogenation of the highly symmetric oligomers. The products are investigated by scanning tunneling microscopy and supported by ab initio theoretical modeling.

O 9: Surface Reactions

Time: Monday 10:30–12:30 Location: H25

O 9.1 Mon 10:30 H25

Co_2 reduction by solvated electrons at the NH_3/Cu(111) interface. — •Maya Heine, Lukas Gierster, and Julia Stähler — Humboldt-Universität zu Berlin, Institut für Chemie

Understanding CO_2 reactivity is crucial; the amount of CO_2 in the atmosphere continues to rise with no imminent peak in fossil emissions in sight [1]. Previously, solvated electrons (e_s) have been suggested to activate CO_2 , e.g. by forming surface bound CO_2^- radicals [2]. With time-resolved two-photon photoemission and the amorphous NH_3/Cu(111) interface, we can study the energetics and dynamics of e_s on femtosecond timescales [3]. Here, the electrons are localised at the surface and their lifetime depends exponentially on NH_3 coverage. On an ultrafast timescale, we can now use e_s to decipher the fundamental rate and steps of CO_2 activation. We observe a systematic decrease in the e_s lifetime as CO_2 is added and conclude that CO_2 opens a new decay channel for e_s. Further, increases in the work function serve as indicators of possible reactions: electron attachment to CO_2 or activated CO_2^- which has a dipole moment. For thick NH_3 films we see a much larger work function increase and bleaching of e_s. This suggests that the film thickness controls the lifetime of charged reaction intermediates and thus the reaction pathway. Moreover, we show that e_s attachment to CO_2 occurs on a 10s of ps timescale.

[1] Friedlingstein et al. **ESDD** (2024)
[2] Hu et al. **Nat. Commun, 14**, 4767 (2023)
[3] Stähler et al. **Chem. Sci. 2, 5**, 907 (2011)

O 9.2 Mon 10:45 H25

Exploring on hydrogen evolution reaction performance of borophene monolayer — •Jing Liu and Axel Gross — Institute of Theoretical Chemistry, Ulm University, Oberberghof 7, 89081 Ulm, Germany

Borophene, a unique graphene-like 2D material composed of boron atoms, has gained significant attention due to its exceptional properties [1]. This study investigates its performance in catalyzing the hydrogen evolution reaction (HER). We focus on four distinct borophene configurations: α, $\beta12$, $\gamma3$, and trigonal structures [2]. Using density functional theory (DFT), we assess the HER performance of pristine monolayers as well as their interaction with an Ag(111) substrate.

The results show that α, $\beta12$, and $\gamma3$ monolayers possess exceptional HER activity, evidenced by their optimal Gibbs free energy for H-adsorption. However, their performance is markedly suppressed upon interaction with a Ag(111) support, where borophene-support interaction alters the hydrogen binding properties. By contrast, trigonal structure exhibits limited HER activity in both conditions, reflecting structural characteristics unfavorable for HER.

This work highlights the intrinsic catalytic potential of borophene monolayers while emphasizing the critical influence of substrate interactions.

[1] B. Feng, J. Zhang, Q. Zhong, et al. Experimental realization of two-dimensional boron sheets. *Nature Chem.* 8, 563 (2016).
[2] X. Wu, J. Dai, Y. Zhao, et al. Two-Dimensional Boron Monolayer Sheets. *ACS Nano* 6, 7443 (2012).

O 9.3 Mon 11:00 H25

Realistic Representations of IrO2 Catalyst Surfaces through Extensive Sampling — •Hao Wan, Hendrik H. Heenen, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Iridium oxides catalyze the oxygen evolution reaction with unparalleled activity and stability, even under harsh acidic conditions. However, this performance is sensitively correlated to strong structural, compositional and morphological changes of the working catalyst. At the atomic level little is presently known about the true active state, aside from the unlikelihood of it being ideal rutile IrO2.

This situation spans a vast configurational space, the extensive sampling of which (e.g. via parallel tempering) would be intractable with predictive-quality first-principles calculations. Training a machine-learning interatomic potential (MLIP) as an efficient surrogate is challenged by an unprecedented diversity of training structures, as even the bulk structure and composition is unknown. To this end, we create a comprehensive training set by first assembling prototype bulk structures for various IrOx stoichiometries from existing databases. In an active learning loop, this set is then augmented through extensive sampling of diverse surface structures created from the prototypes. The resulting trained MLIP identifies hexagonal ring structures on the rutile (110), (100), (111) facets as most stable configurations under operating potential, aligning with experimental indications. Activity evaluations on these structures using established descriptors effectively capture trends consistent with experimental observations.

O 9.4 Mon 11:15 H25

Hydrogen Atom Scattering from Graphene on Nickel — •Sophia Tödter, Yvonne Dorenkamp, and Oliver Bünermann — Institute of Physical Chemistry, Georg-August University, Göttingen, Germany

Previously, H atom scattering from graphene grown on a Pt(111) substrate was investigated in detail by our group [1]. Depending on the experimental conditions, two energy loss channels were observed, one quasi-elastic and one strongly inelastic. For a C-H bond to form, the delocalized electronic structure of graphene has to be locally destroyed. This gives rise to an adsorption barrier. If the hydrogen atom cannot cross the barrier, it is elastically reflected. However, if the atom can cross the barrier, it loses a large amount of energy, which can lead to it sticking to the surface [1]. Pt(111) was chosen because it is a weakly interacting substrate. This allows comparison of the experimental data with simulations of H atom scattering from free-standing graphene. Although good qualitative agreement is achieved between experiment and theory, quantitative agreement cannot be achieved because of the non-negligible substrate effect.

To experimentally study the substrate effect we chose Ni(111) as an additional substrate and performed the same experiments. Ni(111) is a strongly interacting substrate and a much larger substrate effect is expected.

[1] H. Jiang et al., Imaging covalent bond formation by H atom scattering from graphene, Science 264, (2019).

O 9.5 Mon 11:30 H25

On-Surface Photoreactivity via Reactive Intermediates on a Metal Versus an Insulator — •Iheb Baklouti[1], Julien F. Rowen[2], Dave Austin[3], Lilian N. Alsayed[1], Talat S. Rahman[3], Wolfram Sander[2], and Karina Morgenstern[1] — [1]Ruhr-Universität Bochum, Chair of Physical Chemistry I, Bochum, Germany — [2]Ruhr-Universität Bochum, Chair of Organic Chemistry II, Bochum, Germany — [3]University of Central Florida, Department of Physics, Orlando, FL, USA

Organic azides play a pivotal role in click chemistry, serving as versatile precursors in synthesizing complex molecules across synthetic chemistry, pharmacology, materials science, and catalysis. Despite their importance, investigations into the surface reactivity of azides remain sparse. This study elucidates the behavior of 2-azidofluorene (2AF) on two distinct surfaces: metallic Ag(100) and ionic NaBr(100), under cryogenic conditions (7 K). Utilizing Infrared Reflection

Absorption Spectroscopy (IRRAS) and Scanning Tunneling Microscopy (STM), reactions initiated by ultraviolet illumination are analyzed. Nitrene formation from 2AF is hindered by charge transfer interactions with Ag(100), emphasizing the need for low-interaction surfaces like NaBr(100). Illumination at 254 nm induces 2AF dissociation, forming 2-fluorenylnitrene. Subsequent exposure to 450 nm light leads to didehydroazepines, a process reversible under 405 nm. This study sheds light on azide surface-mediated dynamics and introduces a framework for investigating reactive intermediates in surface chemistry.

O 9.6 Mon 11:45 H25

Sustainable argon irradiated MWNT-based filters for efficient remediation of methylene blue dye from wastewater: characterization and mechanism — •Emad Elsehly — Physics Department, Faculty of Science, Damanhour University, 22516, Damanhour, Egypt

This study handles the irradiation of the multi-walled carbon nanotubes by argon ion beam and their potential application for dye removal from wastewater. The obtained data revealed that Argon ion irradiation can induce various structural changes and defects in MWNTs as confirmed by Raman spectroscopy. Moreover, the structural integrity of R-MWNTs is preserved during irradiation as shown by SEM. R-MWNTs yielded smaller crystallites, reaching a size of 4.4 nm. The adsorption efficiency of R-MWNTs was examined by remediation of methylene blue (MB) from wastewater. The results demonstrated that the remediation percentage of R-MWNTs enhanced and could reach 98%. The adsorption mechanism of methylene blue onto R-MWNTs is spontaneous, and almost chemical adsorption process. R-MWNTs have greater surface area and more active sites for adsorption. The irradiation tool offers an alternative approach to enhance the structure of MWNTs-based filters and present a highly effective solution for the removal of dyes from wastewater.

O 9.7 Mon 12:00 H25

On-surface Synthesis of Non-Benzenoid Nanographenes Embedding Azulene and Stone-Wales Topologies — •Qifan Chen[1], Kalyan Biswas[2], Sebastian Obermann[3], Ji Ma[3], Diego Soler-Polo[1], Jason Melidonie[3], Ana Barragán[2], Ana Sánchez-Grande[1], Koen Lauwaet[2], Rodolfo Miranda[2], David Écija[2], Pavel Jelínek[1], Xinliang Feng[3], and José Urgel[2] — [1]Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic — [2]IMDEA Nanoscience, C/Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain — [3]Center for Advancing Electronics Dresden & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, D-01069 Dresden, Germany

The incorporation of non-benzenoid motifs in graphene nanostructures significantly impacts their properties. Understanding of the specific reaction mechanism of forming non-benzenoid nanographene structures with tailored electronic/magnetic properties remains limited. In this work, we report a theoretical study addressing an on-surface synthetic strategy toward fabricating non-benzenoid nanographenes containing different combinations of pentagonal and heptagonal rings. We employ the Quantum Mechanics/Molecular Mechanics (QM/MM) approach to analyze the optimal reaction pathways on Au(111) surface and explore the roles of an adatom on the activation energy barrier of the reaction. Our work provides atomistic insight into the reaction mechanism of single gold atom-assisted synthesis of novel NGs containing nonbenzenoid motifs.

O 9.8 Mon 12:15 H25

Enhanced Sampling of Chiral Molecules on Chiral PdGa Surfaces Using Machine Learning — •Raymond Christopher Amador[1,2], Umberto Raucci[3], Peilin Kang[3], Enrico Trizio[3], Hannah Bertschi[4], Jacob Wright[2], and Daniele Passerone[1,2] — [1]nanotech@surfaces laboratory, Empa, Zürich, Switzerland — [2]ETH Zürich, Zürich, Switzerland — [3]Italian Institute of Technology, Genova, Italy — [4]Max Planck Institute, Hamburg, Germany

The interaction of chiral molecules with chiral surfaces plays a fundamental role in enantioselective catalysis and molecular recognition processes. In this work, we present a novel machine learning-assisted framework for enhanced sampling of chiral molecule dynamics on chiral PdGa surfaces. Using high-dimensional descriptors of molecular-surface interactions and leveraging state-of-the-art neural network potentials, our approach significantly accelerates the exploration of configurational space while maintaining chemical accuracy. Detailed analysis reveals how chiral PdGa surfaces influence molecular adsorption, orientation, and reaction pathways, providing new insights into the enantioselective mechanisms. These findings demonstrate the potential of integrating machine learning techniques with surface science to address challenges in heterogeneous catalysis.

O 10: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit II

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Monday 15:00–17:45 Location: H2

Invited Talk O 10.1 Mon 15:00 H2

Probing coherent optical emission processes with ultrafast scanning electron microscopy — •Albert Polman — NWO Institute AMOLF, Amsterdam, the Netherlands

High-energy electron beams are unique probes of optical materials properties as their time-varying electric field can create strong materials polarizations. The subsequent light emission (cathodoluminescence, CL) provides a fingerprint of the local optical density of states at the nanoscale.

CL from plasmonic and dielectric nanostructures has a coherent phase relation with the excitation process, which enables self-referenced measurements to perform holography and metrology. Electron excitation of semiconductors creates a sequence of fs-ps-ns materials excitations, that lead to bunched CL photon emission.

New developments in ultrafast electron microscopy enable the creation of picosecond electron pulses and pump-probe spectroscopy where light and electrons serve as pump and probe or vice versa. The interaction of pulsed electrons with optical metasurfaces enables novel ways to shape the quantum mechanical electron wavepackets in space and time and may eventually create entirely new forms of ultrafast materials spectroscopy.

O 10.2 Mon 15:30 H2

Spectrally resolved free electron-light coupling strength in a transition metal dichalcogenide — •Soufiane El kabil[1], David Lerchenberger[1], Niklas Müller[1], Jonathan Weber[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany

In ultrafast transmission electron microscopy (UTEM), combining precisely controlled free-electron beams with localized light fields enables the creation of intricate electronic states and the visualization of transient optical near-fields via PINEM [B. Barwick, et al. Nature 462.7275 (2009): 902-906]. However, optical nearfields in photonic structures typically exhibit a strong wavelength dependence, which has so far only been partially captured by PINEM approaches.

To address this, we use strongly chirped broadband light pulses to explore the spectrally resolved interaction between free electrons and light at the edge of a

MoS2 thin film [N. Müller, et al. arXiv preprint arXiv:2405.12017(2024).]. As a fast electron traverses the optical field near the MoS2 flake, it absorbs or emits multiple photons, producing photon sidebands in its energy spectrum. By varying the electron-light delay at the sample, different spectral components of the near-field can be investigated. Numerical simulations reveal that the observed spectral and spatial modulations stem from interactions between incident and reflected light fields, as well as guided thin-film optical modes. Our results highlight the ability of PINEM to resolve the optical properties of semiconductors spatially and spectrally.

O 10.3 Mon 15:45 H2

Simulating Quantum Spin Dynamics in Transmission Electron Microscopy — •Santiago Beltrán Romero[1,2], Dennis Rätzel[3], Stefan Löffler[2], and Philipp Haslinger[1,2] — [1]VCQ, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria — [2]University Service Centre for Transmission Electron Microscopy,TU Wien, Wiedner Hauptstraße 8-10/E057-02, 1040 Wien, Austria — [3]ZARM, Unversität Bremen, Am Fallturm 2, 28359 Bremen, Germany

Transmission Electron Microscopy (TEM) has revolutionized nanoscale research by enabling unprecedented simultaneous spatial and temporal resolutions, thanks to advancements such as aberration correction, cryogenic techniques, and ultra-fast probing. However, the capabilities of TEM to probe spin dynamics – critical for understanding quantum materials – are, to date, quite limited and could be significantly improved by novel microwave spectroscopic tools [1, 2]. Building on recent innovations in that direction, we present a framework that integrates scattering theory and multislice simulations to describe the probing of spin samples on the nanoscale with time-resolved TEM. Our simulations offer insights into both elastic and inelastic processes - including the electrons backaction on the spin. They reveal how the choice of set-up parameters influence the precision of spin detection, identifying optimized conditions for enhancing the signal-to-noise ratio (SNR) and contrast. This work sets the stage for combining spin resonance tools with cutting-edge TEM capabilities, paving the way for breakthroughs in spin imaging and manipulation at the atomic level.

O 10.4 Mon 16:00 H2

Ultra-Nonlinear Subcycle Photoemission of Few-Electron States from Sharp Gold Nanotapers — •Germann Hergert, Rasmus Lampe, Andreas Wöste, and Christoph Lienau — Institut für Physik, Carl-von-Ossietzky Universität, 26129 Oldenburg, Germany

Generating attosecond electron pulse trains by coherent modulation of swift electrons enabled attosecond resolution in ultrafast transmission electron microscopy [1,2]. The possibility to transfer photon statistics to the electron number statistics in multiphoton photoemission (MPP) from nanotapers [3], opens up a window to increase photoemission nonlinearities of few-electron states and generating subcycle electron pulses. This provides an alternative road to reach subcycle resolution in electron microscopy.

Here, we present MPP of few-electron wavepackets triggered by near-infrared pulses from gold nanotapers, demonstrating 20th-order nonlinearities for electron triplets. Event-based interferometric autocorrelations of the photoemission yield are quenched to single-peak traces with 0.8 fs duration. We observe a modulation of the electron yield by the carrier-envelope phase, indicating the emission of subcycle isolated electron beams, with prospects to improve the temporal resolution in ultrafast point-projection electron microscopy.

[1] D. Nabben, Nature, 619, 63 (2023)
[2] J. Gaida, Nat. Photon., 18, 509 (2024)
[3] J. Heimerl, Nat. Phys., 20, 945 (2024)
[4] G. Hergert, Nano Lett., 24, 11067 (2024)

Invited Talk O 10.5 Mon 16:15 H2

Ultrafast exciton dynamics in momentum space — Alexander Neef[1], Tommaso Pincelli[1,2], Lawson Lloyd[1], Shuo Dong[1], Samuel Beaulieu[1], Tania Mukherjee[1,2], Sebastian Hammer[3], Malte Selig[2], Dominik Christiansen[2], Andreas Knorr[2], Martin Wolf[1], Jens Pflaum[3], Laurenz Rettig[1], and •Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Julius-Maximilian-Universität Würzburg, 97070 Würzburg, Germany

Time- and angle-resolved photoemission spectroscopy (trARPES) provides a quantum-state-resolved picture of the ultrafast dynamics of many-body states like excitons in non-equilibrium states of matter. Following the formation and scattering of excitons in momentum space in real time reveals all key properties of the excitons like binding energy, exciton-phonon coupling, and the real-space distribution of the many-body wave functions. Additionally, information about the orbital properties and Berry curvature is encoded in the multidimensional trARPES signals. Applied to heterostructures, the ultrafast exciton and charge dynamics across interfaces reveal the mechanism of charge and energy transfer processes. We will exemplify this approach for transition metal dichalcogenides heterostructures, molecular crystals, and layered semiconducting antiferromagnets.

S. Dong et al., Nature Commu. 14, 5057 (2023); T. Pincelli et al., Adv. Mater. 2209100 (2023), A. Neef et al., Nature 616, 275 (2023), S. Beaulieu et al., Sci. Adv. 10, eadk3897 (2024).

O 10.6 Mon 16:45 H2

Subcycle band-structure videography of quantum materials — •Vincent Eggers[1], Manuel Meierhofer[1], Jakob Helml[1], Lasse Münster[1], Robert Wallauer[2], Giacomo Inzani[1], Sarah Zajusch[2], Suguru Ito[2], Leon Machtl[1], Yin Hao[3], François C. Posseik[3], Changhua Bao[1], Jens Güdde[2], F. Stefan Tautz[3], Rupert Huber[1], and Ulrich Höfer[1,2] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Philipps-Universität Marburg, 35037 Marburg, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

We introduce the next generation of subcycle band-structure videography. By combining atomically strong few-cycle mid-infrared lightfields with sub-10-femtosecond XUV pulses in a momentum microscope, lightwave-driven dynamics can now be investigated throughout the entire Brillouin zone. Here, we observe electrons driven by carrier fields of light reaching amplitudes as high as MV/cm in graphene. Subcylce analysis of the timing of these lightwave-driven currents reveals femtosecond scattering times. Our novel setup provides a new platform to explore strong-field phenomena ranging from inter- and intraband dynamics to Bloch oscillations and the emergence of Floquet-Bloch states directly in subcycle videos covering the full band structure.

O 10.7 Mon 17:00 H2

Approaching Atomic Resolution in Ultrafast Transmission Electron Microscopy — •Sophie Schaible[1,2], Till Domröse[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) [1] extends the study of structural heterogeneity in conventional TEM by introducing femtosecond temporal resolution, providing the means to map structural phase transitions at the nanoscale. However, access to atomic-scale ultrafast dynamics remains a major challenge due to the limited brightness of pulsed photoelectron beams. In this contribution, we explore approaches to atomic-resolution imaging of a structural transformation in a UTEM employing a high-coherence photoelectron source. Highly dose-efficient imaging is crucial to make optimum use of the available electron signal. We further gauge the impact of experimental parameters on the achievable spatiotemporal resolution such as sample drift, acquisition time, repetition rate and electron pulse length with and without optical excitation of the specimen.

[1] Feist *et al.* Ultramicroscopy **176** (2017)

O 10.8 Mon 17:15 H2

Towards Detection of Spin Resonance Excitations with TEM — •Antonín Jaroš, Johann Toyfl, Benjamin Czasch, Michael Stanislaus Seifner, Isobel Claire Bicket, Santiago Belrán-Romero, and Philipp Haslinger — VCQ, Atominstitut, TU Wien, USTEM, Stadionallee 2, 1020 Vienna, Austria

Microwave (MW) excitations of spin systems induce precessional spin motion at GHz frequencies. Traditional spin resonance spectroscopy techniques, such as Electron Spin Resonance (ESR) and Ferromagnetic Resonance (FMR), are employed to determine key parameters like gyromagnetic ratios and damping constants in magnetic materials. However, these methods often lack the spin sensitivity and spatial resolution required for spin studies at the atomic level. We present a novel approach that synergistically combines spin resonance techniques with Transmission Electron Microscopy (TEM). Spin state polarization is induced by the magnetic field of the TEM pole piece, while spin system excitation is achieved through an impedance-matched micro-resonator integrated into a custom-designed sample holder. The detection of spin resonance excitations in TEM might represent an important step towards MW driven spin studies with highly controlled electron probe at the nanoscale.

O 10.9 Mon 17:30 H2

Laser-driven cold-field emission source for ultrafast transmission electron microscopy — Alexander Schröder[1], •Andreas Wendeln[1,2], Jonathan Weber[1,2], Masaki Mukai[3], Yuji Kohno[3], and Sascha Schäfer[1,4] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Insitute of Physics, Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Germany — [3]JEOL Ltd., Tokio, Japan — [4]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

In recent years ultrafast transmission electron microscopy (UTEM), which combines the nanometer spatial resolution of a TEM with the femtosecond temporal resolution of a pump-probe approach, has become an increasingly important tool for investigating nanoscale dynamics. Further improving the spatiotemporal resolution in time-resolved electron imaging experiments requires femtosecond photoelectron sources with a higher degree-of-coherence. Here, we present the development of a laser-driven cold field electron source integrated in a UTEM instrument [1]. This approach yields 220-fs electron pulses with elec-

tron energy widths down to 360 meV, photoelectron spot sizes of 2 Å, and a peak normalized beam brightness exceeding $6.5 \cdot 10^{13}$ A/m^{2}sr, providing a new level of spatial and spectral precision in observing ultrafast nanoscale dynamics for UTEM applications. Lastly, we discuss the implementation of laser-driven cold-field emitters in a probe-aberration-corrected electron microscope potentially leading to smaller spot sizes with less coherent beams and significantly increased electron currents. [1] Schröder et al., arXiv:2410.23961, (2024).

O 11: Electronic Structure of Surfaces: Spectroscopy, Surface States I

Time: Monday 15:00–18:00 Location: H4

O 11.1 Mon 15:00 H4

Optimizing the photon detection in inverse photoemission — •Jan Willermann, Fabian Schöttke, and Markus Donath — Physikalisches Institut, Universität Münster, Münster, Germany

The detection of vacuum-ultraviolet photons ($\hbar\omega$ = 9.9 eV) in inverse-photoemission experiments is usually carried out with gas-filled counting tubes. Commonly, iodine/argon gas fillings were used for Geiger-Müller type photon detection. Recently, the gas filling was replaced by acetone to increase stability and the operation was changed to proportional mode [1]. While doing this, the counting tube geometry must not necessarily be changed. We carried out systematic measurements to understand the photon detection process in acetone-filled counting tubes and optimize the geometry accordingly. In the range of optimal gas pressures, we found that the photon mean free path in acetone is in scale of a few millimeters instead of a few centimeters as in iodine/argon. Furthermore, we observed that the electron mean free path in proportional-type counting tubes is also reduced to few millimeters. In comparison, the mean free path of electrons in Geiger-Müller-type counting tubes is in the range of the radius of the counting tube. As a consequence, the position of the cathode wire close to the entrance window becomes a critical parameter for the detection efficiency.

[1] C. Thiede *et al.*, Meas. Sci. Technol. **29**, 065901 (2018).

O 11.2 Mon 15:15 H4

Excitation-Mediated Transport through Nano-scale Josephson Junctions in the Coulomb Blockade Regime — •Zhengyuan Liu, Sebastian Scherb, Werner M.J. van Weerdenburg, Daniel Wegner, Nadine Hauptmann, and Alexander A. Khajetoorians — IMM, Radboud University Nijmegen, the Netherlands

Josephson junctions (JJs) are essential for superconducting quantum computing and sensing technologies. It has been shown that superconductivity in elemental BCS superconductors, including those typically used for JJs [1], can persist down to the 2D limit. However, the effects of such quantum confinement on both the electronic structure of a JJ and its subsequent transport remains unclear, and fabricating conventional source-drain JJ devices at the nanometer scale is challenging. Here, we use low-temperature scanning tunneling microscopy and spectroscopy to study the electronic structure and transport of model nano-JJ stacks grown on Si(111) surface. We first characterize the quantum well states and superconducting gap of the underlying layer. Then, we explore how both the dielectric and overlying metallic layer affect the electronic and superconducting states. We study the tunneling transport in the Coulomb blockade limit for a number of JJ stacks, revealing that the conductance is dominated by an excitation mediated process. We also discuss the superconducting properties of these stacks, and the potential to detect superconductivity through their charge transport. [1] Werner M. J. van Weerdenburg et al. Sci. Adv. 9, eadf5500 (2023).

O 11.3 Mon 15:30 H4

Double Photoemission Spectroscopy of C_{60} on $SrTiO_3$ (001) with high efficiency high-order harmonic light source — •Kathrin Plass[1], Robin Kamrla[1], Frank O. Schumann[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The photoemission spectroscopy is one of the main tools for studying the electronic structure of solids. However, the effects of electron correlation can only be inferred indirectly. In contrast, double photoemission spectroscopy (DPE) enables the direct observation of such phenomena by detecting pairs of correlated photoelectrons ejected following the absorption of a single photon [1].

C_{60} is considered a strongly correlated material, exhibiting a highly structured valence band spectrum. Recently, we discovered orbital-resolved correlation-induced two-electron binding energy shifts in C_{60}. In this study, we analyzed DPE data from C_{60} thin films on $SrTiO_3$(001) obtained using a laboratory-based high-order harmonic generation (HHG) light source operating at MHz repetition rates [2]. By boosting the HHG light source to higher photon energies and repetition rates, we are now able to investigate plasmon-assisted double photoemission in C_{60}, predicted recently [3].

[1] J. Berakdar et al., Phys. Rev. Lett. **81**, 3535 (1998)
[2] C.-T. Chiang et al., ELSPEC **200**, 15 (2015)
[3] M. Schüler et al., Sci. Rep. **6**, 24396 (2016)

O 11.4 Mon 15:45 H4

Surface Orbitroscopy: Emergent Phenomena of Orbital Angular Momentum — •Maximilian Ünzelmann[1], Tim Figgemeier[1], Begmuhammet Geldiyev[1], Hendrik Bentmann[2], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [2]QuSpin, NTNU Trondheim, Norway

Quantum degrees of freedom in electronic states are a key facet of modern quantum materials. Recently, the orbital angular momentum (OAM) — an orbital analogue of electron spin — has attracted broad attention in condensed matter and surface physics. For instance, orbitronics has been predicted as a promising route towards new functionalities, such as low-dissipation orbital currents or magnetization switching by orbital torques. In this talk, I will present orbital-sensitive angle-resolved photoemission spectroscopy experiments that demonstrate three key features of the OAM: (i) it acts as a central mediator between lattice and spin in spin-orbit-coupled systems, such as Rashba-type surface states [1,2], (ii) it might be associated with orbital currents, and (iii) its momentum texture carries topological information, giving rise to intriguing paradigms like OAM monopoles [3] or momentum-space quantum vortices [4].

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2021), [2] B. Geldiyev, M.Ü., *et al.*, Phys. Rev. B **108**, L121107 (2023), [3] M. Ünzelmann *et al.*, Nat. Commun. **12**, 3650 (2021), [4] T. Figgemeier, M.Ü., *et al.*, arXiv:2402.10031 (2024)

O 11.5 Mon 16:00 H4

Computationally Efficient First-Principles Treatment of Scattering States in Photoemission: A Pseudo-potential Approach — •Gian Parusa[1,2,3] and Michael Schüler[1,2,3] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

The calculation of photoemission matrix elements requires the consideration of several key factors, including Bloch states, light-matter coupling, and scattering states. The evaluation of scattering states in solids from first-principles, particularly within a plane-wave basis, is computationally demanding due to the large number of plane waves required at high energies. A well-established strategy for reducing the computational cost in the treatment of valence states involves the use of pseudo-potentials. In this work, we extend the concept of optimized norm-conserving pseudo-potentials to scattering states, utilizing a non-local Vanderbilt projector to restore the wave function properties at a specified target energy. This approach is applied to scattering states, specifically for energies above 1 Rydberg. The method is validated by simulating the photoemission spectrum of graphene and hexagonal boron nitride (h-BN) with the results compared to all-electron calculations, demonstrating both the accuracy and computational efficiency of the proposed technique.

O 11.6 Mon 16:15 H4

Electronic structure of ferromagnetic CrTe — •Chien-Wen Chuang[1], Muthu P.T. Masilamani[1], Hibiki Orio[1], Maximilian Ünzelmann[1], Chia-Nung Kuo[2,3], Chin-Shan Lue[2,3], Ashish Chainani[4], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [3]Taiwan Consortium of Emergent Crystalline Materials, National Science and Technology Council, Taipei, Taiwan — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Recent studies showed that CrTe and doped CrTe exhibit various emergent properties, such as a large magnetocaloric effect, spontaneous skyrmions and ferromagnetism with high Curie temperature T_C~340 K. We carried out Cr L-edge ($2p$-$3d$) X-ray absorption spectroscopy (XAS) and resonant photoemission spectroscopy (Res-PES) with right and left circularly polarized light on single crystal CrTe to investigate the role of Coulomb correlations in Cr $3d$ density of states(DOS). The Res-PES spectra showed a resonantly enhanced sharp peak at a binding energy of 1.5 eV, which corresponds to the Cr main $3d$ DOS, while states at the Fermi level do not show a clear resonance enhancement. A small circular dichroism of Cr $3d$ DOS was observed. In addition, we observed the Cr $3d$ two-hole L_3VV Auger feature which corresponds to a correlation satellite. Using the Cini-Sawatzky method, we estimate the on-site Coulomb interaction energy in Cr $3d$ states to be U_{dd}~3 eV.

O 11.7 Mon 16:30 H4

Unveiling the Role of Inelastic Mean Free Path in Photoelectron Diffraction: A Computational Study by Multiple Scattering — •Trung-Phuc Vo[1,2], Olena Tkach[3], Sylvain Tricot[4], Didier Sébilleau[4], Aimo Winkelmann[5], Olena Fedchenko[3], Yaryna Lytvynenko[3,6], Dmitry Vasilyev[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Ján Minár[1] — [1]Univ. West Bohemia, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Czech Republic — [3]Univ. Mainz, Germany — [4]Univ. Rennes, IPR, France — [5]AGH Univ. Krakow, Poland — [6]Institute of Magnetism of the NAS of Ukraine and MES of Ukraine, Ukraine

The inelastic mean free path (IMFP) of electrons near solid surfaces describes the average distance an electron travels through a solid before losing its kinetic energy via inelastic collisions. In surface analysis techniques such as photoelectron diffraction (PED), a short IMFP makes photoelectrons highly surface sensitive, allowing precise structural determination of surfaces. Conversely, a longer IMFP allows access to deeper layers, facilitating the study of bulk properties. The influence of the IMFP on PED is particularly evident with the advent of advanced time-of-flight (ToF) measurements. Controlling this key parameter is crucial. In this work, we summarize the PED implementation within the SPRKKR package and systematically explore its application over a wide kinetic energy range (106-1036 eV) for Ge 3d core levels. Our computational efforts provide insight into both Kikuchi diffraction patterns and their relation to valence band mapping, thus bridging PED analysis with electronic structure studies.

O 11.8 Mon 16:45 H4

Towards accessing the initial state by dichroic photoemission — •Jakub Schusser[1,2], Hibiki Orio[1], Maximilian Ünzelmann[1], Johannes Hessdörfer[1], Muthu Prasath Thirugnanasambandam Masilamani Masilamani[1], Florian Diekmann[3,4], Kai Rossnagel[3,4], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg- Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]University of West Bohemia, Pilsen, Czech Republic — [3]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [4]Institute of Experimental and Applied Physics, Kiel University, Germany

Despite its many advantages, photoemission has so far not allowed direct experimental access to detailed information about the initial state of solids. Dichroism in angle-resolved photoemission spectroscopy arises inherently from the matrix-element effects that depend on the initial and final states as well as the light field perturbation. By comparing both experimental and theoretical soft X-ray data in bulk WSe_2 we show the robustness of the newly introduced dichroic technique against variation of photon energy, light polarization and angle of incidence. Such robustness of the matrix-element effect represents a leap towards accessing the initial state by this differential technique with high relevance in the field of topological materials, layered systems and other material classes.

O 11.9 Mon 17:00 H4

Surface electronic structure of Te chains on Au(100) via ARPES — •Begmuhammet Geldiyev[1], Maximilian Ünzelmann[1], Tim Figgemeier[1], Hendrik Bentmann[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7 and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Center for Quantum Spintronics, Department of Physics, NTNU, Norway

In this talk, we will provide a comprehensive description of the surface electronic band structure in epitaxial Te chains grown in the submonolayer regime on a Au(100) substrate. First, the deposition of 0.25 ML Te results in an adlayer square lattice superstructure with $p(2\times2)$ periodicity. Particularly, the band structure of this system features an interface state – derived from hybrid Te-Au orbitals – that exhibits an anisotropic spin and orbital Rashba effect [1]. Second, by slightly increasing the Te coverage to 0.30 ML, the earlier square arrangement evolves into a chain structure with c(10 × 2) periodicity [2]. Here, we will address whether the latter system inherits an analogous Rashba effect scenario. Furthermore, we will unravel a flat electronic band with a bandwidth of ≈ 20 meV, indicating an almost perfect one-dimensional character.

[1] B. Geldiyev et al., Phys. Rev. B 108, L121107 (2023)
[2] L. Hammer et al., Surf. Sci. 750, 122589 (2024)

O 11.10 Mon 17:15 H4

Unoccupied electronic structure of the AgTe/Ag(111) surface alloy: A spin-resolved inverse photoemission study — •Marcel Holtmann, Carolin Benfer, and Markus Donath — Physikalisches Institut, Münster University, Germany

The AgTe/Ag(111) surface-alloy system has recently been investigated to understand the microscopic origin of the Rashba effect [1]. ARPES measurements suggest that tellurium p orbitals hybridize with states of the Ag(111) substrate resulting in two p_{xy} valence bands. For the unoccupied band structure, a third hybridization state with out-of-plane symmetry is detected using two-photon photoemission. Apart from this, the unoccupied electronic structure of AgTe/Ag(111) remains unexplored.

We employed spin- and angle-resolved inverse photoemission (IPE) to measure the unoccupied electronic structure with a broader scope. Using our rotatable spin-polarized electron source, we were able to measure the three-dimensional spin texture of the unoccupied states. As expected in [1], we found that the hybridization state shows a large Rashba-type spin splitting, which is untypical for non-heavy-metal systems. Using several photon detectors at different take-off angles to measure the angular distribution of the emitted photons, we gained access to the orbital symmetries of the involved electronic states. In addition, like the pristine Ag(111) surface, the AgTe/Ag(111) surface hosts an image-potential state.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

O 11.11 Mon 17:30 H4

Surface Sensitivity of the VLEED Scattering Process at Pt(111) — •Hannah Unterberg, Christoph Angrick, and Markus Donath — Universität Münster, Germany

The diffraction pattern of low-energy electrons (LEED) from Pt(111) shows a three-fold symmetry, although the surface layer exhibits a six-fold symmetry. This result proves the non-neglible influence of the second and deeper atomic layers resulting from the finite probing depth of the electrons. Here, we report on a spin-polarized very-low-energy electron diffraction (VLEED) [1,2] experiment on Pt(111). The reflected specular beam is measured at a fixed polar angle of incidence $\Theta = 45°$, while the azimuthal angle of incidence is varied over a wide range. This allows us to probe the surface sensitivity of the VLEED scattering process.

Our measurements at the non-reconstructed Pt(111) surface reveal distinct differences in the electron reflectivity and the spin-orbit-induced reflection asymmetry along the high symmetry directions $\overline{\Gamma}\,\overline{M}$ and $\overline{\Gamma}\,\overline{M}'$. These directions are equivalent (non-equivalent) in the case of six (three)-fold rotational symmetry. Our result indicates a substantial contribution from both the first and subsequent atomic layers to the VLEED scattering process. In contrast, results for the Au(111) surface, which hosts the prominent herringbone reconstruction, exhibit only minor differences between $\overline{\Gamma}\,\overline{M}$ and $\overline{\Gamma}\,\overline{M}'$. The different results for Pt(111) and Au(111) are discussed in view of the reconstruction.

[1] U. Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)
[2] C. Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020)

O 11.12 Mon 17:45 H4

Broadband THz Non-Linear Response In Topological Noble Metal Dichalcogenides — George de Coster[1,2], Lucas Lafeta[3], Stefan Heiserer[1], Zdeněk Sofer[4], Achim Hartschuh[3], Georg Duesberg[1], and •Paul Seifert[1] — [1]Institute of Physics, University of the Bundeswehr Munich, EIT, Werner-Heisenberg-Weg. 39, 85577 Neubiberg, Germany — [2]DEVCOM Army Research Laboratory, 2800 Powder Mill Road, Adelphi, Maryland, United States — [3]Department of Chemistry and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Butenandtstraße 5-13 (E), 81377 Munich, Germany — [4]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Noble metal dichalcogenides belong to the material class of layered 2D materials and were shown to host type-II Dirac semi-metallic behavior, as well as topological surface states and superconductivity. Intriguingly, noble metal dichalcogenides display strong second harmonic generation and second order photocurrent response despite their centrosymmetric crystal structure. We investigate the spectrally-resolved optical response and reveal second and third order nonlinear response at both, optical frequencies as well as in the THz range. The latter is analyzed in polarization resolved spectroscopy, that points towards spin-polarized bands at the symmetry broken surface as origin of the non-linearities. Our results elucidate the spectral opto- electronic response at low energies and discuss its anisotropy in light of underlying symmetry constraints.

O 12: Nanostructures at Surfaces I

Time: Monday 15:00–17:45 Location: H6

O 12.1 Mon 15:00 H6

Imaging standing phonons within topological defect in strong coupling superconductor by scanning tunneling microscopy — •Qili Li, Thomas Gozlinski, Rolf Heid, Jörg Schmalian, and Wulf Wulfhekel — Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron-phonon coupling plays an important role in conventional superconductors. Understanding the behavior of phonons will promote the applications of conventional superconductors. However, it is difficult to observe the spatial behavior of phonons. Here, we utilize inelastic scanning tunneling microscopy (ISTS) at 45 mK to investigate phonons within topological defect, i.e. stacking fault tetrahedron (SFT), in the strong coupling superconductor Pb(111) [1]. We find that the local Eliashberg function [2,3] is significantly enhanced by SFTs. Moreover, lateral standing waves of phonon are also observed on SFTs. Compared with phonon bandstructure, we find that the SFTs have strong confinement on transverse acoustic phonons, while the longitudinal acoustic phonons are less confined. Our findings pave the way to phonon engineering in strong coupling superconductors. [1] PRL 14, 108 (1965). [2] Sov. Phys. JETP 11, 696 (1960). [3] PRL 114, 047002 (2015).

O 12.2 Mon 15:15 H6

Directing far- and nearfield scattering with dielectric Mie Voids — •Benjamin Reichel[1], Mario Hentschel[1], Adrià Canós Valero[2], Thomas Weiss[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Physics, University of Graz, and NAWI Graz, Graz 8010, Austria

Controlling the behavior of light at the nanoscale is a significant challenge in various applications such as metadevices, diffraction gratings, and resonant surfaces. Recently, Mie voids created in high-index dielectric host materials have emerged as a promising platform for confining electromagnetic waves in small values, possibly extending down to ultraviolet wavelengths in air. Therefore understanding and theoretical modeling the electromagnetic scattering behavior of Mie voids are crucial for their effective use.

In this study, we perform a spectral multipolar decomposition for the far- and near-field scattering behavior of dielectric Mie voids upon plane wave or local point dipole illumination. Dielectric Mie voids exhibit strong forward far-field scattering behavior, whereas in the near-field strong backscattering behavior is observed. These insights will be important in the development of resonance and meta structure designs, especially when deriving a generalized Kerker condition. Finally, leveraging the full resolution of electromagnetic Mie voids will open avenues for embedding quantum emitters in high index substrates.

O 12.3 Mon 15:30 H6

Influence of Plasma on the Electrode and the Electrolyte during Plasma Electrolysis — •Lukas Forschner[1], Jan-Luca Gembus[2], Peter Awakowicz[2], Andrew R. Gibson[3], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Ulm University, Institute of Electrochemistry, Ulm, Germany — [2]Ruhr University Bochum, Chair of Applied Electrodynamics and Plasma Technology, Bochum, Germany — [3]University of York, York Plasma Institute, Heslington, United Kingdom

During plasma electrolysis, a plasma is ignited in a thin vapor layer between the powered electrode and the liquid electrolyte. The plasma interacts with both the electrode[1] and the electrolyte, which can modify their properties.[2] In this work, we focus on a metal electrode used as a cathode, where nanoparticle formation can be observed during plasma electrolysis. To gain fundamental insight into nanoparticle formation, we studied the gas sheath surrounding the electrode (including the plasma) and the respective interfaces in detail. Specifically, we use optical emission spectroscopy and high-speed camera imaging to analyze the processes on a milli- to microsecond time scale. We elucidate the structural changes on the electrode induced by the plasma under these conditions with scanning electron microscopy imaging. Based on these results, we discuss mechanisms leading to the formation of nanoparticles in the solution from the electrode.

[1] Artmann et al., *ChemPhysChem* **22** (2021) 2429.
[2] Forschner et al. *J. Phys. Chem. C* **127** (2023) 4394.

O 12.4 Mon 15:45 H6

Structural, morphological and chemical characterization of plasma-treated NiCoO electrolyzer anodes — •Timo Wagner[1], Nicolas Wöhrl[1], Vineetha Vinayakumar[2], Christian Marcks[3], Anna Mechler[3], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]IVG-PST and CENIDE, University of Duisburg-Essen — [3]AVT.ERT, RWTH Aachen University

Plasma surface pre and post treatment are important steps to tailor characteristics for later manufacturing steps, or as a finishing step to engineer surface characteristics for later applications. We developed a nitrogen microwave plasma process to be used as pre and post treatment for NiCoO coatings for electrolyzers. The plasma treatment resulted in significant modification of the NiCoO films. For example a porous structure, as measured by AFM, SEM and TEM, leads to enhanced accessibility of the active material. Organic species from the spray coating were removed and the plasma-treated NiCoO layers also exhibited a highly hydrophilic surface, which facilitated better interaction with the electrolyte. X-ray absorption spectroscopy (XAS) studies indicated a higher Fe uptake from the electrolyte, which is beneficial for the oxygen evolution reaction (OER). Raman studies showed a more reversible oxidation behavior in the plasma-treated layers. Overall, these modifications contributed to an enhanced OER performance of the NiCoO anodes due to the plasma post-treatment as characterized electrochemically by cyclic voltammetry (CV) and measuring the electrochemically active surface area (ECSA).

O 12.5 Mon 16:00 H6

Artificial Atoms: Energy-Level Engineering and Shape-Dependent Reactivity — •Marco Weiss, Fabian Stilp, Michael Roessner, Max Reinhart, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg

Artificially arranged nanostructures can confine the quasi-free two-dimensional electron gas present on noble metal surfaces, giving rise to a series of resonant eigenstates [e.g. 1-3]. These structures, often referred to as artificial atoms, exhibit remarkable parallels to natural atoms, including the ability to form chemical bonds with natural atoms or repulsive interactions with chemically inert molecules. [4] In our previous investigations using atomic force microscopy (AFM), we successfully identified the occupation of resonant eigenstates that intersect the Fermi level. Notably, we observed a probe-tip-induced energy shift of these states during the measurements. [4] Building on these findings, we developed a method to estimate the energy of artificial atomic states based on their electron occupation. This approach enables precise tuning of the energy levels of these states with meV-scale accuracy. Additionally, we discovered that the distance-dependent repulsive interaction between a chemically inert molecule and the resonant eigenstates of the artificial atom is influenced by the geometric shape of the nanostructure. This holds the potential to tailor nanoscale interactions through precise structural design. [1] Crommie et al., Science 262 (1993), [2] Manoharan et al., Nature 403 (2000), [3] Freeney et al., SciPost Phys. 9 (2020), [4] Stilp et al., Science 372 (2021)

O 12.6 Mon 16:15 H6

Increasing the lifetime of confined electronic states in an artificial quantum structure — Marco Weiss, •Michael Schelchshorn, Fabian Stilp, Alfred J. Weymouth, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Understanding and tuning the factors influencing the lifetime of confined electronic states is a basic concept of quantum mechanics, whereas achieving large lifetimes in artificial nanostructures holds great potential for advancing quantum technologies. An example of such artificial structures are CO-based quantum corrals. In this study, tunneling spectroscopy measurements reveal a strong correlation between the size of the quantum corral and spectral width, characterized by a predominant Gaussian line shape. We attribute this dominant Gaussian-shaped lifetime broadening to the interaction of surface state electrons with the corral boundary. To further investigate this phenomenon, we constructed corrals of varying wall densities. Our findings indicate that elastic processes, such as tunneling, are more sensitive to the wall density than coupling to the bulk.

O 12.7 Mon 16:30 H6

Template-Assisted Synthesis of Fe_3O_4 Nanodots for High-Density Resistive Switching Memory — •Yifan Xu[1,2], Connie Bednarski-Meinke[2], Erkai Wang[3], Asmaa Qdemat[2], Emmanuel Kennzinger[2], Felix Gunkel[3], Regina Dittmann[3], Yen-Po Liu[3], Oleg Petracic[2,1], and Mai Hussein Hamed[2,4] — [1]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, 40225 Düsseldorf, Germany — [2]Jülich Centre for Neutron Science (JCNS-2), JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany — [4]Faculty of Science, Helwan University, 11795 Cairo, Egypt

The growing demand for high-density memory solutions has driven the exploration of innovative fabrication techniques. We introduce a bottom-up approach for synthesizing ordered Fe_3O_4 nanodots for nanoscale resistive switching memory applications. Using anodic aluminum oxide (AAO) templates as masks, Fe_3O_4 nanodots on Nb:$SrTiO_3$ substrate were fabricated via pulsed laser deposition. Scanning electron microscopy (SEM) confirms the nanodots' uniformity. Grazing incidence X-ray scattering (GISAXS) reveals a high degree of long-range ordering. Magnetometry measurements show that the Verwey transition temperature (T_V) and coercivity are preserved compared to continuous thin films. Conductive atomic force microscopy (cAFM) confirms well-defined nanodots using current maps. By sweeping the voltage on a single nanodot, set and reset processes are observed within ±2V.

O 12.8 Mon 16:45 H6

Intercalation of graphene nanoribbons — •Lüthi Dominik[1], Lin Yang[2], Ji Ma[2], Akimitsu Narita[3,4], Xinliang Feng[2], Klaus Müllen[3], Pascal Ruffieux[1], Roman Fasel[1], and Gabriela Borin Barin[1] — [1]Empa, Ueberlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [3]Max Plank Institute for Polymer Research, 55128 Mainz, Germany — [4]Okinawa Institute of Science and Technology, Okinawa 904-0495, Japan

Atomically precise graphene nanoribbons (GNRs) exhibit unique properties due to electron confinement and tunable band gaps, making them ideal for applications ranging from transistors to spintronics. Precise fabrication is critical, and on-surface synthesis enables the creation of various GNR types with tailored edge topologies, giving rise to intriguing properties such as spin-polarized edges and topological quantum states.

For device integration, GNRs must be transferred from metallic to insulating substrates. However, the high chemical reactivity of zigzag edges has hindered studies of their transport properties. To address this, we explore intercalation to decouple GNRs from metallic substrates, enabling dry-transfer in ultra-high vacuum. This preserves intrinsic properties and facilitates integration into device architectures.

We investigate intercalation with transition metal halides, providing a platform to study interactions with magnetic layers, combining decoupling benefits with potential applications in quantum technologies.

O 12.9 Mon 17:00 H6

Facilitating On-Surface Synthesis on Inert Surfaces by Using a Noble Gas Atmosphere — •Lukas Grossmann[1], Sascha Korn[2], Rochus Breuer[3], Michael Schmittel[3], Heiko Weber[2], Wolfgang Heckl[1], and Markus Lackinger[1] — [1]Deutsches Museum, Munich, Germany — [2]Friedrich-Alexander University, Erlangen, Germany — [3]University of Siegen, Siegen, Germany

A decisive milestone of On-Surface Synthesis (OSS) is the transition from reactive to inert surfaces for the covalent coupling of molecules. This is desirable, because conventionally used metal surfaces strongly interact with organic adsorbates. Thus, adsorption on metals alters the intrinsic properties of the synthesized nanostructures, compromising their applicability. In contrast, inert surfaces leave the adsorbed nanostructures unperturbed. But synthesis is aggravated since activation energies for coupling reactions on inert surfaces are generally higher than on metals. Consequently, reactants desorb before the activation temperature required for their covalent coupling is reached. Here, we explore the OSS of covalent thioether-linked Sierpinski triangles from 1,3,5-tris(4-mercaptophenyl)benzene on inert graphite surfaces. As shown by Scanning Tunneling Microscopy, covalent coupling is feasible by annealing in an argon atmosphere of 1 bar instead of in a vacuum. This protocol kinetically inhibits the premature desorption of reactants, and could be successfully transferred to even more weakly interacting graphene surfaces. The adsorbed Sierpinski triangles exhibit superior thermal stability compared to identical structures on gold and are air stable, underscoring the advantages of inert surfaces.

O 12.10 Mon 17:15 H6

Functionalization of Surfaces with Ordered Arrays of Fullerenes — •Lukas Spree, Caroline Hommel, Pierre Josse, and Andreas Heinrich — IBS Center for Quantum Nanoscience, 52 Ewhayeodae-gil, Daehyeon-dong, 03760 Seoul, South Korea

Endohedral fullerenes are a fascinating class of compounds that facilitate the stabilization of exotic configurations of few-atom structures within the confines of a carbon cage. Depending on the combination of carbon cage and encapsulated species, they provide very stable compounds with highly desirable physical properties. Among the compounds isolated and characterized so far are single molecule magnets with high blocking temperatures and promising candidates for spin qubits with long coherence times.

The exceptional chemical stability of endohedral fullerenes makes them very promising candidates for real-world applications. To achieve their full potential as nanometer sized magnets or quantum sensors, it is necessary to characterize and control the spatial orientation and surrounding of each individual molecule. Scanning probe microscopy techniques lend themselves well for the characterization of ordered assemblies on atomically flat substrates, as they offer an unparalleled combination of spatial and energy resolution.

In this presentation we will show our ongoing efforts of preparing ordered low-dimensional assemblies of endohedral fullerenes on surfaces through chemical functionalization and on-surface synthesis approaches, and discuss possibilities to preserve their desirable properties, like slow magnetic relaxation and potentially long coherence times.

O 12.11 Mon 17:30 H6

Well-defined nanostructures for energy storage and conversion applications — •Ningxiang Wu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Template-based technique provides a perfect approach to realize well-defined arrayed nanostructures within large-scale.[1]We have developed nanostructuring techniques mainly using anodic aluminum oxide templates with scalable, parallel and fast processes for fabricating different three-dimensional and surface nanostructures.[2]The obtained well-defined nanostructures possess large-scale arrayed configuration, high structural density, perfect regularity and cost-effectiveness, and are highly desirable for constructing different nano-devices especially for energy storage and conversion applications, including rechargeable sodium-ion and potassium-ion batteries, supercapacitors, and photo electrochemical devices.[3-4]The device performances demonstrated that the obtained nanostructures benefit these applications through the precise control over the structural features enabled by the geometrical characteristics of the templates. These achievements indicate the high potential and importance of template-based nanostructuring techniques for both basic research and device applications.[1] Nat.Commun.,2022,13,2435, [2] Nat.Nanotechnol.,2017,12,244, [3] Nat.Commun.,2018,9,1720, [4] Nat.Commun.,2016,7,10348

O 13: Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Monday 15:00–17:30 Location: H8

O 13.1 Mon 15:00 H8

Identical Fe-N4 Sites with Different Reactivity: Elucidating the Effect of Support Curvature — •Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Azin Shahsavar[1], Jiří Pavelec[2], and Jan Čechal[1,3] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Institute of Applied Physics, TU Wien, Vienna, Austria — [3]Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic

Understanding the atomic-scale mechanisms of single-atom catalysts (SACs) is pivotal for advancing their design and application. Using a 2D metal-organic framework (MOF) featuring Fe-N4 sites on a graphene/Ir(111) support, we uncover how the curvature of an inert substrate can significantly influence adsorption properties. We show that a 0.4 Å corrugation induced by the inert graphene/Ir(111) moiré leads to pronounced variations in adsorption energy of TCNQ (tetracyanoquinodimethane) molecules adsorbed on the 2D MOF. Molecules adsorbed above the "valleys" of the graphene/Ir moiré exhibit binding energies significantly stronger than those above the "hills," resulting in a temperature stability difference of over 60 °C. Our findings based on STM and DFT highlight those small structural distortions in SAC structure can profoundly impact the adsorption properties.

O 13.2 Mon 15:15 H8

Small atoms – large influence: Structural evolution upon dehydrogenation — •Jonas Brandhoff[1], Alina Preibsch[1], Richard Berger[2], Felix Otto[1], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Solid State Physics, Technical University Graz, Petersgasse 16, 8010 Graz, Austria

Molecular self-assembly is governed by the delicate balance between molecule-substrate and intermolecular interactions. Surface reactions can modulate this balance, enabling the engineering of tailored molecular architectures. Dehydrogenation is one of such surface reactions. Despite hydrogen being often overlooked as the smallest atom, its removal can significantly alter molecular interactions. In this study, 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) serves as a prototypical molecule to investigate dehydrogenation processes on surfaces. HHTP contains six equivalent hydroxy groups, allowing for varying degrees of dehydrogenation. These can be controlled via variation of the substrate temperature during deposition or using annealing steps post-deposition. Utilizing distortion-corrected Low-Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and Density Functional Theory (DFT), we examine the structural properties of (dehydrogenated) HHTP monolayers on Cu(111). Our analysis reveals distinct HHTP motifs and elucidates their interactions, providing deeper insights into the design of molecular architectures through controlled surface chemistry.

O 13.3 Mon 15:30 H8

Optical and Electronic Properties of Epitaxial Lead Phthalocyanine Monolayers and Bilayers on Graphite and Graphene — •Roman Forker, Marco Gruenewald, Matthias Spoddeck, and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The optical and electronic properties of the near-infrared absorber lead phthalocyanine (PbPc) on graphitic surfaces are measured by means of differential reflectance spectroscopy (DRS) and scanning tunneling spectroscopy (STS), respectively. This is corroborated by a thorough structural characterization using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), demonstrating the similarity of the adlayer structures on graphite and graphene substrates. The dielectric function of PbPc monolayers (ML) extracted from our DRS measurements exhibits monomer character, and thus provides evidence that there is no significant electronic coupling between the molecular film and graphite or graphene. From 1 to 2 ML the dielectric function changes drastically, indicating the formation of physical dimers. Concomitantly, for PbPc bilayers the electronic properties are found to be caused by the formation of face-to-face stacked molecules, resulting in a splitting of the dI/dV-features associated with the PbPc HOMO and LUMO upon bilayer formation. Our results are compared to previous photoelectron spectroscopy data of this system, where a similar splitting of the HOMO-related features was reported.

O 13.4 Mon 15:45 H8

Growth of N-heterocyclic carbenes on modified silicon surfaces — •Marie-Louise Fraser[1], Milan Kubicki[1], Ankita Das[2], Mowpriya Das[2], Preeti Chahar[2], Martin Franz[1], Frank Glorius[2], and Mario Dähne[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Universität Münster, Organisch-Chemisches Institut, Münster, Germany

Today's semiconductor industry is mainly based on silicon, thus the growth of organic films on silicon surfaces is a highly promising research field. However, the high number of dangling bonds typically present on silicon surfaces renders them often less suitable for molecular growth. With surface modifications more suitable silicon substrates can be produced. One such modification is a rare earth silicide layer on the Si(111) surface enabling growth of highly ordered monolayers [1]. Another suitable substrate is Si(111) modified by boron, as demonstrated e.g. for N-heterocyclic carbenes (NHCs) [2]. NHCs have been demonstrated to be particularly promising ligands for surface modification and functionalization. Here, scanning tunneling microscopy is used to examine the growth of the NHC molecule BIMe on both boron and rare-earth modified Si(111) surfaces. On both substrates, films with coverages ranging from submonolayers to complete monolayers could be successfully grown, allowing the determination of the adsorption geometry and of the ordering behavior in the monolayer. [1] M. Kubicki et al., *J. Phys. Chem. C* **128**, 13347 (2024). [2] M. Franz et al., *Nat. Chem.* **13**, 828 (2021).

O 13.5 Mon 16:00 H8

Imaging Dihydrogen Bond-Driven Assembly of Borazine on Au(111) — •Matthias Zeilerbauer, Marco Thaler, Barbara Obwaller, Milan Ončák, and Laerte L. Patera — Universität Innsbruck, Austria

Dihydrogen bonding (DHB) is a peculiar type of attractive interaction occurring between a partially positively charged hydrogen atom and a partially negatively charged hydrogen atom. Borazine represents a prototypical molecule exhibiting dihydrogen bonding in both gas phase, as well as in its crystalline form. For borazine assemblies on solid surfaces, a direct observation and characterization of dihydrogen bonding has remained elusive, possibly due to an intricate interplay of substrate-molecule and intermolecular interactions. Here we present evidence of dihydrogen bonding occurring in borazine assemblies on a Au(111) surface. By means of low-temperature scanning tunneling microscopy, we unveiled distinct configurations, exhibiting single and double dihydrogen bonding. Density functional theory calculations elucidate the interplay between substrate adsorption and intermolecular interactions to stabilize the formation of borazine dimers on Au(111), being the building blocks for the formation of larger assemblies.

O 13.6 Mon 16:15 H8

From Physical Trends to Structural Control: Insights into Phase Transition Times at Metal-Organic Interfaces — •Anna Werkovits, Simon B. Hollweger, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

At many metal-organic interfaces, molecules in the wetting layer undergo lying-standing transitions, significantly altering interface properties. Understanding the kinetics governing these transitions is essential for controlling structural evolution over time. This knowledge is particularly critical for tailoring interfaces based on either kinetically trapped or thermodynamically favoured structures.

To facilitate the design of interfaces, we develop a physically motivated surrogate model that estimates the phase transition times across a wide range of metal-organic interfaces. Using a systematic set of kinetic Monte Carlo simulations, incorporating variations in energetic landscapes and relative molecule sizes (representing hypothetical interface systems), we extract the physical relationships governing the timescales of phase transitions. These dependencies are analysed as functions of adsorption energies (lying and standing), kinetic barriers for reorientation and diffusion, molecule sizes, and environmental parameters such as temperature and pressure. This approach yields a formula that serves as a foundation for understanding trends, controlling structural evolution, and estimating timeframes for experiments and applications to ensure phase stability. Additionally, it enables the design of systems that remain stable over long periods, even in metastable states, advancing experimental and practical applications.

O 13.7 Mon 16:30 H8

Controlled Ion Beam Deposition supplied by Electrospray (ES-CIBD) - enabling UHV deposition of large, reactive or fragile building blocks for functional nano-architectures — •Andreas Walz[1,2], Annette Huettig[1,2], Michael Walz[1,2], Hartmut Schlichting[1,2], and Johannes V. Barth[2] — [1]pureions GmbH, Gilching, Germany — [2]Technical University of Munich, Germany

Cutting-edge research in the field surface- and nano- science using organic molecules requires control and unbiased understanding of structure and composition. Standard deposition techniques for the underlying building blocks restrict possible candidates: Thermal evaporation in vacuum (MBE, OMBE) is limited to volatile substances. Solution-based techniques such as drop casting, spin coating or inkjet printing are versatile but often lack purity and quality. Electrospray ionization (ESI) combined with mass selection and soft-landing of molecules unravels the vast potential of large, reactive or bio-relevant building blocks. The pool of possible molecules spans a wide spectrum from small organic molecules, over graphene nanoribbons (GNRs) up to several kilo- and megadalton proteins, DNA, but also inorganic clusters and larger nanoparticles may be possible. In-line with this, we present an UHV ion beam deposition device and its functionalities. Deposited layers are analyzed via STM. The main body of the device contains RF-driven ion guides with high transmission (>80% efficiency). A digital square-wave quadrupole mass filter (dQMF) provides virtually unlimited m/z-range. The footprint is benchtop in size, 0,5 x 1 m.

O 13.8 Mon 16:45 H8

Reactions of benzoporphyrins with Cu(111) — •Maximilian Muth, Majid Shaker, Julien Steffen, Alexander Wolfram, Simon Steinbach, Andreas Görling, Hans-Peter Steinrück, and Ole Lytken — Friedrich-Alexande-Universität Erlangen-Nürnberg, Germany

Porphyrins are molecules with many interesting properties that change upon adsorption on solid substrates. This can lead to something as simple as a change in conformation of the molecule or something more drastic as a reaction with - or catalyzed by - the substrate. We have focused on three molecules: free-base tetraphenyl transdibenzoporpyhrin, copper tetraphenyl transdibenzoporpyhrin and free-base tetraphenyl tetrabenzoporpyhrin adsorbed on Cu(111). Using temperature-programmed desorption, X-ray photoelectron spectroscopy, scanning tunneling microscopy and density-functional theory calculations, we have identified three reactions in the temperature range from 280 to 1000 K. In the first reaction step at 350 - 480 K the free-base benzoporphyrins react with copper atoms from the substrate, forming metalloporphyrins. At 480 - 650 K, the phenyl rings and pyrrole/benzo rings undergo a ring fusion reaction. Finally, at 650 - 950 K, the molecules polymerize and all remaining hydrogen atoms desorb from the surface as H2.

O 13.9 Mon 17:00 H8

Supercharging Polymorphism of Organic/Inorganic Interfaces — •Christoph Wachter and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, 8010, Austria

The polymorphism of organic/inorganic interfaces heavily influences a multitude of their properties. Therefore, altering the polymorphism by changing the substrate or modifying the intermolecular interactions has been studied extensively. However, the extent to which charge transfer affects polymorphism has yet to be investigated systematically. Based on the hypothesis that there is a link between the band width of polymorphs and their relative energy, we expect that polymorphs with larger band width are preferred if charge is transferred uniformly across the organic monolayer.

Conversely, it is also possible for charge to localize in individual adsorbates instead of spreading out across the monolayer. Such localized charge transfer occurs when the electronic coupling of the organic molecules to each other and to the substrate is small. In that case the relation stated above is not well-defined anymore.

To investigate the impact of both localized and delocalized charge transfer on polymorphism, we employ density functional theory in conjunction with a machine-learning based structure search algorithm. To properly capture charge localization, we go beyond the standard semi-local functionals by utilizing hybrid functionals and report whether the expected relation still holds in the case of localized charge transfer.

O 13.10 Mon 17:15 H8

Towards 2D metal-organic frameworks on weakly interacting substrates: FeDCA on coinage metals and Bi_2Se_3(111) surfaces — •Anna Kurowská[1], Matthias Blatnik[1], Veronika Stará[1], Pavel Procházka[1], Čestmír Drašar[2], and Jan Čechal[1,3] — [1]Central European Institute of Technology, Brno University of Technology — [2]Faculty of Chemical technology, University of Pardubice — [3]Institute of Physical Engineering, Brno University of Technology, Czech Republic

The formation of 2D metal-organic frameworks (MOFs) on a surface of topological insulator (TI) is a promising path to design quantum materials with exotic properties. MOFs featuring ferromagnetically coupled metal atoms are theoretically predicted to induce an exchange gap in the TI's surface band structure, potentially leading to a quantum anomalous Hall effect. However, the knowledge of self-assembly on TI substrates is still scarce. Here, we demonstrate the first experimental realization of 2D MOF, Fe-dicyanoanthracene (FeDCA), on the surface of a strong TI Bi2Se3. The structure and morphology were studied via scanning tunneling microscopy (STM) and low-energy electron microscopy (LEEM) and diffraction (LEED). We compare the growth of FeDCA on the Bi_2Se_3(111) surface with coinage metals and gr/Ir(111) surfaces, and discuss the conditions at which we obtain typical mixed Kagomé-honeycomb lattice and at which a new hexagonal lattice appears. The demonstration of 2D MOF/TI hybrid material presents a milestone on the way toward their application in fault-tolerant spin interconnects in future quantum devices.

O 14: 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Monday 15:00–18:00 Location: H11

O 14.1 Mon 15:00 H11

Hexagonal structures of europium oxides on Pd(111) studied with LEED and STM — •Muriel Wegner, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

With an increasing interest in technological applications of oxide materials, also two-dimensional (2D) oxides came into focus. The large flexibility in the variation of the cationic species, including even a combination of different cations, promises a rich variety of properties [1,2]. So far, the center of attention has been on transition metal sesquioxides M_2O_3 of corundum structure.

Here, we expand this field towards lanthanides. We present a combined scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) study of the growth of submonolayer coverages of europium oxide on a Pd(111) surface. Upon annealing the as deposited Eu in oxygen containing environments at temperatures above 800 K, long-range ordered multilayer islands of Eu_2O_3 are obtained. From LEED a $\begin{pmatrix} 8/3 & 4/3 \\ -4/3 & 4/3 \end{pmatrix}$ superstructure on Pd(111) is derived, which corresponds to a hexagonal lattice with a lattice parameter of 6.35 Å. This structure exhibits a large stability range. Only upon annealing to 1175 K in UHV an additional (2×2) superstructure evolves, which is seen as a hexagonal array of pores at a distance of 12.70 Å in STM.

By addition of small amounts of Ti atoms, the transformation into planar two-dimensional films is achieved. These mixed-metal oxides form a honeycomb lattice with a lattice parameter of 7.2 Å. In contrast to pristine Eu_2O_3, the Ti containing honeycomb can easily be resolved in STM.

[1] M. Van den Bossche, J. Goniakowski, and C. Noguera, Nanoscale **13**, 19500 (2021)

[2] P. I. Wemhoff, N. Nilius, C. Noguera, and J. Goniakowski, J. Phys. Chem. C **126** (10), 5070 (2022)

O 14.2 Mon 15:15 H11

Growth of an Fe buckled honeycomb lattice on Be(0001) — Hermann Osterhage[1], Abid H. Khan[2], Karoline Oetker[1], Radek Dao[1], Samaneh Setayandeh[2], Patrick Burr[2], Roland Wiesendanger[1], and •Stefan Krause[1] — [1]University of Hamburg, Germany — [2]University of New South Wales, Sydney, Australia

The Be(0001) surface is considered to be an ideal model system to host a 2D electron gas with pronounced electron-electron and electron-phonon interactions that are decoupled from the bulk [1,2]. In a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study the growth of Fe on a clean Be(0001) surface is investigated on the atomic scale [3]. At low Fe coverage, the nucleation of terraced nanoislands with a disordered surface is observed experimentally with STM. Increasing the Fe coverage results in the growth of extended films exhibiting a well-ordered p(2×2) superstructure. DFT is applied to investigate the growth of Fe on a Be(0001) surface from individual atoms to extended films.

The Fe buckled honeycomb lattice formation on Be(0001), as derived from our study, provides evidence for the realization of a very peculiar non-trivial electronic and magnetic model system. The results will be presented and discussed in terms of their implications for the emergence of novel electronic and magnetic phases resulting from the interactions between the 2D electron gas and the magnetic atoms.

[1] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).

[2] H. Osterhage *et al.*, Phys. Rev. B **103**, 155428 (2021).

[3] H. Osterhage *et al.*, Surf. Sci **752**, 122609 (2025).

O 14.3 Mon 15:30 H11

Electronic structure and edge states in the 2D Kagome lattice Ta_2S_3 / Au(111) — •Thais Chagas[1], Alessia Bardazzi[1], Samuel M. Vasconcelos[2], Alan C. R. Souza[3], Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Daniel Weber[1], Mario S. C. Mazzoni[3], Michael Rohlfing[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Germany — [2]Institute of Solid State Theory, Universität Münster, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Brazil

Kagome structures are a key model system in quantum physics, representing one of the most geometrically frustrated 2D magnetic lattices. In these systems, magnetic moments condense into a spin liquid phase at low temperatures, leading to intriguing physical phenomena. The characteristic Kagome bands in this lattice consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, in contrast, leads to fermions with infinite effective mass.

In this work, we investigate the 2D Ta_2S_3 Kagome phase on Au(111) using scanning tunneling microscopy (STM). STM images reveal bright island edges as a consequence of an enhanced density of states, indicating the presence of edge states. Additionally, we observe a significant dependence of atomic contrast on tunneling conditions, suggesting a complex electronic band structure near the Fermi level. Furthermore, we analyze the impact of growth parameters on defect formation. Finally, density functional theory (DFT) was employed to study the electronic structure of this material on Au(111), providing deeper insight into its electronic properties and interactions.

O 14.4 Mon 15:45 H11

Spectroscopic and microscopic study of (car)borane based 2D materials — •Martha Frey[1], Julian Picker[1], Jakub Visnak[2], Christof Neumann[1], Tomas Base[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec-Rez, c.p. 1001, Czech Republic

Boranes are electron-delocalized molecular clusters containing boron and hydrogen. Their electron-deficient bonding and structural diversity as well as their high thermal stability make them attractive for applications ranging from optoelectronics to energy storage. Here we present the fabrication of a novel boron-based, carbon free two-dimensional (2D) material via electron-induced crosslinking of borane-based self-assembled monolayers (SAMs) on silver substrates. The SAMs, crosslinking process and resulting nanomembranes were analyzed using complementary surface-sensitive techniques including X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), low-energy electron diffraction (LEED) and scanning tunneling and electron microscopies (STM, SEM). Furthermore, the results were compared with carborane-based 2D nanomaterials studied previously in our labs. The results demonstrate that properties of the 2D (car)borane nanosheets can be adjusted and tailored by the respective SAM constituents and that these structurally diverse cluster molecules open up new avenues for engineering novel functional 2D materials.

O 14.5 Mon 16:00 H11

Growth and Structure of Titanium Ditelluride Films on Au(111) — •Andreas Raabgrund, Alexander Wegerich, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Aiming at the MBE growth of transition metal ditelluride (MTe_2) films particularly in the single-layer limit, the formation of and interaction with the interface is of fundamental interest. The growth of a MTe_2 film can be achieved either by the tellurization of the desired metal substrate [1] or by the reactive deposition of Te and the corresponding transition metal M on a suitable substrate [2].

In this contribution we follow the latter approach and investigate both single-

and multilayer $TiTe_2$ films on Au(111) by LEED-IV, DFT, and STM. At first glance, LEED suggests a (4×4) superstructure with three $TiTe_2$ on four Au(111) unit cells. STM topography, however, reveals a mismatch of about 1% of the growing film w.r.t. the Au(111) substrate which indicates a relaxed $TiTe_2$ layer. LEED-IV results favor a film in close contact with Au substrate (Te-Au layer distance: ≈ 2.7 Å). By DFT total energy calculations we find that neither Te nor Ti substitution is favored in the topmost Au layer. Continuing the reactive deposition of Ti and Te a multilayer $TiTe_2$ film grows epitaxially as found by LEED-IV with a Pendry R factor of 0.12. Further, we discuss the transferability of this growth recipe to other MTe_2 films on Au(111).

[1] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)
[2] K. Lasek et al., ACS Nano **14**, 8473 (2020)

O 14.6 Mon 16:15 H11

Growth and Edge Reconstruction of 2D MnI_2 on Ag(111) — •Daniel Rothhardt[1,2,3], Christopher Penschke[4], Hans Josef Hug[1,2], Regina Hoffmann-Vogel[3], and Amina Kimouche[3] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [4]Institute of Chemistry, University of Potsdam, 14476 Potsdam, Germany

The reduced dimensionality of thin transition metal dihalide films on single-crystal surfaces enables a wide array of magnetic and electronic phenomena. However, producing stoichiometric monolayer islands demands thorough control over growth parameters. In this work, we utilize scanning probe microscopy (SPM) to explore the growth of MnI_2 on Ag(111) through single-crucible evaporation. The Ag(111) surface's catalytic activity promotes dehalogenation of MnI_2, resulting in a reconstructed iodine adlayer that serves as a template for the formation of truncated hexagonal MnI_2 islands. These islands display alter-nating edge lengths and distinctive Kelvin potentials, as revealed by Kelvin Probe Force Microscopy (KPFM). Density Functional Theory (DFT) calculations corroborate the experimental observations, including island heights, lattice parameters, and edge formation energies for both pristine and reconstructed edges. The asymmetry in edge lengths arises from differences in formation energies, determined by the orientation (up or down) of iodine atoms at the edges, as confirmed by DFT.

O 14.7 Mon 16:30 H11

Low defect density in MoS_2 monolayers grown on Au(111) by metal-organic chemical vapor deposition — •Julian Picker, Ziyang Gan, Christof Neumann, Antony George, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany

Monolayers of transition metal dichalcogenides (TMDs) possess high potential for applications in novel electronic and optoelectronic devices and therefore the development of methods for their scalable growth is of high importance. Among different suggested approaches, metal-organic chemical vapor deposition (MOCVD) is the most promising one for technological applications because of its lower growth temperature compared to most other methods, e.g., conventional chemical vapor or atomic layer deposition (CVD, ALD). Here we demonstrate the epitaxial growth of MoS_2 monolayers on Au(111) by MOCVD at 450 °C. We confirm the high quality of the grown TMD monolayers down to the atomic scale using several complementary methods. These include Raman spectroscopy, non-contact atomic force microscopy (nc-AFM), X-ray photoelectron spectroscopy and scanning tunneling microscopy (STM). The topographic corrugation of the MoS_2 monolayer on Au(111), revealed in a moiré structure, was measured as 20 pm by nc-AFM. The estimated defect density calculated from STM images of the as-grown MoS_2 monolayers is in the order of 10^{12} vacancies/cm^2. The defects are mainly caused by single sulfur vacancies.

J. Picker *et al.*, Micron **186**, 103708 (2024).

O 14.8 Mon 16:45 H11

Characterization of a large-scale single-domain MoS_2 monolayer — •Fabian Schöttke[1], Luka Pirker[2], Martin Vondráček[3], Michaela Hanušová[2], Václav Valeš[3], Jan Honolka[3], Otakar Frank[2], Matěj Velický[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

To fully utilize the outstanding optical and electronic properties of single-layer transition metal dichalcogenide (TMDC) in devices, a perfect single-domain film is needed. From the wealth of available preparation methods, exfoliation seems to provide the highest film quality. This method, however, commonly results in small flakes within the micrometer regime only. Exfoliation onto, or assisted by, a Au(111) surface is able to result in large-scale single-domain samples of several millimeters in diameter. We experimentally confirm the high quality of a MoS_2 monolayer on Au(111) by characterizing several sample properties: optical appearance, long-range structural order, work function changes, and the occupied & unoccupied electronic structure. Optical inspection and diffraction patterns easily identify millimeter-sized single domains. The electronic structure of MoS_2 is clearly distinguished from Au(111) states, especially measured by inverse photoemission in the L gap of Au(111). In summary, our experimental data of a MoS_2 monolayer exfoliated onto Au(111) demonstrate the capability of this procedure to produce large-scale single-domain TMDC samples.

O 14.9 Mon 17:00 H11

Kinetics of borophene growth on Ir(111) via boron segregation from the bulk — •Marin Petrović[1], Sherif Kamal[1], Borna Radatović[1], Marko Kralj[1], Matteo Jugovac[2], Iulia Cojocariu[2], Andrea Locatelli[2], and Tevfik Onur Menteş[2] — [1]Centre for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia — [2]Elettra - Sincrotrone Trieste S.C.p.A, 34149 Trieste, Italy

Segregation of boron atoms to the Ir(111) surface and their self-assembly into a borophene monolayer were tracked by low-energy electron microscopy (LEEM). Real-time monitoring of sample temperature, boron adatom concentration and borophene coverage reveals the kinetics of boron segregation from the iridium bulk and different modalities of borophene epitaxial growth. It is found that the temperature-triggered boron segregation to the surface is accompanied by instantaneous nucleation of borophene islands and condensation of boron adatoms, followed by rapid propagation of island perimeter along the iridium terraces. Subsequent growth of borophene proceeds by displacement of iridium surface steps, which is energetically expensive and thus relatively slow process that heavily depends on the step morphology. By identifying and analyzing quasi-equilibrium conditions on the sample surface during borophene growth, formation enthalpy of a boron monomer from borophene was estimated, which agrees well with the available theoretical calculations of the boron-iridium system.

O 14.10 Mon 17:15 H11

Growth and etching of hBN on Cu(111): Impact on substrate step dynamics and morphology — •Patrick Seleš[1,2], Marin Petrović[1], Smruti Ranjan Mohanty[3], and Frank Meyer zu Heringdorf[3] — [1]Center for Advanced Laser Techniques, Institute of Physics, Bijenička 46, Zagreb, Croatia — [2]Faculty of physics, University of Rijeka, Radmile Matejčić 2, Rijeka, Croatia — [3]Faculty for Physics, University of Duisburg-Essen, Lotharstrasse 1-21, Duisburg, Germany

The interaction of precursors and oxygen molecules with metal surfaces plays an important role in the growth dynamics of two-dimensional material such as graphene and hexagonal boron nitride (hBN). By using low-energy electron microscopy (LEEM), in this study we investigate the influence of hBN growth on Cu(111) step dynamics at various stages ranging from borazine precursor dosing to oxygen etching. Real-time monitoring of Cu step displacement underneath and next to hBN islands revealed step pinning and a significant decrease in step velocities compared to the pristine Cu surface, highlighting the stabilizing effect of hBN. After the removal of hBN islands by oxygen etching, Cu steps accelerated back to the pre-growth velocities and rearranged into a new surface morphology. Our findings elucidate the interplay between surface dynamics and step motion during hBN growth on Cu(111). By analyzing step displacement and morphological evolution, we contribute to a deeper understanding of metal-catalyzed chemical vapor deposition growth of hBN.

O 14.11 Mon 17:30 H11

In-situ growth and characterization of 2D $TaSe_2$ on Au(111) — •Cathy Sulaiman[1], Lars Buss[1], Raquel Sánchez-Barquilla[1], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany

Group V dichalcogenides such as TaX_2 (X = S, Se, T) have extensively been investigated in recent decades due to their diverse electron correlation effects, including the occurrence of charge density waves and Mott-Hubbard transitions. In 2D, two polytypes, 1T and 1H, exist, which exhibit distinct properties, making selective growth of each polytype crucial. Using low-energy electron microscopy (LEEM), we have successfully observed the growth of two $TaSe_2$ phases on Au(111) *in situ* after the co-deposition of Ta and Se. At elevated temperature, micron-sized, triangle-shaped islands with bright contrast nucleate first and grow at a higher rate. However, this phase turns out to be meta-stable as it suddenly transitions into a more stable phase (with dark contrast) and continues to grow at a reduced rate. Low-energy electron diffraction shows the presence of $TaSe_2$; bandstructure-sensitive I(V)-LEEM analysis reveals substantial differences in electron reflectivity between both phases. A comparison with TaS_2 suggests that the metastable and stable phases are 1T- and 1H-$TaSe_2$, respectively.

O 14.12 Mon 17:45 H11

CVD growth of monolayer transition metal dichalcogenides heterostructures using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Julian Picker[1], Christof Neumann[1], Moritz Quincke[2], Johannes Biskupek[2], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena 07743, Germany — [2]Central Facility of Electron Microscopy, Electron Microscopy Group of Material Science, University of Ulm, Ulm 89081, Germany

Heterostructures (HSs) formed of transition metal dichalcogenide (TMD) monolayers have attracted substantial research interest due to their unique physical properties. However, engineering the HS configurations (lateral and vertical) including the domain size for each TMD remains challenging. Here we present a facile route for the synthesis of different types of HSs of TMD monolayers using liquid precursors for transition metals. We characterized the TMD HSs by several complementary spectroscopy and microscopy techniques. Our results suggest that the HS configurations, lateral length and area of each TMD can be tuned by varying concentration ratios of the precursors. In addition, the overall heterostructure sizes can also be tuned from few to hundreds of micrometers. The developed method paves the way to obtaining high-quality lateral and vertical HS of $MoSe_2$-WSe_2 with controllable domain sizes.

O 15: Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)

The electron spin, a fundamental quantum mechanical property, plays a crucial role in determining the electronic and magnetic properties as well as the dynamics of matter. Its role becomes even more important at surfaces, 2D materials and nanomagnets as the low-dimensionality increases electron correlation. A fundamental understanding of spin excitations is significant for both fundamental science and modern applications. For decades, the interpretation of experimental signatures of spin excitations were focused on the Kondo effect paradigm, with Co atoms on the (111) surface of noble metals as the prototypical example. However, recent first-principles predictions and spin-polarized scanning tunnelling spectroscopy in high magnetic fields have demonstrated the existence of many-body states, called spinarons. These states arise from the binding of electronic states to spin excitations in the presence of spin-orbit coupling. Such findings, along with other studies, challenge the Kondo interpretation. Furthermore, related non-trivial many-body states may emerge in thin-film geometries, as shown by photoemission spectroscopy and first-principles manybody investigations or in quantum spin liquids. These examples testify that many-body phenomena are not only critically important for the fundamental understanding of spin excitations, they also impact a wide range of material characteristics, including electronic, magnetic, thermodynamic, and transport properties. This focus session will provide a forum to discuss intriguing many-body states driven by spin excitations, and serve as a forum to discuss the current knowledge on their origins, unique properties, and implications.

Organized by Matthias Bode (Würzburg University), Yujeong Bae (Swiss EMPA), and Stefan Blügel (FZ-Jülich).

Time: Monday 15:00–18:15 Location: H24

Invited Talk O 15.1 Mon 15:00 H24

Kondo and Yu-Shiba-Rusinov resonances: transport and coupling — •Laëtitia Farinacci[1,2,3], Gelavizh Ahmadi[3], Gaël Reecht[3], Benjamin W. Heinrich[3], Contanstin Czekelius[3], Felix von Oppen[3], and Katharina J. Franke[3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Germany

The exchange coupling between a magnetic impurity and a superconducting substrate leads to the formation of magnetic bound states, known as Yu-Shiba-Rusinov (YSR) states, inside the superconducting gap, as well as a Kondo resonance outside the gap. Studying these two many-body phenomena in parallel provides valuable insights into their characteristic properties.

We observed striking correlations between the asymmetries of the YSR state and the Kondo effect induced by FeTPyP molecules on Pb(111) in a scanning tunneling microscope (STM) [1]. We show that both asymmetries originate from interfering tunneling paths via a spin-carrying orbital and the highest occupied molecular orbital.

Additionally, we studied the formation of YSR bands in a self-assembled kagome lattice of magnetic molecules on Pb(111) and track YSR hybridization from kagome precursors to larger islands [2]. This work will motivate further studies to resolve possible spin-liquid or Kondo-lattice-type behavior.

[1] PRL 125, 256805 (2020). [2] Nat. Comm. 15, 6474 (2024).

Invited Talk O 15.2 Mon 15:30 H24

Electron delocalization in a 2D Mott insulator — •Amadeo L. Vazquez de Parga[1,2,4,5], Cosme G. Ayani[1,2], Michele Pisarra[3], Iván M. Ibarburu[1], Clara Rebanal[1], Manuela Garnica[2,4], Fabián Calleja[2], and Fernando Martín[1,2] — [1]Universidad Autónoma de Madrid, Madrid, Spain — [2]IMDEA Nanociencia, Madrid, Spain — [3]Universitá della Calabria, Rende, Italy — [4]Instituto Nicolás Cabrera, Madrid, Spain — [5]Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We follow by means of low temperature Scanning Tunneling Microscopy and Spectroscopy, the buildup of a 2D Kondo lattice in a system composed by a 2D Mott insulator, a single 1T-TaS2 layer, stacked on the surface of a metallic crystal, 2H-TaS2. When the sample temperature is lower than 27K, the magnetic moments present in the Mott insulator experience the Kondo screening by the conduction electrons of the metal, leading to the appearance of a Kondo resonance at the Fermi level. Below 11 K, a gap opens within the Kondo resonance, which is the signature of the formation of a coherent quantum state that extends all over the sample, i.e., a Kondo lattice [1]. Quasi particles interference maps reveal the emergence of a Fermi contour in the 2D Mott insulator when the temperature drops below 11K, indicating the delocalization of the highly correlated Mott electrons [2]. The observed modifications in the LDOS are well explained by state-of-the-art Density Functional Theory calculations.

[1] Small 20, 2303275 (2024) [2] Nat. Commun. 15, 10272 (2024)

Invited Talk O 15.3 Mon 16:00 H24

Kondo or no Kondo, that is the question — •Alexander Weismann, Neda Noei, Niklas Ide, and Richard Berndt — Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

The spin properties of individual atoms and molecules can produce distinctive spectral features in tunneling spectra near zero bias. Among these features, Kondo resonances and inelastic spin-flip excitations are often challenging to distinguish, despite their markedly different spectral line shapes. A Kondo resonance indicates a non-magnetic ground state, where the atomic spin is screened by conduction band electrons. In contrast, spin-flip excitations observed in zero-field tunneling spectra require magnetic anisotropy, which arises from spin-orbit coupling (SOC), to play a significant role. In this study, we demonstrate that the well-known Co/Cu(111) system, long believed to exhibit a Kondo resonance, instead adopts a magnetic ground state that is protected from Kondo screening by substantial magnetic anisotropy. The zero-bias anomaly in scanning tunneling spectra undergoes significant modification when Co atoms are attached to monoatomic Cu chains. Measurements conducted at 340 mK in a magnetic vector field reveal clear signatures of inelastic spin-flip excitations, with the anisotropy axis tilted away from the surface normal. The magnitude and orientation of this anisotropy are consistent with density functional theory (DFT) calculations. Moreover, quantum Monte Carlo many-body simulations confirm that the Kondo effect is suppressed when SOC is properly accounted for.

Invited Talk O 15.4 Mon 16:30 H24

Evidence for spinarons in Co atoms on noble metal (111) surfaces — •Artem Odobesko — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The zero-bias anomaly in the tunnelling differential conductance of Co atoms on Au(111) [1], long attributed to the Kondo effect, has recently been reinterpreted [2] as evidence of the spinaron – a novel many-body excitation arising from the interplay between spin excitations and conduction electrons. In our study, we used spin-polarized scanning tunneling spectroscopy (STS) on Co atoms on Cu(111) and Au(111) under high magnetic fields, revealing field-induced energy shifts and spin-resolved spectral features that challenge the conventional Kondo interpretation. Instead, our findings provide the first experimental confirmation of the spinaron [3].

We also investigated the role of hybridization with the substrate in spinaron formation, focusing on the reconstructed Au(111) surface. The unique local electronic environments created by the herringbone reconstruction strongly influ-

ence the hybridization strength and spectral features of Co adatoms, revealing a clear link between adsorption site, hybridization, and spinaronic excitations. Our results shed light on the fundamental mechanisms driving spinaron formation.

[1] V. Madhavan, et al., Science 280, 567 (1998)
[2] J. Bouaziz, et al., Nat. Comm. 11, 6112 (2020)
[3] F. Friedrich, et al., Nat. Phys. (2023)

Invited Talk O 15.5 Mon 17:00 H24

Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures — •Samir Lounis — Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Many-body phenomena are crucial in physics, particularly in condensed matter, influencing electronic, magnetic, thermodynamic, and transport properties. They leave distinct spectroscopic signatures, such as Kondo, excitonic, and polaronic features, arising from specific degrees of freedom. Since more than two decades Cobalt atoms on the (111) surfaces of noble metals have been a paradigm for the Kondo effect in scanning tunnelling spectroscopy experiments [1]. However, our recent first-principles predictions [2] followed by STS experiments in high magnetic fields [3,4] challenge this notion. Our findings reveal that the observed transport anomalies stem from spin excitations of Co atoms, forming a new many-body state – the spinaron – distinct from the Kondo resonance. I will delve into the spinaron origins, their unique properties, and implications explored through the recent atomic manipulation experiments. This work opens pathways to investigate and engineer these hybrid states in nanostructures, offering new insights into fundamental many-body states.

[1] V. Madhavan et al., Science 280, 567 (1998); [2] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [3] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [4] N. Noei et al., Nanoletters 23, 8988 (2023)

O 15.6 Mon 17:30 H24

Emergence of spinaronic states in Fe adatoms — Ilias Klepetsanis[1,2], Juba Bouaziz[4], •Philipp Rüssman[1,3], and Samir Lounis[1,2] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]University of Würzburg, Germany — [4]Research Center for Advanced Science and Technology, University of Tokyo, Japan

In recent years, spinarons, predicted from first-principles calculations [1], have been observed in Co adatoms on the Cu(111) surface, using spin-polarized scanning tunnelling spectroscopy (STS) in high magnetic fields [2]. Spinarons leave a non-trivial spectroscopic signature, for long interpreted to originate from the Kondo effect [3]. Here, we employ relativistic time-dependent density functional and many-body perturbation theory, to investigate the case of Fe adatoms on the Cu(111) surface, which carry a large magnetic moment of $3.25\mu_B$ preferring an out-of-plane orientation as dictated by a magnetic anisotropy energy of 2meV. In contrast to the Co adatom, the spinarons in Fe do not overlap with trivial spin-excitations. We discuss the spinaronic response to an out-of-plane magnetic field, the orbital character and the impact of spin-orbit coupling. [1] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [2] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [3] V. Madhavan et al., Science 280, 567 (1998)

O 15.7 Mon 17:45 H24

Revising the Superconductivity in Iron Based Superconductors from the Perspective of Electron Phonon Coupling — •Lanlin Du[1,2] and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong, China

There are currently two mainstream superconducting pairing mechanisms, namely electron phonon coupling and spin fluctuation, which are believed to play a dominant role in conventional superconductors like simple metal superconductors and unconventional superconductors like Copper oxides, respectively. Iron based superconductors are believed to connect these two aspects, that is, both mechanisms are important in it. In fact, some studies have shown that electron phonon coupling is also important in cuprates, and even provide evidence for s-wave pairing symmetry in them. Therefore, it is important to consider the role of electron phonon coupling in unconventional superconductors. Here, we revise the superconductivity in Iron based superconductors using Migdal-Eliashberg formalism and electron phonon coupling strength corrected by many body method from the two perspectives of doping and pressurization. Our results are in good agreement with the experiments. Based on this, we predict a new two-dimensional high-Tc Iron based superconductor.

O 15.8 Mon 18:00 H24

Theoretical model for multiorbital Kondo screening in strongly correlated molecules with several unpaired electrons — •Manish Kumar[1], Aitor Calvo-Fernandez[2], Diego Solar-Polo[1], Asier Eiguren[2], Maria Blanco-Rey[3], and Pavel Jelinek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic , Cukrovarnicka 10, Prague 6, CZ 16200, Czech Republic — [2]Department of Physics, University of the Basque Country UPV-EHU, 48080 Leioa, Spain — [3]Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, University of the Basque Country UPV-EHU, 20018 Donostia-San Sebastián, Spain

The mechanism of Kondo screening in strongly correlated molecules with several unpaired electrons on a metal surface is still under debate. Here, we provide a theoretical framework that rationalizes the emergence of Kondo screening involving several extended molecular orbitals with unpaired electrons. We introduce a perturbative model, which provides simple rules to identify the presence of antiferromagnetic spin-flip channels involving charged molecular multiplets responsible for Kondo screening. The Kondo regime is confirmed by numerical renormalization group calculations. In addition, we introduce the concept of Kondo orbitals as molecular orbitals associated with the Kondo screening process, which provide a direct interpretation of experimental dI/dV maps of Kondo resonances. We demonstrate that this theoretical framework can be applied to different strongly correlated open-shell molecules on metal surfaces, obtaining good agreement with previously published experimental data.

O 16: Scanning Probe Techniques: Method Development

Time: Monday 15:00–18:00 Location: H25

O 16.1 Mon 15:00 H25

Fast and quantitative nanomechanical mapping using photothermal off-resonance tapping atomic force microscopy (AFM) — •Gunstheimer Hans[1,2], Fläschner Gotthold[1], Adams Jonathan[1], Hölscher Hendrik[2], and Hoogenboom Bart[1] — [1]Nanosurf AG, Gräubernstrasse 12-14, 4410 Liestal, Switzerland — [2]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology, Karlsruhe, Germany

Multifunctional imaging, makes AFM a powerful tool for nanoscale surface analysis. However, most scanner-based methods for measuring mechanical properties are slow, limiting their use in fast mapping of mechanical characteristics. The main source of limitation is the piezo scanner, used to modulate tip-sample distance. This can be overcome by direct cantilever actuation, such as photothermal excitation. By moving the cantilever's comparably smaller mass, higher actuation bandwidths are accessible, enabling new approaches for AFM-based nanomechanical characterization. Here, we share insights on applying photothermal off-resonance tapping to fast nanomechanical property mapping. Based on simulations of cantilever bending due to laser-induced heating, we predict the cantilever response and propose a procedure to convert thermomechanical cantilever behavior into a calibrated nanomechanical measurement. We present the experimental method validation by measurements of polymer samples and reference structures. This novel photothermal off-resonance tapping mode enables quantitative nanomechanical mapping at frequencies of several tens of kHz, unlocking new insights into dynamic sample behavior.

O 16.2 Mon 15:15 H25

Multifrequency Excitation and High Dynamic Range Tunneling Spectroscopy — Philipp E.J. Maier, Ajla Karić, Carolina A. Marques, Berk Zengin, and •Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

The massive number of spectra required for high-resolution quasiparticle interference of low-dimensional quantum materials motivates the development of faster point spectroscopies. While the advent of parallel spectroscopy and compressive sensing enhancements has provided welcome speed boosts, these come at a cost. The application of a sinusoidal voltage on the nonlinearities in the current-voltage characteristics of a tunneling junction generates a frequency comb of higher order current-harmonics. While their parallel measurement enables faster tunneling spectroscopy, it unfortunately averages longest where the currents are largest, leading to poor signal-to-noise ratios for smaller signals associated with features close to the Fermi level. Here, we introduce a multifrequency excitation mode that increases the averaging time for small currents, enabling fast and high-resolution spectroscopy. Additionally, the AC excitation of our method can be used to dramatically increase the dynamical current range by exactly and deliberately suppressing the large amplitude, low order harmonics that would otherwise saturate the preamplifier stage.

O 16.3 Mon 15:30 H25

Dynamics on the atomic-scale: Use and limitations of stochastic resonance spectroscopy — •Nicolaj Betz[1,2], Vivek K. Rajathilakam[1], Laëtitia Farinacci[1,3], Susan N. Coppersmith[4], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany — [3]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [4]School of Physics, University of New South Wales, Sydney, Australia.

Stochastic dynamics offer valuable insight into the internal structure of a system and its interactions with the environment. However, in atomic-scale systems investigated using scanning tunneling microscopy, comprehensive and accurate characterization is often a significant challenge. In this talk, we discuss a new type of measurement technique, stochastic resonance spectroscopy (SRS), that provides comparatively large signals over a wide range of timescales down to the picosecond range. It uses the effect of stochastic resonance, where the system's state synchronizes with an external harmonic drive. This encodes information about the dynamics in a time-independent signal. Such drive-induced imprinting of time-independent signals can alter the system's dynamics, but this limitation can be mitigated in SRS by its ability to identify and even tune these drive-induced dynamics. This enables targeted investigation of driven quantum systems on the atomic scale.

O 16.4 Mon 15:45 H25

From experiments to insights: processing tool for SPM images with periodic pattern — •Farzin Irandoost[1], Fillippo Federici Canova[2], Tobias Dickbreder[3], Franziska Sabath[3], Angelika Kühnle[3], and Adam S. Foster[1,4] — [1]Department of Applied Physics, Aalto University, Helsinki, Finland — [2]Nanolayers Research Computing Ltd., London, England — [3]Physical Chemistry I, Bielefeld University, Germany — [4]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

Big datasets of Scanning Probe Microscopy (SPM) images are potentially valuable, but robust algorithms are required for preprocessing them due to the high levels of defects and noise introduced during experiments. These issues often render many images unusable, especially for in-liquid SPM studies.

As part of a study on hydration patterns using a dataset of in-liquid calcite, we developed a versatile workflow to clean the data and extract features for further analysis. This workflow automatically corrects non-linear defects, ensuring the outputs closely resemble ideal periodic patterns. Consequently, many previously discarded raw images can be recovered to prepare a large, clean dataset ready for analysis. Afterward, the features of interest could be extracted using pattern decomposition facilitated by Fourier transforms.

This approach provides access to invaluable information about the lattice and hydration patterns for our study. Additionally, it offers a versatile tool for broader analyses of images with periodic structures.

O 16.5 Mon 16:00 H25

True Alternating Current Scanning Tunneling Microscope (ACSTM): tunneling on insulators — •Marcel Rost[1] and Milan Allan[1,2] — [1]Leiden Institute of Physics (LION), Leiden, NL — [2]University of Munich (LMU), Munich, Germany

Scanning Tunneling Microscopy has revolutionized our atomic scale understanding of surfaces and accelerated progress in nanotechnology. This technique, however, is restricted to metal or semiconducting samples, as it requires a tiny current to stabilize the tip-sample distance with atomic scale precision.

We developed a new imaging and feedback method that relies on true alternating current (AC) without any direct current (DC) component. This technique does not only enable the imaging on non-conducting surfaces with atomic resolution, like (thin) glass and oxides, it provides also access to high-frequency electronic sample information. We demonstrate that it is possible to measure on 22nm thick silicon oxide with 10 MHz tunneling current.

O 16.6 Mon 16:15 H25

STM-induced luminescence with a parabolic mirror - millions of counts — •Yannis Hilgers, Andreas Reutter, Mike Stummvoll, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics - LENA, TU Braunschweig, Germany

In recent years, scanning tunneling microscopy-induced luminescence (STML) has become a powerful technique allowing to record topography with atomic resolution and simultaneous spatially resolved photon count maps. We have built a Photon STM with a large parabolic mirror which was specifically designed for high photon collection efficiency. With this system we detected so far unreached photon counts of about 6 million photons per second at 1 nA tunnelling current that result from the decay of plasmon-polariton excitations between a Ag(111) surface and a Ag tip. Considering losses due to geometry, shadowing, optical components and detectors, we estimate a yield of approximately $5 \cdot 10^{-3}$ photons per tunnelling electron. This is scratching on the theoretical predictions by Johansson et al. [1], Persson and Baratoff [2] and others who all reported conversion factors in the range of 10^{-4} to 10^{-3} at most. In this talk we discuss these results, the instrumental calibrations and assumptions necessary for this estimation and speculate about possible explanations of the high observed excitation efficiency.

1 P. Johansson, R. Monreal, P. Apell - Phys. Rev. B 42, 9210 (1990)
2 B.N.J. Persson, A. Baratoff - Phys. Rev. Lett. 68, 3224 (1992)

O 16.7 Mon 16:30 H25

Momentum-polarized microscopy with van der Waals scanning probe tip. — •Abhisek Kole[1,2,4], Frank Stefan Tautz[1,2,4], Markus Ternes[1,2,3], Jose Martinez Castro[1,2,3], and Felix Lüpke[1,2,5] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Germany — [3]Institut fur Experimentalphysik II B, RWTH Aachen, Aachen, Germany — [4]Institut fur Experimentalphysik IV A, RWTH Aachen, Aachen, Germany — [5]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

Van der Waals materials are celebrated for their remarkable 2D physics, which includes correlated phenomena and topological effects. In this work, we present momentum-polarized microscopy using a van der Waals scanning probe tip. We developed and implemented a novel fabrication method to fabricate van der Waals scanning tunneling tips from exfoliated graphite flakes. The fabricated tips were characterized by atomically resolved scanning tunneling microscopy (STM) on an Ag(111) surface, where differential conductance measurements provided direct evidence of tunneling through the zigzag edge states of graphene. In addition, Friedel oscillations on the Ag(111) surface revealed clear signs of momentum-dependent tunneling, manifesting as anisotropic tunneling conductance. To further validate and investigate the momentum selective properties of the zigzag graphene tips, we have resolved the momentum dependent superconducting gap on FeSe lattices.

O 16.8 Mon 16:45 H25

Image-to-molecule translation for high-resolution SPM images — •Lauri Kurki[1], Jie Huang[1], Niko Oinonen[1,2], and Adam S. Foster[1,3] — [1]Aalto University, Finland — [2]Nanolayers Research Computing Ltd., UK — [3]WPI-NanoLSI, Kanazawa University, Japan

Scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) functionalized with a CO molecule on the probe apex capture sub-molecular level detail of the imaged sample [1]. However, the produced images are often difficult to interpret due to complex tip-sample interactions. To accelerate image analysis, we propose machine learning tools to extract sample properties directly from SPM images.

In recent years, there has been rapid development in image analysis methods in SPM in general and in particular for extracting atomic positions from AFM and STM images [2,3,4]. We build upon these models and achieve improved chemical and physical sensitivity compared to previous results [2]. Additionally, we explore equivariant neural networks [5] and compare their data efficiency and accuracy to traditional deep learning models.

[1] Cai et al., J. Am. Chem. Soc. 2022, 144, 44, 20227-20231 [2] Kurki et al., ACS Nano 2024, 18, 17, 11130*11138 [3] Alldritt et al., Sci. Adv. 2020; 6 : eaay6913 [4] Carracedo-Cosme et al., Nanomaterials 2021, 11, 1658. [5] Cesa et al., arXiv:1911.08251

O 16.9 Mon 17:00 H25

Scanning Quantum Microscopy for 2D Superconductors — •Ruoming Peng[1], Malik Lenger[1], Sreehari Jayaram[1], and Joerg Wrachtrup[1,2] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Visualization of nanoscale dynamics in 2D superconductors provides critical insights into pairing mechanisms and topological electronic responses. Using state-of-the-art scanning quantum microscopy based on nitrogen-vacancy (NV) centers in diamonds, we investigate the local magnetic behavior of the 2D superconductor 2H-NbSe2 with high sensitivity and spatial resolution. This approach enables the first spatial-temporal measurements of vortex dynamics in thin exfoliated 2H-NbSe2, revealing a strong correlation between vortex arrangements and geometric confinement. We observe the melting transition of vortex solids near the critical temperature, alongside cooling-rate-dependent vortex rearrangements across thermal cycles. Additionally, through local magnetic noise probing via spin coherence time (T2) measurements, we uncover unexpected supercurrent fluctuations in reduced dimensionality. These findings highlight the potential of scanning quantum microscopy in advancing our understanding of vortex physics and emergent phenomena in 2D superconducting systems.

O 16.10 Mon 17:15 H25

A high-throughput ESR-STM setup at mK temperatures — •Máté Stark, Jonas Arnold, Luise Renz, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Characterizing and controlling single spins using Electron Spin Resonance Scanning Tunneling Microscopy (ESR-STM) [1] benefits from ultra-low tempera-

tures, minimal noise, and efficient RF transmission to the junction. This work details upgrades to an ESR-STM system operating at mK temperatures within a compact dilution refrigerator under UHV conditions. We achieved an electronic temperature below 200 mK while maintaining effective RF transmission up to 40 GHz. In addition, we developed a compact UHV chamber with an automated sputter-annealing stage, allowing for efficient sample preparation and quick exchange of samples with various atoms and molecules atop. In combination with the fast cooldown of the dilution refrigerator, these upgrades greatly streamline the experimental workflows allowing for rapid and high quality ESR-STM measurements. [1] Baumann, S. et al., 350(6259), 2015.

O 16.11 Mon 17:30 H25

Molecular Identification via Molecular Fingerprint extraction from Atomic Force Microscopy images — •Manuel González Lastre[1], Pablo Pou[1,2], Miguel Wiche[3,4], Daniel Ebeling[3,4], Andre Schirmeisen[3,4], and Rubén Pérez[1,2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany — [4]Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Previous works have already shown that deep learning (DL) models can retrieve the chemical and structural information encoded in a 3D stack of constant-height HR–AFM images, leading to molecular identification.

In this work, we overcome their limitations by using a well-established description of the molecular structure in terms of topological fingerprints, the Extended Connectivity Fingerprints, which provide local structural information of the molecule. In this work, we train a DL model to extract this optimized structural descriptor from the 3D HR–AFM stacks and use it, through virtual screening, to identify molecules from their predicted ECFP4 with a retrieval accuracy on theoretical images of 95.4%. This approach, unlike previous DL models, assigns a confidence score, the Tanimoto similarity, to each of the candidate molecules, thus providing information on the reliability of the identification.

O 16.12 Mon 17:45 H25

The Josephson effect in the dynamical Coulomb blockade regime with high energy resolution — •Xianzhe Zeng[1], Janis Siebrecht[1], Haonan Huang[1], Sujoy Karan[1], Klaus Kern[1,2], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Josephson effect can be used as a good quantitative indicator of the energy resolution of scanning tunneling microscopy (STM). Recently we have upgraded our mK-STM with low-temperature filtering on our scan head. We measured the Josephson current and found an improvement of the energy resolution by almost an order of magnitude. The high resolution allows us to measure several spectroscopic features in detail, including the superconducting coherence peaks with extreme sharpness and the environmental resonances in the Josephson current at low frequency due to the dynamical Coulomb blockade.

O 17: Poster Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation

Time: Monday 18:00–20:00 Location: P2

O 17.1 Mon 18:00 P2

Synthesis and characterization of a non-planar cyclophenylene on Au(111) — Sergio Salaverria[1], Martin Irizar[2,3,4], Jesus Janeiro[5], Paula Angulo-Portugal[6], Tao Wang[2], Jan Patrick Calupitan[6], •Jonathan Rodriguez-Fernandez[1,7], Aran Garcia-Lekue[2,8], Martina Corso[6], Emilio Artacho[2,3,8,9], Diego Peña[5], Dolores Perez[5], and Dimas G. de Oteyza[1,2] — [1]CINN, CSIC-UNIOVI-PA, El Entrego, Spain — [2]DIPC,San Sebastián, Spain — [3]CIC nanoGUNE, San Sebastián, Spain — [4]PMAS, UPV/EHU, San Sebastián, Spain — [5]CiQUS, Universidade de Santiago de Compostela, Spain — [6]CFM-MPC, CSIC-UPV/EHU, San Sebastián, Spain — [7]Physics Department, University of Oviedo, Spain — [8]Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [9]TCM, University of Cambridge, Cambridge (UK)

Cyclophenylenes, i.e., macrocycles composed of linked benzene rings, have attracted intensive interest because of their appealing structures and potential applications.

In this work, we report the on-surface synthesis of a non-planar Au-coordinated cyclophenylene, containing four meta- and two para- connections, on a Au(111) surface, by undergoing hierarchical, metal-assisted double Ullmann coupling of a 1,10-dibrominated angular phenylene, and subsequent selective C-C bond cleavage of the four-membered rings in the resulting phenylene dimer. The chemical structure was characterized by bond-resolving (BR) STM and further supported by STS and DFT. This study offers the first approach for the synthesis of non-planar cyclophenylenes on surfaces.

O 17.2 Mon 18:00 P2

Experimental benchmark for configuration monitoring during scanning-probe-microscope manipulation — •Mong-Wen Gu[1], Jonas Lederer[2], Joshua Scheidt[1,2], Hadi H. Arefi[1], Kristof T. Schütt[2], Michael Gastegger[2], F. Stefan Tautz[1], Klaus-Robert Müller[2], and Christian Wagner[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Machine Learning Group, Technische Universität Berlin, Berlin, Germany

The scanning probe microscope (SPM) allows nano-objects to be manipulated with single-molecule precision. A critical challenge of this SPM-based technique is to simultaneously manipulate molecules and monitor their configuration. Here, an experimental protocol is developed and evaluated that predicts the molecular configuration based on the physical observables continuously acquired by the SPM. A PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule on the Ag(111) surface is manipulated to move along a predefined tip trajectory. The measured observables (force gradient) are compared with the results of a DFT trained machine learning model. This work paves the way for the fabrication of a wide variety of nanostructures.

O 17.3 Mon 18:00 P2

Exploring supramolecular rings by scanning tunneling microscopy — •Cagri Turan[1], Elie Benchimol[2], Guido Clever[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr-Universität Bochum, Germany — [2]Inorganic Chemistry, Technische Universität Dortmund, Germany

Enzymes inspire the design of supramolecular systems, mimicking their catalytic functions for advanced material applications. Among these systems, supramolecular rings and cages are one of the most suitable candidates for mimicking enzyme-like behavior. The use of two different ligands in the heteroleptic supramolecular rings enhances their complexity, enabling the creation of structures that resemble the sophisticated architectures of enzymes. This study reports deposition, self-assembly and inelastic electron tunneling manipulation of PdL2 rings on the Ag(111) surface. The ring molecules were characterized using low-temperature scanning tunneling microscopy in ultra-high vacuum at 7 K. By utilizing an atomic layer injection system, the acetonitrile solvent, used as a solvent during the self-assembly of ligands, will evaporate before the molecules reach the surface, ensuring that only the ring molecules are deposited onto the substrate. Through inelastic electron tunneling manipulation, site-specific manipulations and ligand dissociation processes were explored, offering insights into reaction mechanisms and molecular dynamics on rings on the metallic substrate. The findings contribute to understanding the interaction of supramolecular systems with metal surfaces, enabling advancements in nanoscale functional materials.

O 17.4 Mon 18:00 P2

Autonomous chemical reactions in scanning tunneling microscopy — •Nian Wu[1], Peter Liljeroth[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

Scanning tunneling microscopy (STM) has shown great promise in manipulating atoms or molecules in on-surface molecular synthesis. However, the selection of proper parameters for various manipulations requires extensive explorations and strongly depends on domain knowledge. In particular, the coupling of fragments, as a critical step for polymerizations, necessitates more precise control in rotations and distances. To address this problem, we designed a deep reinforcement learning approach to automate the C-C coupling from Zn(II)-5,15-bis(4-bromo-2,6-dimethylpheny)porphyrin (ZnMe4DPP2.) through learning manipulation parameters in STM, thus enabling the assembly of large polymers based on the building blocks.

O 17.5 Mon 18:00 P2

Steering intermolecular interaction and ordering of N-heterocyclic carbenes on metal surfaces — •Duong Tran[1,2], Philipp Wiesener[1,2], Lacheng Liu[1,2], Ankita Das[3], Alex-Cristian Tomut[4], Nikos Doltsinis[4], Frank Glorius[3], Harald Fuchs[1,2], and Harry Mönig[1,2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Center for

Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany — [3]Organisch-Chemisches Institut, Universität Münster, Corrensstrasse 40, 48149 Münster, Germany — [4]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

N-Heterocyclic carbenes (NHCs) are established ligands for the chemical and electronic functionalization of surfaces and nanoparticles. Controlling their nucleation and aggregation mechanisms provides valuable opportunities to tune their catalytic- and electro-optical properties. In the present work, we investigate the effect of hydroxyl-side groups on the self-assemblies of IMes on Au(111) and Ag(111) substrates by scanning tunneling microscopy with sub-molecular resolution. Our results are complemented by X-ray photoelectron spectroscopy (XPS) and first-principles calculations. We find that the OH groups can drastically enhance the molecular order, especially on the Ag(111) substrate where extended 2D networks are found. Our findings are essential for robust NHC-based supramolecular networks with tailored properties.

O 17.6 Mon 18:00 P2

Controlling on-surface chemical reactions through photochemistry — •Hao Jiang, Yu He, Jiayi Lu, Zhiwen Zhu, and Qiang Sun — Materials Genome Institute, Shanghai University, 200444 Shanghai , China

On-surface synthesis targets extended nanostructures by covalent coupling of organic molecules on surfaces. The most common way to induce reactions of precursor molecules on the surface is by heating, which will however increase the possibility of forming side reactions and lacks selectivity in many cases, thus limiting wider applications of on-surface synthesis. In contrast to the thermally triggered chemistry, photochemistry provides an alternative way to activate molecules. Light has been demonstrated to break certain covalent bonds in a less constructive fashion. Moreover, light has more adjustable parameters such as intensity, wavelength, polarization, etc., to control reactions more finely. Recently, we demonstrated the use of light polarizations to reveal the mechanism of dehalogenation reaction and realized photo induced dechlorination reactionon metal surfaces.

In this poster, we will showcase the wavelength dependence in on-surface synthesis and demonstrate how to harness photochemistry to achieve reaction selectivity in on-surface reactions. Three organic molecules, each with the same functional group, exhibit different chemical reactivities under photon excitation. Our work provides fundamental insights into photoinduced on-surface reactions and illustrates the potential of photochemistry for achieving highly selective and controllable reactions.

O 17.7 Mon 18:00 P2

Reaction intermediates, organometallic polymers and graphene nanoribbons in on-surface Ullmann-type coupling on coinage metals — R.S. Koen Houtsma[1], Jeanne van Zuilen[1], Floris van Nyendaal[1], Mihaela Enache[1], and •Meike Stöhr[1,2,3] — [1]University of Groningen, Netherlands — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Applied Sciences of the Grisons, Switzerland

Ullmann-type coupling has been so far the most often employed on-surface reaction for the controlled fabrication of molecular nanoarchitectures in a bottom-up manner. For the case of the prochiral precursor molecule 6,12 dibromochrysene, we compared the influence of substrate material/orientation, annealing temperature and reaction conditions on the reaction outcome. While on Au(111) achiral chevron-type graphene-nanoribbons are formed [1], on Cu(111), Ag(111) [2] and Ag(110) [3] only 1D organometallic polymers were obtained. These 1D polymers are homochiral when Cu(111) was used as substrate whereas they were heterochiral on Ag(111). In the case of Ag(110), their chirality could be even steered via the reaction conditions. With the help of reaction intermediates observed on Ag(111), we obtained key insights into the formation process of the organometallic polymers which is based on the breaking and re-establishing of C-Ag bonds. References: [1] R.S.K. Houtsma et al., Nanoscale Adv. 2022, 4, 3531. [2] R.S.K. Houtsma et al., Adv. Mater. Interfaces 2024, 11, 2300728. [3] R.S.K. Houtsma et al., Commun. Chem. 2024, 7, 51.

O 17.8 Mon 18:00 P2

LT-STM investigations of subphthalocyanine based vertical molecular rotors on Au (111) — •Franz Plate[1], Natasha Khera[1], Suchetana Sarkar[1], Soyoung Park[2,3], Ningwei Sun[2,3], Ebru Cihan[1], Dmitry Ryndyk[1,4], Franziska Lissel[2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Leibniz Institute of Polymer Research Dresden, TU Dresden, 01069 Dresden Germany — [3]Institute of Applied Polymer Physics (IAPP) TU Hamburg, Kasernenstraße 12, 21073 Hamburg Germany — [4]Professur für Theoretische Chemie, TU Dresden, 01062 Dresden, Germany

We present a vertical rotor based on borsubphthalocyaninchloride (SubPC) platforms adsorbed on Au(111), investigated by low temperature scanning tunneling microscopy. SubPC is a well-investigated molecule which is known to form well-ordered structures, to adsorb flat on the surface and to be highly mobile as a single molecule. The boron atom carries an axial ligand. In this study, SubPC was functionalized with different axial ligands, aiming to create a vertical molecular rotor. The adsorption behavior of SubPC functionalized with azobenzene and 2-methylnaphthalene after thermal evaporation and flash deposition on a cold (5K) surface is presented in high resolution STM images supported by density functional theory (DFT) simulations. In addition, the stabilization through co-deposited pure SubPC and SubPC functionalized with 2-methylnaphthalene is presented.

O 17.9 Mon 18:00 P2

Adsorption behavior of organoboroxine and organoborthiine based molecules on Au(111) — •Natasha Khera[1], Franz Plate[1], Karen Marlenne Garcia Alvarez[2], Suchetana Sarkar[1], Andreas Schneemann[2], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Inorganic Chemistry I, TU Dresden, 01069 Dresden, Germany

In this study, we investigate the adsorption behavior of organoboroxine and organoborthiine based molecules on Au (111) surface, employing low temperature scanning tunneling microscopy (LT-STM) and spectroscopy in ultra-high vacuum (UHV) conditions. Organoboroxines provide a model system for constructing Covalent Organic Frameworks (COFs) and are well studied for their applications in catalysis, material science, optoelectronics and energy storage. In contrast, organoborthiines, due to their sulfur mediated interactions, hold promise, making them a compelling area for future research. In this work, a comparative analysis of the adsorption geometries, self-assembled structures and spectroscopic properties of both these molecules is presented.

O 17.10 Mon 18:00 P2

Chemical activation of a single melamine molecule via isomerization and metalation with a copper atom — •Karl Rothe[1], Manex Alkorta[2], Nicolas Néel[1], Thomas Frederiksen[3], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Centro de Física de Materiales and Fisika Aplikatua Saila, University of the Basque Country, E-20018 Donostia - San Sebastián — [3]Donostia International Physics Center, E-20018 Donostia San Sebastián and IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao

The entire sequence of chemically activating an educt, identifying its reactive site, running a chemical reaction and quantifying the involved forces and energies was performed by means of scanning probe methods. The organic molecule melamine adsorbed on Cu(100) serves as a single-molecule model system for activation via tautomerization and consecutive metalation with a single Cu atom. An atomic force microscope with a CO-decorated tip probes the reactive sites of the isomers at which the subsequent single metal atom transfer is initiated using a Cu-terminated probe. Following the interaction between the mutually approached reaction partners up to the verge of chemical-bond formation enables the access to the force and energy involved in the single-molecule metalation process. Total-energy calculations from density functional theory support the experimental findings and illustrate the structure of the reactants.

Funding by the DFG through KR 2912/18-1 and the BMBF through Forlab is acknowledged.

O 17.11 Mon 18:00 P2

Metallocorroles: On-Surface Synthesis, Adsorption Geometry, and Electronic Structure — •Cong Guo, Jan Herritsch, Anastasiya Beliakouskaya, and J. Michael Gottfried — Philipps-Universität Marburg, Fachbereich Chemie, 35043 Marburg, Germany

Tetrapyrrolic macrocycles are widely recognized as fundamental building blocks for interfacial covalent architectures with remarkable stability and atomic precision. Corrole complexes are particularly notable due to their nature as trianionic ligands providing a contracted coordination environment. Herein, we report the on-surface formation and reaction of an octaalkyl-substituted magnesium corrole and an iron triphenylcorrole (FeTPC) on Ag(111). The free-base octaalkylcorrole forms a well-ordered overlayer . Upon vapor deposition of Mg, the metal atoms incorporate into the corrole cavity, forming Mg-corrole complexes. However, XPS and STM studies show that excessive Mg deposition induces structural deformation and alters the electronic properties of the complex. FeTPC forms different long-range ordered adsorbate structures on Ag(111). During annealing, the degradation of FeTPC occurs, with cyclodehydrogenation leading to the planarization of the ligands, as indicated by XPS and STM. In addition, the ligation of nitric oxide at the Fe center, resulting in significant changes in the electronic properties of the complex, was investigated. These findings highlight the tunability of corrole complexes for tailored applications in catalysis and materials science.

O 17.12 Mon 18:00 P2

Theoretical investigation of 3,3"-dibromo-p-terphenyl on copper substrate — •Kevin Eberheim[1], Simone Sanna[1], Michael Dürr[2], and Mohit Jain[2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Institut for Applied Physics, Justus-Liebig-University Gießen, Germany

Chemoselectivity is a key parameter for building customized organic nanostructures via bottom-up approaches. Therefore, strategies are needed that allow con-

necting molecular entities at a specific stage of the assembly process in a chemoselective manner. Studying the mechanisms of such reactions is the key to apply these transformations for the buildup of organic nanostructures on surfaces. Especially, the knowledge about the precise adsorption geometry of intermediates at different stages during the reaction process and their interactions with surface atoms or adatoms is of fundamental importance, since often catalytic processes are involved. With first-principles simulations we can determine the adsorption geometry of the 3,3"-dibromo-p-terphenyl as well as adsorbed mono/diradicals and the halogens. For further comparability with experimental results simulations of Nudged Elastic Band (NEB) have been calculated for transitions between the observed linear chain and ring structures.

O 18: Poster Focus Session Ultrafast Electron Microscopy at the Space-Time Limit

Time: Monday 18:00–20:00 Location: P2

O 18.1 Mon 18:00 P2

Extending machine-learning-based band structure reconstruction into the time domain. — •Mirko Myksa[1], Rui Patrick Xian[1], Vincent Stimper[2], Martin Wolf[1], Ralph Ernstorfer[1], and Laurenz Rettig[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for Intelligent Systems, Tübingen, Germany

Reliably extracting the electronic band dispersion from angle-resolved experimental photoemission (ARPES) data poses a challenging task, which often relies on specific line shape models and underlying assumptions, and thereby limiting a systematic and large-scale band structure extraction from volumetric ARPES data. For such purposes, we recently developed a band-structure reconstruction pipeline, including probabilistic machine learning and the associated data processing [1]. This pipeline shows an excellent performance on benchmarks for the reconstruction of three-dimensional photoemission (kx, ky, E) data from various materials. Here, the prospect for extending such analysis towards further dimensions such as pump-probe delay time-resolved ARPES will be discussed.

[1] R.P. Xian, et al., Nat. Comput. Sci. 3, 101 (2023)

O 18.2 Mon 18:00 P2

Accessing energy- and momentum-dependent electron-phonon coupling from multidimensional photoemission data — •Hossein Yousofniadarzi, Julian Maklar, Martin Wolf, Ralph Ernstorfer, and Laurenz Rettig — Fritz Haber Institute of the Max Planck Society

Time- and angle-resolved photoemission spectroscopy (trARPES) provides a powerful method for probing ultrafast electron dynamics and their interactions with lattice vibrations. The electron-phonon (e-ph) interaction and its momentum dependence play an important role in many quantum materials, e.g., at the origin of charge-density-wave (CDW) formation. Here, we present an approach based on Fourier analysis, combined with a fitting procedure [1], that allows access to the energy and momentum dependence of the e-ph coupling strength for various coherent phonon modes in several CDW compounds. We discuss how these interactions vary across the Brillouin zone and contribute to the electronic structure modifications characteristic of the CDW phase. This work demonstrates the effectiveness of trARPES as a valuable technique for studying interactions in complex quantum materials.

[1] H. A. Hübener, et al., Phys. Rev. Lett. 125, 136401 (2020)

O 18.3 Mon 18:00 P2

Machine learning-based denoising and artefact removal for multidimensional photoemission data — •Joshka Laird, Tommaso Pincelli, and Laurenz Rettig — Fritz haber institute of the Max Planck Society, Berlin, Germany

Angle-Resolved Photoemission Spectroscopy (ARPES) is a powerful tool for investigating the electronic structure of materials. While modern approaches such as momentum microscopy provide rich, multidimensional photoemission data, they pose challenges for achieving high statistics data and good signal-to-noise ratios. Additionally, image distortions such as mesh artefacts often complicate the analysis. Traditional denoising techniques, while effective in specific scenarios, can fail to preserve the fine structural details essential for accurate interpretation.

Here, we present a machine learning-based denoising and artefact removal approach for multidimensional photoemission data. Based on recent results using convolutional neural networks [1], we discuss how to extend such networks to higher dimensions to cope with data e.g. from time-resolved momentum microscopy.

[1] Y. Kim et al., Rev. Sci. Instrum. 92, 073901 (2021)

O 18.4 Mon 18:00 P2

Towards the Investigation of Spin Systems With Electron Microscopy Tools — Antonín Jaroš[1,2], Johann Toyfl[1,2], Benjamin Czasch[1,2], •Michael Stanislaus Seifner[1,2], Isobel Claire Bicket[1,2], and Philipp Haslinger[1,2] — [1]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria — [2]University Service Centre for Transmission Electron Microscopy, TU Wien, Stadionallee 2, 1020 Wien, Austria

Electron spin resonance (ESR) spectroscopy is a method for studying unpaired electrons in various samples with applications in medicine, biology, chemistry, and physics. Typically, the spatial resolution of classical ESR is limited to a few micrometers preventing studying spin systems and their dynamics at the atomic level. To obtain a better understanding of such dynamics, this project aims to develop an ESR setup inside a transmission electron microscope by using the magnetic field created by the objective lens of the microscope to generate energetically separated spin states. A specially designed microcoil integrated into a standard specimen holder allows for exciting spin systems, and various approaches for measuring the resulting resonances are presented. Our results point out potential ways of investigating spin dynamics with sub-nanometer spatial resolution and high temporal resolution. The developed setup will enrich the field of electron microscopy by providing a non-invasive tool to investigate spin systems as well as certain electron beam-induced sample damage.

O 18.5 Mon 18:00 P2

Characterization and Improvement of the Electron Beam Stability and the Measurement Noise in Ultrafast Low-Energy Electron Microscopy — •Ole Böttger[1,2], Johannes Otto[1,2,3], Leon Brauns[1,2], and Claus Ropers[1,2,3] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Max Planck School of Photonics

Ultrafast Low Energy Electron Microscopy (ULEEM) promises to uncover real-space dynamics on surfaces with few-picosecond temporal and nanometer spatial resolutions. Our group is currently developing such an instrument and has obtained first promising results [1]. The extended measurement durations required in this scheme require a high degree of long-term stability of the system. Here, we present results of energy, beam position and intensity stability measurements under various operating conditions, applied to both the laser pump and electron probe beam used. Moreover, we show results of state-of-the-art drift correction algorithms [2] applied to first ULEEM data [1].

[1] J. Otto et al., in preparation (2024).
[2] T. A. de Jong et al., Ultramicroscopy 213, 112913 (2020).

O 18.6 Mon 18:00 P2

Monochromatization of Electron Beams with Spatially and Temporally Modulated Optical Fields — •Neli Laštovičková Streshkova[1], Petr Koutenský[1], Tomáš Novotný[2], and Martin Kozák[1] — [1]Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, CZ-121 16 Prague, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, Prague CZ-12116, Czech Republic

Inelastic interaction between coherent light and free electrons is a powerful tool for modulating electron wave packets, typically resulting in periodic sidebands in the electron energy spectra. We present a novel approach leveraging a time-dependent frequency modulation of light fields to achieve spectral squeezing and monochromatization of free electron pulses. This method compensates for the energy chirp inherent to dispersive propagation in electron sources like TEMs and SEMs, where finite coherence lengths lead to broadened energy spectra. By correcting the chirped wave packet in the energy-time domain through inelastic interaction with tailored optical fields, we enable significant spectral narrowing. Up to 26% of the electron distribution is concentrated within a narrowed energy band, achieving spectral compression by a factor of five. This advancement has implications for high-resolution quantum sensing and electron-based spectroscopy, addressing a critical need for low-loss electron monochromatization.

O 18.7 Mon 18:00 P2

Spatio-Temporal Electron Propagation Dynamics in Au/Fe/MgO(001) in Nonequilibrium — Markus Heckschen[1], Yasin Beyazit[1], Elaheh Shomali[1], Florian Denizer[1], J. Jayabalan[1], Ping Zhou[1], Detlef Diesing[2], Markus Gruner[1], Rossitza Pentcheva[1], Axel Lorke[1], Björn Sothmann[1], and •Uwe Bovensiepen[1] — [1]University of Duisburg-Essen, Faculty of Physics and CENIDE, 47048 Duisburg — [2]University of Duisburg-Essen, Faculty of Chemistry, 45141 Essen

Since the mean free path of hot electrons is only a few nanometer, insights into the spatio-temporal electron dynamics are desired for the analysis of ultrafast microscopy. We determine the energy-dependent electron propagation time through epitaxial Au/Fe(001) as a function of Au layer thickness [1] by femtosecond time-resolved two-photon photoemission spectroscopy at energies 0.5-2.0

eV above E_F. By combining real-time time-dependent density functional theory and microscopic electron transport simulations we identify ballistic transport of minority electrons of the optically excited electron population. At lower energy, superdiffusive transport with 1-4 scattering events dominates. The effective electron velocity accelerates from 0.3 to 1 nm/fs with an increase in the Au layer thickness from 10 to 100 nm which is explained by electron transport that becomes preferentially aligned with the interface normal for thicker Au layers. On this basis the electron momentum or energy can be selected by the choice of the propagation layer thickness. We acknowledge funding by the DFG through SFB 1242. [1] Heckschen et al., PRX ENERGY **2**, 043009 (2023).

O 19: Poster Surface Magnetism

Time: Monday 18:00–20:00 Location: P2

O 19.1 Mon 18:00 P2

Studying Higher-Order Interaction Driven Non-Coplanar Spin Structures Using SP-STM — •Arved Heilmann, Roland Wiesendanger, and Kirsten von Bergmann — Universität Hamburg, Germany

Complex magnetic order arises from competing interactions between magnetic moments. Higher-order interactions (HOI), involving more than two spins, can lead to three-dimensional magnetic configurations known as multi-Q states. Spin-polarized scanning tunneling microscopy (SP-STM) is a powerful tool for studying these systems, enabling real-space imaging of atomic-scale magnetic structures. HOI-driven hexagonal 3Q states have been observed at the atomic and nanoscale in Rh/Mn/Re(0001) and Fe/Rh/Ir(111), respectively [1,2].

To identify further HOI-driven magnetic states, we investigate other systems with Mn/Rh and Fe/Rh interfaces grown on Re(0001). Our findings reveal distinct spin structures that depend on the layer sequence of the pseudomorphic layers. Mn monolayers grown on single or double Rh layers form the Néel state, while Mn grown directly onto the substrate exhibits a non-coplanar 3Q state [3]. For Fe, deposition on two Rh layers results in a distorted quasi-hexagonal magnetic lattice, contrasting with the substrate's ideal hexagonal symmetry. This two-dimensional modulation of the spin texture suggests it also arises from HOI.

[1] F. Nickel, et al., Phys. Rev. B **108**, L180411 (2023).
[2] M. Gutzeit, et al., Nat. Commun. **13**, 5764 (2022).
[3] J. Spethmann, et al, Phys. Rev. Lett. **124**, 227203 (2020).

O 19.2 Mon 18:00 P2

Design of a STM/ nc-AFM head to quantify the magnetic exchange interaction between individual atoms — •Karoline Oetker, Zhengyuan Liu, Henning von Allwörden, Alexander A. Khajetoorians, and Nadine Hauptmann — IMM, Radboud University, Nijmegen, The Netherlands

STM methods are highly powerful tools to quantify the magnetic coupling between single adatoms and with the atom at the tip [1,2]. These current-based methods prohibit to probe the atomic-scale magnetic properties of adatoms on thick insulating layers. However, it was shown that thicker insulating layers with a 4-fold symmetry, as MgO, can prohibit single-electron induced ground state transitions and only allow higher-order excitation processes, which stabilizes the magnetic moment of the adatom [3]. Therefore, a force-based method, such as magnetic exchange force microscopy (MExFM), is a promising tool to quantify the different magnetic coupling mechanisms between individual adatoms on thick insulating layers. We present the design of a 1K STM/nc-AFM setup dedicated for MExFM measurements in magnetic fields up to 9T, based on the tuning fork design. Our goal is to quantify the different distance-dependent magnetic interactions between different magnetic atoms, e.g. 3d and 4f elements. We will utilize functionalized tips with different magnetic atoms, to probe the distance-dependent magnetic exchange force between the tip and adatoms on thick insulating layers. 1.Meier, F. et al., Science 320, 82-86 (2008), 2. Baumann, S. et al., Science 350, 417-420 (2015). 3.Donati, F. et al., Science 352, 318-321 (2016).

O 20: Poster Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale

Time: Monday 18:00–20:00 Location: P2

O 20.1 Mon 18:00 P2

Generation of single cycle terahertz pulses for a THz-STM and improvement of the current measurement noise — •Paul Wiechers, Christian Lotze, Florian Faaber, Vibhuti Rai, and Katharina J. Franke — Freie Universität Berlin, Fachbereich Physik,Arnimallee 14, 14195 Berlin, Germany

Terahertz Scanning Tunneling Microscopy (THz-STM) aims to combine the atomic spatial resolution of STM with the sub-picosecond time resolution commonly achieved through optical pump-probe techniques.

We generate single-cycle terahertz pulses by optical rectification and short optical pulses of various wavelengths. Particular care is taken to minimize pointing deviations of the beams, ensuring proper focusing in the STM junction, even under varying beam delay positions.

In a THz-STM experiment, the measured quantity is the low-bandwidth tunneling current. The THz-induced part of that current, due to the low duty cycle ($\sim 10^{-5}$) of the THz pulses, is very small. Thus, a thorough understanding of the limiting noise sources in the measurement is important. Here, we characterize a cryogenic low-noise ammeter and increase its prohibitively low bandwidth by more than two orders of magnitude.

O 20.2 Mon 18:00 P2

Local excitation of coherent phonons in 2H-$MoTe_2$ by THz driven scanning tunnelling microscope — Vibhuti Rai, Junyoung Sim, •Florian Faaber, Sergey Trishin, Nils Bogdanoff, Tom Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The coupling of THz pulses into a scanning tunnelling microscope has emerged as a unique technique to achieve picosecond time resolution while maintaining sub nanometer spatial resolution [1,2]. By delaying one THz pulse with respect to the other while recording the current rectified by the two pulses, a pump-probe scheme can be realized [3]. In this work, we use this scheme to investigate the quasi 2D semiconducting transition metal dichalcogenide (TMD) 2H-$MoTe_2$ at 7K in ultra-high vacuum and find a large oscillatory rectified current that is slowly decaying over 50 ps. We attribute these oscillations to the excitation of coherent phonons and discuss the effect of defects and DC bias voltage on the excited modes.

[1] Cocker, et al., Nature Photonics 7, 620*625 (2013)
[2] V. Jelic et al., Nature Physics 13, 591 (2017)
[3] T. L. Cocker et al., Nature 539, 263 (2016)

O 20.3 Mon 18:00 P2

Charging of atomic defects in 2H-$MoTe_2$ under infrared illumination — •Friedemann Lohss, Florian Faaber, Vibhuti Rai, Junyoung Sim, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The electronic properties of semiconductors are heavily shaped by the concentration and type of defects present in the material. The sub-nanometer resolution of scanning tunneling microscopy (STM) allows to locally probe such defects. Here we characterize the response of the semiconductor 2H-$MoTe_2$ to infrared illumination in an STM at cryogenic temperature. We observe the formation of disc-shaped regions of increased conductivity around some local defects, likely stemming from charging and tip-induced band bending. We characterize the different defect states occuring in this material.

O 20.4 Mon 18:00 P2

Two-Color Pump-Probe STM of Coherent Phonon Dynamics in Ultrathin ZnO/Ag(111) — •Henrik Wiedenhaupt[1], Shuyi Liu[2], Akitoshi Shiotari[1], Adnan Hammud[1], Daniel Wegkamp[1], Martin Wolf[1], Takashi Kumagai[3], and Melanie Müller[1] — [1]Fritz Haber Institute of MPG, Berlin, Germany. — [2]Huazhong University of Science & Technology, Wuhan, China. — [3]Institute for Molecular Science, Okazaki, Japan.

We use photon-assisted ultrafast scanning tunneling microscopy (ph-USTM) to study coherent phonon (CP) dynamics in optically excited ZnO/Ag(111). In recent work, we have shown that resonant single-color ph-USTM enables CP spectroscopy on 3ML-ZnO/Ag(111) with nanometer spatial resolution [1], where the optical resonance between an interface state (IS) and the ZnO conduction band edge (CBE) appears to play an important role, as also observed in tip-enhanced Raman spectroscopy (TERS) [2]. However, the detailed mechanisms by which the CPs modulate the photocurrent and of their local excitation remain unclear. To gain further insight, we implement two-color ph-USTM for the selective on- and off-resonant ultrafast excitation of the IS-CBE transition on 2ML-ZnO and 3ML-ZnO. Besides demonstrating local CP spectroscopy also on 2ML-ZnO, our results show that CPs can also be excited off-resonantly, while optically resonant photon-assisted tunneling seems to be more crucial for local CP detection via ph-USTM. We explain our observations by phonon-induced transient changes in the local dielectric response.

[1] S. Liu et al., Sci. Adv. 8, 42, eabq5682 (2022)
[2] S. Liu et al., Nano Lett. 19, 8, 5725 (2019)

O 20.5 Mon 18:00 P2

Plasmonic STM-luminescence driven by a high-power spintronic THz emitter — •Alkisti Vaitsi, Luis Enrique Parra López, Vivien Sleziona, Martin Wolf, and Melanie Müller — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We demonstrate THz-induced STM-luminescence (THz-STML) from a plasmonic tunnel junction driven by broadband single-cycle THz pulses generated from a high-power rotating spintronic THz emitter (STE). By measuring the dependence of the plasmonic luminescence on the static STM bias and the THz-STM bias, we aim for a purely data-driven approach to calibrate the THz peak bias via reconstruction of the THz-STML spectra from the static reference STML spectra. Our results proof the capability of the rotating STE to generate several Volts peak THz bias in a metallic STM junction and pave the way for future time-resolved gating of STM-luminescence from excitonic quantum emitters.

[1] Kimura et al., ACS Photonics 8, 4, 982-987 (2021)
[2] Vaitsi et al., Appl. Phys. Lett. 125, 071107 (2024)

O 20.6 Mon 18:00 P2

Scanning Quantum Microscopy for Emergent Phases of Matter — •Ruoming Peng[1], Sreehari Jayaram[1], Malik Lenger[1], King Cho Wong[1], Xuankai Zhou[1], Yan Tug Kong[1], and Joerg Wrachtrup[1,2] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Scanning quantum microscopy using NV centers in diamond enables direct visualization of condensed matter phenomena. Applying this technique, we uncover the emergence of a super-Moiré magnetic texture in twisted double bilayer CrI3, distinct from the geometric Moiré periodicity at small twist angles. Additionally, we investigate vortex dynamics in thin-layer 2H-NbSe2, revealing vortex melting behaviors during different thermal cycling and unconventional magnetic noise arising from the vortex dynamics. Our findings highlight the strong capability of scanning quantum microscopy to unravel nanoscale magnetic interactions and dynamic phases in 2D materials.

O 20.7 Mon 18:00 P2

A theoretical perspective on electroluminescence, photoluminescence and photocurrent generation in a scanning tunneling microscope — •Tomáš Neuman[1], Sofia Canola[1], Rodrigo Ferreira[1], Anna Rosławska[2], Katharina Kaiser[3], Alex Boeglin[4], Andrei Borisov[5], Guillaume Schull[4], and Martin Švec[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czechia — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Georg-August-Universität Göttingen, Göttingen, Germany — [4]Université de Strasbourg, IPCMS, CNRS, UMR 7504, Strasbourg, France — [5]Université Paris-Saclay, Institut des Sciences Moléculaires d'Orsay, CNRS, UMR 8214, Orsay, France

The phenomena occurring in a scanning tunneling microscope (STM) that lead to the generation of light or are triggered by light (STM+light, STM+L), including the STM-induced luminescence and photocurrent generation in single molecules, allowed for studying excited states of molecules in a STM. As the underlying principles of these phenomena involve electron tunneling, plasmon-enhanced optical absorption and spontaneous emission, and vibronic effects, interpreting these STM+L experiments hinges on the development of theoretical models. I will show such modelling strategies and showcase its application to recent experiments. In particular, I will focus on the theory of mapping of orbitals of a multireference excited state of a small molecule (perylene tetracarboxylic dianhydride - PTCDA) via photocurrent generation, whose explanation requires all the mentioned ingredients.

O 20.8 Mon 18:00 P2

Neutral Exciton-Libron Coupling via Resonant Energy Transfer in Single Molecules — •Thiago G. L. Brito[1], Klaus Kuhnke[1], Klaus Kern[1,2], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The optical properties of single molecules can vary depending on their environment. In some surroundings, vibrations due to frustrated rotations (librations) may occur if the molecules feature some rotational freedom. In this study, we provide evidence of coupling between neutral excitons and libration modes (librons). We observed this coupling through light emission resulting from resonant energy transfer (RET). We measured neutral and charged exciton emissions in isolated zinc phthalocyanine (ZnPc) and ZnPc-platinum phthalocyanine (PtPc) assemblies deposited on NaCl/Ag(111) using scanning tunneling microscopy induced luminescence (STML). For isolated ZnPc, we observed a broad peak from the neutral exciton and exciton-libron coupling for the charged exciton. In contrast, in ZnPc-PtPc structures, we found libronic signatures in the neutral emission of ZnPc when excited via RET from PtPc. This study is providing deeper insights into exciton-libron dynamics in single molecules.

O 20.9 Mon 18:00 P2

Mapping adsorbed states of iron(II) phthalocyanine on Ag surfaces by plasmon-enhanced Raman spectroscopy — Borja Cirera[1], •Rodrigo Cezar de Campos Ferreira[2,3], Amandeep Sagwal[2], Jiří Doležal[3], Martin Švec[2,3], and Pablo Merino[1] — [1]Instituto de Ciencia de Materiales de Madrid, Spain — [2]Institute of Physics, Czech Academy of Sciences, Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic

The high spatial confinement of a plasmonic field in LT-SPM has become a valuable tool for near-field spectroscopies. Among the techniques, Raman scattering enables chemical identification, investigation of relations between adsorption geometry and vibrational fingerprints in real space at single-molecule level.[1,2] Here we studied different adsorption configurations of iron(II) phthalocyanines (FePc) on Ag(110) and Ag(111) crystal surfaces. Real-space mapping reveals the appearance of shifted Raman states when adsorbed in specific geometries. Results and simulations suggest that the breaking in symmetry with respect to the main crystallographic directions of the substrates are the leading reason for this phenomenon. [1] Y. Zhang et. al. Nature 498, 82-86 (2013). [2] R. Zhang et. al. National Science Review, Volume 6, 2019, 1169-1175.

O 20.10 Mon 18:00 P2

Investigations of the plasmon excitation of C60 multilayers on Au(111) using STM induced luminescence — •Andreas Reutter, Yannis Hilgers, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics - LENA, TU Braunschweig

In recent years, Scanning Tunneling Microscopy induced luminescence (STML) has gathered great interest, as it allows to investigate optical properties in addition to normal STM measurements, both with atomic spatial resolution. Since its development, the main challenge of this method is to obtain reasonable photon intensities.

We succeeded in building a setup with a greatly increased detection efficiency by using a parabolic mirror inside the STM, that covers 75% of the upper hemisphere.

Here, we present STML measurements of surface plasmons on C60 on Au(111) as a model system for the effects of an organic semiconductor on a metal surface [1]. We will present conductance and optical spectroscopy measurements as well as photon yields for different number fo C60 layers and different applied voltages.

[1] Große, Christoph; Merino, Pablo; Rosławska, Anna; Gunnarsson, Olle; Kuhnke, Klaus; Kern, Klaus; ACS Nano, 11, 1230 (2017).

O 20.11 Mon 18:00 P2

Resonant energy transfer as a function of distance between metal-phthalocyanine molecules — •Roel Burgwal, Nikhil Seeja Sivakumar, Joëlle J. A. Schrijer, Alexander A. Khajetoorians, and Daniel Wegner — Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, The Netherlands

Resonant transfer of energy (RET) between molecules is a process ubiquitous in nature that also has interesting technological applications. The rate of RET decreases as the molecules involved are spaced further apart, with the distance dependence determined by the exact mechanism responsible for energy transfer. Two possible mechanisms are electrodynamical Förster energy transfer (FRET) and the electron tunneling-based Dexter energy transfer (DET). Recent advances in scanning tunneling microscope-induced luminescence (STML) have made it possible to observe energy transfer between single molecules and to control the spacing between these with sub-nanometer precision. So far, STML measurements of RET distance dependence resemble more the exponential behavior of DET, in contrast with the commonly assumed FRET mechanism. However, it has been proposed this apparent behavior may be a plasmonic effect arising from the varying distance between STML-tip and acceptor molecule. Here, we study RET between different metal-phthalocyanine molecules while elucidating the role of the plasmon through complementary measurements.

O 21: Poster Heterogeneous Catalysis

Time: Monday 18:00–20:00 Location: P2

O 21.1 Mon 18:00 P2

Disentangling Transport and Kinetics in Complex Reaction Chambers by Novel Reduced-Order Modeling Approaches — •Tobias Hülser[1], Maryke Kouyate[1], Uzair Qureshi[2], Daniel Runge[3], Georg Brösigke[2], Christian Merdon[3], Jürgen Fuhrmann[3], Karsten Reuter[1], Christoph Scheurer[1], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Unviversität Berlin — [3]Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin

Operando catalytic characterization chambers are governed by mass transport interplaying with highly-nonlinear chemical kinetics, which needs to be accounted for by corresponding coupled simulations. Often, these chambers can not be modelled with established reactor models, instead requiring high-cost Computational Fluid Dynamics simulations. We have developed reduced-order methods which disentangle the computational treatment for transport and kinetics into an offline (OffPh) and online phase (OnPh). In the OffPh, we determine a suitable solution space of the transport operator, which is independent of the employed kinetic model and therefore reusable. In the OnPh, the solution from this space is determined from the balance of transport and kinetics at the catalytic surfaces. This drastically reduces the costs as the OffPh is a linear problem and, particularly, the nonlinear online phase typically involves only very few degrees of freedom. We demonstrate this idea on mesoscale core-shell particles, an asymptotic expansion for small catalyst samples and a quasi-exact reduced basis strategy for general problem settings.

O 21.2 Mon 18:00 P2

Bayesian Inference of Kinetic Models of Heterogeneous Catalysis by Normalizing Flows — •Andreas Panagiotopoulos[1], Javed Mudassar[2], Jens-Uwe Repke[2], Georg Brösigke[2], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technical University Berlin

Estimating kinetic parameters is typically done by classical fitting a model to experimental reactor data, which, however, suffers from a number of fundamental problems like ill-posedness, multiple possible solutions and the lack of reliable uncertainty estimates. By reformulating the problem in a probabilistic language, Bayesian inference cures these problems, but also requires to sample from a high-dimension probability distribution. Because of their high non-linearity and sensitivity, this becomes challenging for kinetic models and established sampling approaches become inefficient. We investigate Normalizing Flows in conjunction with Quasi Monte Carlo sampling to address this problem. In this approach, a bijective nonlinear parameter transformation is sequentially learned such that a uniform sampling from the transformed parameters leads to a good importance sampler of the Bayesian posterior. We investigate the performance of the proposed approach on an empirical model for methanol synthesis on Cu based catalysts using synthetic and experimental data.

O 21.3 Mon 18:00 P2

Model Catalytic Studies on the Thermal Dehydrogenation of the Benzaldehyde/Cyclohexylmethanol LOHC System on Pt(111) — •Marius Steinmetz[1], Valentin Schwaab[1,2], Felix Hemauer[1,2], Eva Marie Freiberger[2], Natalie J. Waleska-Wellnhofer[2], Hans-Peter Steinrück[2], and Christian Papp[1] — [1]Angewandte Physikalische Chemie, Freie Universität Berlin (FU Berlin), Arnimallee 22, 14195 Berlin, Germany — [2]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Egerlandstr. 3, 91058 Erlangen, Germany

We investigated the dehydrogenation reaction and the thermal decomposition of the liquid organic hydrogen carrier (LOHC) pair benzaldehyde/cyclohexylmethanol on a Pt(111) model catalyst via temperature-programmed desorption experiments and synchrotron radiation photoelectron spectroscopy. The LOHC pair has a hydrogen storage capacity of 7.0 mass%, stored in a cyclohexyl ring and a primary alcohol group. We observed a stepwise dehydrogenation mechanism, starting with the dehydrogenation of the alcohol group, followed by the dehydrogenation of the cyclohexyl ring. We also observed different dehydrogenation behaviors for low and high coverages, probably caused by steric hindrance for high coverages. Even though the LOHC pair achieves high hydrogen storage capacity, early decomposition at low temperatures between 250 and 350K limits the use of the molecule pair as a reversible hydrogen carrier.

O 21.4 Mon 18:00 P2

Size-selected metal nanoparticles on tungsten: influence of the deposition angle — •Sumanasa Begur Prakash and Mathias Getzlaff — Institute of Applied Physics, University of Düsseldorf

Metal nanoclusters and nanoparticles, especially those composed of iron (Fe), nickel (Ni), and their alloys, are fascinating due to their unique electronic and magnetic properties which vary significantly with particle size. This feature makes them not only interesting for fundamental research but also highly promising for advanced technologies including catalysis, magnetic storage, and sensing. However, interaction with the substrate during and after deposition significantly influences the particle's properties.

Our contribution is focused on size-selected Fe, Ni, and Fe-Ni alloy nanoparticles which are deposited on a W (110) substrate. Using a magnetron sputter source (Haberland-type) we vary the deposition angle to understand how this parameter influences the particle size, structure, and overall distribution of nanoparticles on the substrate surface. This approach allows us to probe the relationship between deposition conditions and particle characteristics. The size and structural properties are investigated by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) under ultra-high vacuum (UHV) conditions.

O 21.5 Mon 18:00 P2

Optimized BiVO4/g-C3N4 Heterojunctions for Efficient Photocatalytic Green Ammonia Production — •Susana D. Rojas[1], Nicolás A. Soto[1], Pablo E. Salinas[1], Daniel Saavedra[2], Marcelo A. Cisternas[1], and Ulrich G. Volkmann[2] — [1]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Santiago, Chile — [2]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile

BiVO4 nanostructures were synthesized via a hydrothermal method, and g-C3N4 nanosheets by urea pyrolysis. The materials were characterized using Fourier transform IR spectroscopy (FTIR), UV-Vis and X-ray photoelectron spectroscopy, X-ray diffraction, and scanning electron microscopy to confirm their chemical and morphological structures. Photocatalytic ammonia production was evaluated in a cylindrical reactor with a Xenon discharge lamp, using an aqueous catalyst dispersion under magnetic stirring and a nitrogen flow at atmospheric pressure. Ammonia production was analyzed via the Nessler method with ammonium chloride (NH4Cl) calibration curves for the aqueous phase and in situ FTIR spectroscopy with a 16 m optical path gas cell for the gas phase [1, 2]. This work advances the understanding of photocatalytic processes for sustainable ammonia production and the development of efficient, eco-friendly methods for synthesizing this essential compound. Acknowledgements: ANID project SIA77210032 (SR, MC), UVA22991 (SR, MC), ANID Fellowship (DS), and Puente UC 2024-25 (UV). Ref.: [1] P. Huang, et al., Nature Comm. 13, 7908 (2022). [2] S.Z. Andersen, et al., Nature 570, 7762, 504-508 (2022).

O 21.6 Mon 18:00 P2

Tuning the ceria island orientation: from (111) to (100)-oriented islands — •Maja Atlas, Raquel Sanchez-Barquilla, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

Inverse catalysis systems, where the reducible oxide is anchored on the metallic support, have shown a better performance compared with its traditional counterparts due to the strong metal support interaction. Among catalytic materials, ceria (CeO_2) is used in a wide range of applications, due to its oxygen storage and redox properties. In particular, the catalytic activity of Cu(111) can be substantially enhanced when depositing CeO_x on top, achieving direct methanol production from CO_2. In situ near ambient pressure X-ray photoemission spectroscopy (NAP-XPS) measurements have shown that the activated CO_2 molecule is stabilized by Ce^{3+} sites during the reaction. Moreover, epitaxially grown CeO_2 islands can have two different orientations on Cu(111): the (111)-oriented islands appear first and with lower oxygen pressure, while the (100)-oriented phase can be enhanced by increasing the oxygen exposure. Here, we present a structural and chemical study of the ceria islands growth as a function of temperature, oxygen pressure and deposition rate. By varying these parameters, we can study the relation between the phase and the Ce^{3+}/Ce^{4+} ratio, using XPS, low energy electron diffraction (LEED) and scanning tunneling microscopy (STM).

O 21.7 Mon 18:00 P2

Structure and chemical properties of Pt clusters and particles deposited on CeO_2(111) — •Shuang Chen, Zairan Yu, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

CeO_2-supported Pt nanoparticles are of significant technological interest due to their unique catalytic properties and wide range of applications in numerous chemical reactions. However, the catalytic performance of various Pt species remains a highly debated topic. This arises primarily from the complexity of Pt/CeO_2 powder catalysts and the scarcity of accurate reference data obtained from well-defined model systems. Here, we report systematic IR reflection absorption spectroscopic (IRRAS) investigations of Pt deposited on oxidized CeO_2(111) single-crystal surfaces. By employing polarization-resolved IRRAS with CO as a probe molecule and grazing-emission XPS, we were able to track the structural and electronic evolution of Pt on CeO_2(111) as a function of the deposition amount. Various Pt species, ranging from single atoms to small clus-

ters and large particles, were identified. Our results provide solid evidence of strong electronic interactions between Pt and the ceria substrate, offering profound insights into the dynamic behavior of Pt clusters under different conditions. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) -Project-ID 426888090- SFB 1441.

O 21.8 Mon 18:00 P2

Photoelectrochemical nitrate reduction by copper oxide-based semiconductors — •Jasmin A. Zitzmann[1,2], Maximilian Christis[1,2], Saswati Santra[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The photoelectrochemical nitrate reduction reaction (PEC-NO_3RR) offers a route to ambient ammonia (NH_3) synthesis and recycling of NO_3^- pollutants. Copper oxide-based semiconductors, such as Cu_2O, CuO and $CuBi_2O_4$ exhibit suitable band energetics to drive this reaction. While Cu_2O is reported for PEC-NO_3RR, further studies are required to optimize reaction conditions and minimize photocorrosion. With this aim, the PEC-NO_3RR performance characteristics of Cu_2O, CuO and $CuBi_2O_4$ are investigated in alkaline and neutral aqueous electrolytes. The dominant reaction product observed is nitrite (NO_2^-) with Cu_2O producing the highest yields. In addition, NH_3 is generated by Cu_2O, with an increase in selectivity at lower potentials. Photocorrosion is most pronounced for CuO, whereas $CuBi_2O_4$ shows the most consistent PEC stability. Our findings indicate the potential-dependent PEC-NO_3RR product selectivity, with further research necessary to optimize the electrochemical conditions to improve PEC-NO_3RR stability and NH_3 yield using these promising copper oxide-based semiconductors.

O 22: Poster Surface Reactions

Time: Monday 18:00–20:00 Location: P2

O 22.1 Mon 18:00 P2

TRACE/TRIADE: A setup to investigate tritium accumulation of solids — •Marie-Christine Schäfer, Dominic Batzler, James Braun, Robin Grössle, Philipp Haag, Elizabeth Paine, Marco Röllig, Marius Schaufelberger, and Kerstin Trost — Tritium Laboratory Karlsruhe, Eggenstein-Leopoldshafen, Germany

In the context of the KArlsruhe TRItium Neutrino experiment (KATRIN), sufficient knowledge of the accumulation of tritium on surfaces is crucial for minimising systematic effects, thus optimising the experiment. On a bigger scale, the understanding of these specific tritium gas-surface interactions is relevant when it comes to fusion reactors and their fuel cycles. In search of materials with small tritium memory effects, the Tritium Activity Chamber Experiment (TRACE) at Tritium Laboratory Karlsruhe (TLK) provides the possibility of exposing solid samples to high purity tritium gas while monitoring the near-surface activity via beta-induced X-ray-spectrometry (BIXS). Similarly, the TRItium Adsorption Desorption Experiment (TRIADE) also measures the tritium accumulation via the BIXS method but is being upgraded to additionally provide the option of studying adsorption and desorption processes at temperatures down to 100 K. For this, a newly designed sample holder is currently being tested. Besides investigating the tritium accumulating properties of different materials, the compatibility with UV/ozone in the context of decontaminating the surfaces is also of relevance. For this, experiments with an additional setup are set to be conducted in the near future. This contribution will present the TRACE/TRIADE setups as well as their planned modifications.

O 22.2 Mon 18:00 P2

Exploring TiO_2-water-interfaces with AIMD and Machine Learning Force Fields — •Johannes Laurenz Wolf, Christian Dressler, and Malte Grunert — Technische Universität Ilmenau, Department of Physics, 98693 Ilmenau, Germany

Titanium dioxide (TiO_2) is a pivotal material in photocatalysis, particularly for water splitting applications in artificial leaves. In this study, we employ ab initio molecular dynamics (AIMD) and machine learning force fields (MLFF) within the MACE framework to investigate systems comprising, TiO_2 layers in different crystalline phases on indium phosphide (InP) and water. A central focus is placed on the structural and dynamic properties of the TiO_2-water interface.

To enhance our understanding of interfacial interactions, we introduce nanoscale pinholes into the TiO_2 layer, exploring their impact on water adsorption and hydrogen bonding dynamics. AIMD simulations provide atomic-scale insights, while MLFF extends these analyses to longer time scales, enabling a comprehensive investigation of adsorption mechanisms, titanium coordination, and local surface distortions.

O 22.3 Mon 18:00 P2

Investigation of the water-GaN(10$\bar{1}$0) and water-GaN(0001) interface by ab initio molecular dynamics simulations — •Marius Otto, Christian Dressler, Fabian Ullmann, and Stefan Krischok — Technische Universität Ilmenau

We have performed ab initio molecular dynamics simulations to investigate the dissociative adsorption of water at the water-GaN(10$\bar{1}$0) and water-GaN(0001) interfaces. Our results confirm that water undergoes dissociative adsorption on both surfaces, with notable differences in the protonation states of the adsorbed oxygen species. On the non-polar GaN(10$\bar{1}$0) surface, Ga atoms are exclusively coordinated by hydroxyl (OH) groups, whereas the polar GaN(0001) surface shows a mixed coverage of hydroxyl (OH) and water (H_2O) species. The dissociation of water is significantly more pronounced on the GaN(10$\bar{1}$0) surface due to the availability of distinct adsorption sites for both hydrogen and hydroxyl groups. In contrast, on the GaN(0001) surface, steric shielding of the adsorption sites inhibits water dissociation, resulting in reduced reactivity. In addition, we have also compared our simulations to XPS and UPS measurements.

O 22.4 Mon 18:00 P2

kinetics and thermodynamics of dehalogenation on metal surfaces — •Yu He[1], Hao Jiang[1], Zhiwen Zhu[1], Juan Xiang[1], Jinyang Xu[2,3,4], Zhaofeng Liang[2], Lei Xie[2], Fei Song[2], and Qiang Sun[1] — [1]Materials Genome Institute of Shanghai University,Shanghai,China — [2]Shanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai,China — [3]Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai,China — [4]University of Chinese Academy of Sciences, Beijing,China

In the field of on-surface synthesis, dehalogenative aryl-aryl coupling has become the key strategy for the fabrication of covalently bonded carbon-based nanomaterials. However, studies on the kinetics and thermodynamics of these reactions are still scarce. Also, most of the works focus on debromination while overlooking the dechlorination reaction which is a fundamental reaction with significant implications for environmental protection and sustainable chemistry. Here, we combined synchrotron-based x-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) to study the dehalogenative polymerization reactions of chlorinated and brominated aromatic hydrocarbons on the Au(111) surface. We resort to high-resolution surface-sensitive techniques to identify the reactants and products as well as the important reaction intermediates. Using the fast XPS, we are able to extract the kinetic curves of the reactions and obtain detailed insight into the reaction process. Our research deepens the understanding of the reaction mechanism.

O 22.5 Mon 18:00 P2

Self-assembly and reactions of benzonitriles on metal surfaces — •Anran Bao[1] and Wenshao Yang[2] — [1]Physikalische Chemie I, Ruhr-Universität Bochum, Bochum, Germany — [2]Hangzhou Institution of Advanced Studies, Hangzhou, China

Surface synthesis enables innovative material design, with the self-assembly of organic molecules on metal surfaces. Among on-surface reactions, the Ullmann coupling is significant. Notably, despite the considerable differences in the chemical structures of cyanides and halogen atoms, they exhibit similarities in organic reactions. This provides a new perspective on surface synthesis and possibilities for synthesizing novel nanomaterials. This study focuses on the unique self-assembly and chain formation of benzonitrile derivatives, particularly isophthalonitrile (IPN), tere-phthalonitrile (TPN) and ortho-phthalonitrile (OPN), on the Co(0001) surface. We observed that IPN and TPN molecules adsorb randomly at room temperature using Scanning Tunneling Microscopy. However, these molecules undergo significant transformations upon annealing, forming chain-like structures. OPN forms disordered chains at room temperature, which become more linear and ordered upon heating. Compared to Au(111) and Ag(111), where simpler self-assemblies or dimers form, Co(0001) uniquely enables complex, ordered chain formation. This work provides critical insight into the catalytic properties of cobalt, enhancing understanding of molecular assembly on metal surfaces and offering new directions for designing nanostructured materials with precise molecular ordering.

O 22.6 Mon 18:00 P2

Characterization of an unexpected mu3 adsorption of molecular oxygen on Ag(100) with LT-STM — •Merve Ercelik[1], Andrés Pinar Solé[1], Liang Zhang[2], Hua Guo[2], Andreas J. Heinrich[1], Yujeong Bae[1], and Dmitriy Borodin[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul 03760, South Korea — [2]Department of Chemistry and Chemical Biology, Center for Computational Chemistry, University of New Mexico, Albuquerque, New Mexico 87131, USA

The interaction between molecular oxygen and metal surfaces is a key topic in quantum chemistry and surface science, with significant implications for electrochemistry and heterogenous catalysis. Using low-temperature scanning tunneling microscopy (STM), we investigate a previously unknown adsorption state of molecular oxygen on Ag(100), where the molecule binds to three silver atoms simultaneously (mu3-O2). We characterize vibrational excitations through inelastic electron tunneling spectroscopy (IETS): out-of-plane hindered rotation, in-plane hindered rotation, and in-plane hindered translation. Tunneling electron induced rotations reveal a rotational isomerization barrier of 69.3 meV. Interestingly, GGA-level DFT calculations fail to identify mu3-O2 as a stable adsorption state, likely due to self-interaction errors affecting the description of localized charges. We speculate that the mu3-O2 configuration corresponds to a formal molecular oxygen anion, with the 11 meV excitation observed in IETS attributed to a transition between spin-orbit states of the surface-bound molecular anion.

O 23: Poster Ultrafast Electron Dynamics

Time: Monday 18:00–20:00 Location: P2

O 23.1 Mon 18:00 P2

Charge Density Waves and Doublon Lifetime in Doped 1*T*-TaS_2 — •J. Jayabalan[1], Gaël Reecht[1], Florian Diekmann[2], Ping Zhou[1], Walter Schnelle[3], Kai Rossnagel[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Universität Duisburg-Essen, Germany. — [2]Christian-Albrechts-Universität zu Kiel, Germany. — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Below a certain critical temperature, the periodic rearrangement of atoms into a long-range ordered star-like pattern transforms the metallic 1*T*-TaS_2 into an insulating state by opening a band gap [B. Sipos, *et al.*, Nature Materials **7**, 960 (2008)]. This metal-to-insulator transition progresses through distinct charge density wave (CDW) states, driven by the interplay between electron-electron and electron-lattice interactions. In the commensurate CDW state of 1*T*-TaS_2, the carriers excited into its upper Hubbard band (UHB), also known as a doublon state, decay in less than 20 fs due to the presence of unintentionally doped holes in the sample [M. Ligges, *et al.*, Phys. Rev. Lett., **120**, 166401 (2018)]. Through ultraviolet time-resolved photoemission spectroscopy at the Γ point, we identify a long-lived feature near the upper Hubbard band (UHB) energy in 1*T*-$Ta_{(1-x)}W_xS_2$. Through variations in temperature, doping concentration, and pump-induced effects, we identify this observed feature as long-lived doublons. With STM measurements, we show a long living hole dynamics through localized excitations at specific locations of the sample. Funding by the DFG through FOR 5249 QUAST is gratefully acknowledged.

O 23.2 Mon 18:00 P2

Ultrafast low-energy photoelectron diffraction for the study of surface-adsorbate interactions with 100 femtosecond temporal resolution — Hermann Erk[1], Carl Erik Jensen[1], •Stephan Jauernik[1], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

In this contribution a novel method of ultrafast electron diffraction for the study of structural dynamics at surfaces is presented. In our photoemission-based experiment we analyze the energy-momentum distribution of low-energy photoelectrons excited by a near ultraviolet (NUV) ultrafast laser pulse in graphite that are diffracted as they pass through an ordered tin-phthalocyanine adsorbate layer. The probing electron pulse is generated in the immediate vicinity of the surface. This limits the propagation distance of the electron pulse before diffraction to a few nanometers and thus minimizes pulse broadening effects due to space charge and dispersion. We experimentally demonstrate a time resolution of this ultrafast low-energy photoelectron diffraction (ULEPD) of about 100 fs [1], which is only limited by the pulse width of the NUV laser pulse and exceeds reported values of conventional ultrafast low-energy electron diffraction [2] by a factor of 10.

[1] H. Erk *et al.*, Phys. Rev. Lett. **133**, 226201 (2024)
[2] S. Vogelgesang *et al.*, Nat. Phys. **14**, 184 (2017)

O 23.3 Mon 18:00 P2

Studying electron-phonon interaction in $MoTe_2$ using time-resolved and frequency-domain ARPES — •Carl Eric Jensen[1], Stephan Jauernik[1], Petra Hein[1], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

The layered transition metal dichalcogenides $MoTe_2$ and WTe_2 attracted significant attention in the recent years due to the topological properties of their non-centrosymmetric T_d-phase and their manipulation by coherent phonon excitation [1,2]. In this contribution we present time-resolved and frequency-domain ARPES (FD-ARPES) data of 1T'-$MoTe_2$. Optical excitation of the electronic system by a near-infrared (1.5 eV) pump pulse results in the excitation of coherent phonons in this material. The frequencies of the observed coherent phonon modes agree with all-optical measurements of $MoTe_2$ [2,3]. A Fouriertransform of the time-resolved ARPES data into the frequency-domain proviedes further insights into the interaction between electrons and phonons: The FD-ARPES data reveal the electronic band-selectivity of the indivitual coherent phonon modes. The results are compared with published work on WTe_2 [4].

[1] Sie et al. Nature 565, 61-66 (2019)
[2] Zhang et al. Phys. Rev. X 9, 021036 (2019)
[3] Fukuda et al. Appl. Phys. Lett. 116, 093103 (2020)
[4] Hein et al. Nature Communications 11, 2613 (2020)

O 23.4 Mon 18:00 P2

Ultrafast Charge Transfer and Band Renormalization in Bilayer Graphene/single layer Ag/SiC — •Eduard Moos[1], Zhi- Yuan Deng[1], Hauke Beyer[1], Arpit Jain[4], Chengye Dong[4], Joshua A. Robinson[4], Kai Rossnagel[1,2,3], and Michael Bauer[1,2] — [1]Kiel University, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Germany — [3]Electron Synchrotron DESY, Germany — [4]Pennsylvania State University, United States

Intercalated monoelement metals between mono- to multi-layer graphene/SiC interfaces are a new type of van der Waals heterostructures with extraordinary properties. In the monolayer limit, silver (MLAg) exhibits a metal-semiconductor transition and enables ultrafast charge transfer between layers. Due to the twisted arrangement of the Brillouin zones, low binding energy of the valence band maximum of MLAg and the resulting band gap of bilayer graphene (BLGr), this is an interesting model system to investigate charge transfer and interlayer coupling mechanisms.

In this contribution, time- and angle-resolved photoemission spectroscopy (TRARPES) with a time resolution of 35 fs is used. The data show clear evidence for a net charge transfer between Ag and graphene on a time scale of 50 fs. On longer time scales, the electronic structure of BLGr undergoes significant changes, including an enhancement of the intrinsic splitting of the pi band as well as a reduction of the band gap. We associate these with changes in the electronic and/or structural symmetry of BLGr.

O 23.5 Mon 18:00 P2

Ultrafast dynamics of thin films of small PAHs — •Lorenzo Maddii Fabiani, Tobias Reiker, and Helmut Zacharias — Center for Soft Nanoscience, Busso-Peus-Str.10 48149 Münster Germany

Polycyclic aromatic hydrocarbons (PAHs), which are estimated to constitute approximately 10% of the total carbon content in space, are omnipresent in interstellar environments. Molecular reactions of molecules in space, such as ionization, fragmentation and dissociation are fundamental to the chemical evolution of the interstellar medium. To investigate the initial electronic dynamics in alternant and non-alternant PAHs in the condensed phase following optical excitation, we performed time-resolved two-photon photoemission (tr-2PPE) experiments. Thin films of PAHs were prepared on gold-coated quartz substrate. In the range from femtosecond to 200 ps up to three lifetimes after excitation of S1, S2 or S3 were observed. We provide experimental ultrafast lifetimes of nine different alternant and non-alternant small PAH molecules in thin films. For the alternant molecules an increase of the lifetimes with molecular size is found, and the lifetimes decrease generally with increasing of the probe photon energy. In contrast, non-alternant PAHs exhibited less predictable behavior. Overall, the dynamics of excited electronic states provide a fundamental basis for unraveling the reaction processes occurring within the interstellar medium.

O 23.6 Mon 18:00 P2

Transient IR pump-probe spectroscopy on AuNP-TiO_2 structures — •Lisa Mehner[1], Wouter Koopman[1], Felix Stete[1], Steven Berth[1], Alexander von Reppert[1], and Matias Bargheer[1,2] — [1]Insitute for Physics and Astronomy, University of Potsdam — [2]Helmholtz-Zentrum Berlin

Photocatalysts can enhance redox reactions by supplying energetic electrons and holes. Combining gold nanoparticles (AuNP) and TiO_2 nanoparticles (NP) presents a promising route for realizing broad band photocatalysts as AuNP allow broad band absorption and TiO_2NP provide a long excited carrier lifetime. Electrons excited in the AuNP can transfer into the semiconductor if the energy is sufficient to overcome the interfacial Schottky barrier. Transferred electrons are expected to have a prolonged lifetime in the TiO_2 conduction band, since no vacancies are available for recombination in the valence band. Here, we present our initial findings on charge transfer of a TiO_2NP+AuNP sample

measured by transient pump-probe spectroscopy with optical pump-pulses and IR probe-pulses. Our measurements confirm the transfer of charges to the conduction band . Comparing TiO_2NP+AuNP to pure TiO_2NP suggests that both electron transfer from Au to TiO_2 as well as direct excitation of TiO_2 trap states occurs. The decrease in carrier lifetime with increasing fluence moreover indicates back transfer of charges from TiO_2 to Au.

O 23.7 Mon 18:00 P2

Photo-induced electron pressure drives THz phonon in Platinum-Copper superlattice — •Jan-Etienne Pudell[1], Marc Herzog[2], Max Mattern[2], Alexander von Reppert[2], Daniel Schick[3], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Wonhyuk Jo[1], Roman Shayduk[1], Wei Lu[1], Felix Brause[1], Michel Hehn[5], Matias Bargheer[2,4], and Anders Madsen[1] — [1]European XFEL, Germany — [2]Institut für Physik, Uni Potsdam, Germany — [3]MBI, Berlin — [4]HZB Berlin, Germany — [5]IJL, Université Lorraine, France

Using ultrafast X-ray diffraction (UXRD) at the MID end-station at the European XFEL, we investigate the ultrafast lattice dynamics of metal-metal superlattice (SL) with few atomic layers of Pt and Cu upon femtosecond photoexcitation. Our results reveal that the absorbed optical energy is rapidly localizes within the Pt layers, driving the excitation of a coherent artificial THz phonon mode defined by the superlattice period. The signal's amplitude and phase modulation of the SL Bragg peaks induced by the lattice excitation i.e. the artificial THz phonon, are predominantly driven by electron pressure within the first picoseconds. This response is faster than the Debye-Waller effect, which is limited by the electron-phonon coupling time.

O 23.8 Mon 18:00 P2

Ultrafast current response of solids - limits of quasi-classic current formula — •Jelena Schmitz, Adrian Seith, Jan Wilhelm, and Ferdinand Evers — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, D-93053 Regensburg, Germany

In a quasi-classical picture, the velocity of an electron with crystal momentum $\mathbf{k}$ is given by [1] $\mathbf{v}_n(\mathbf{k}) = \partial\epsilon_n(\mathbf{k})/\partial\mathbf{k} + q\,\mathbf{E}(\mathbf{t}) \times \mathbf{\Omega}_n(\mathbf{k})$(1), where $\epsilon_n(\mathbf{k})$ denotes the band structure and $\mathbf{\Omega}_n(\mathbf{k})$ the Berry-curvature associated with the n-th band. Expression (1) is expected to describe the material's current response to a time-dependent external field, $E(t)$, in the limit of slow and weak driving. Motivated by recent progress in generating ultrashort laser pulses, we study the limits of applicability of Eq.(1) in the limit of fast and strong driving. To this end, we adopt the framework of the Semiconductor-Bloch Equations (SBE) [2,3]; we derive Eq.(1) using a perturbative expansion of the SBE leading to analytical expressions for the limits of applicability and compare Eq.(1) with numerical solutions of the full SBE [4].

For massive Dirac Fermions, we find the bandgap energy and the Fermi level as the parameters determining the frequency domain as well as the maximum E-field strength for which the SBEs lead to matching results with Eq.(1).We also calculate corrections to Eq.(1) that enable us to identify Berry-curvature terms at higher frequencies.[1] Xiao, Di et. al., Rev. Mod. Phys. 82, 1959 (2010) [2] Schmitt-Rink, Stefan et. al., Phys. Rev. B 37, 941 (1988) [3] Wilhelm, Jan et. al., Phys. Rev. B 103, 125419 (2021) [4] https://github.com/ccmt-regensburg/CUED/

O 23.9 Mon 18:00 P2

XUV pulses with variable photon energy, pulse duration and bandwidth for time-resolved ARPES — •Isabella Alexandra Hofmeister, Niklas Hofman, Michael Schildbach, and Isabella Gierz — University of Regensburg, Regensburg, Germany

Time- and angle-resolved photoemission spectroscopy (trARPES) provides an unprecedented view on non-equilibrium quasiparticle dynamics and band structures in momentum space. Extreme ultraviolet (XUV) pulses generated by high harmonics generation (HHG) in noble gases are usually required to gain access to the complete first Brillouin zone. HHG yields a broad spectrum containing all the odd harmonics of the driving frequency up to a cut-off energy determined by the intensity and frequency of the drive. Therefore, a single harmonic is typically selected for trARPES using grating monochromators, multilayer mirrors, or a combination of filters. We compare different approaches implemented in a single trARPES setup with respect to their bandwidth and pulse duration and present strategies to enable complementary trARPES measurements with either good energy or good temporal resolution.

O 23.10 Mon 18:00 P2

Terahertz Excitation Source for Next Generation Time-of-Flight Momentum Microscopy at FLASH — Michael Herb[1], •Stefan Miedaner[1], Thomas Seitz[1], Jure Demsar[2], Stephan Winnerl[3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Johannes Gutenberg University of Mainz, Germany — [3]Helmholtz Center Dresden-Rossendorf, Germany

We will combine the broad spectral tunability of the free-electron laser FLASH with Terahertz excitation for next-generation time-of-flight momentum microscopy (ToF-MM). This unique combination will enable unprecedented access to the non-equilibrium electronic and structural properties of novel quantum materials using a variety of time-resolved spectroscopic, diffraction, and microscopic techniques. This requires the design and installation of a compact Terahertz pump source operating at Megahertz repetition rate. Here, we present the current status of the photoconductive-emitter-based source [1] and its characterization by electro-optic sampling.

[1] Optics Express 29, 427247 (2021)

O 23.11 Mon 18:00 P2

table-top source for x-ray absorption spectroscopy with photon energies upto 350 eV — •Rajdwip Bhar, Oscar A. Naranjo-Montoya, Lukas Kalkhoff, Marika Schleberger, Heiko Wende, Alexander Tarasevitch, and Uwe Bovensiepen — University of Duisburg-Essen, Duisburg, Germany

Material science research aims to understand electronic properties and dynamics of complex materials. Performing pump-probe experiments using optical pump and x-ray probe enables capturing element-specific snapshots of the pump induced changes in a material. This contribution describes the development of a tabletop soft x-ray spectroscopy setup based on high harmonic generation using noble gases in a hollow core waveguide (HCW) [1].

To generate high harmonics with higher photon energies, a near-infrared driving laser source based on optical parametric chirped-pulse amplification (OPCPA) was developed [2]. Starting with an 800 nm seed and a 1030 nm pump, the OPCPA generates 1.5 μm and 3 μm pump pulses with pulse energies of 1.8 mJ and 0.8 mJ, respectively. The 1.5 μm pulses, compressed to ~ 40 fs using chirped mirrors, pump the HCW, generating harmonics that reach photon energies up to 350 eV. Near-edge x-ray absorption spectroscopy at the B K-edge in crystalline boron and hexagonal boron nitride (hBN) samples was performed, showing excellent agreement with literature data.

[1] O. A. Naranjo-Montoya et al., Review of Scientific Instruments **95**, 103001 (2024).
[2] M. Bridger et al., Opt. Express **27**, 31330-31337 (2019).

O 23.12 Mon 18:00 P2

New end-station for time- and angle-resolved photoelectron spectroscopy in Artemis facility — •Yu Zhang, Charlotte E. Sanders, Bruce Weaver, Tiffany Walmsley, James O. F. Thompson, Richard T. Chapman, and Emma Springate — Central Laser Facility, STFC Rutherford Appleton Laboratory, Research Complex at Harwell, Harwell, United Kingdom

Artemis, located at the Central Laser Facility in the UK, is a user facility offering time- and angle-resolved photoelectron spectroscopy (TrARPES) utilizing extreme ultraviolet (20-45 eV) photon sources based on high harmonic generation of ultrafast laser. After more than a decade of operation, Artemis has established itself as a leading facility in the research of ultrafast electron dynamics on surfaces. Recently, Artemis received an significant upgrade of its end-station, which will provide users with state-of-the-art techniques in ultrafast time-resolved measurements. These new capabilities include both momentum and real-space mapping, large-angle E-k mapping with a deflector, and a closed-loop cryostat for low-temperature measurements. Detailed information about these features can be found in the poster. Along with the recently upgraded 100kHz laser source, Artemis is committed to delivering high-performance TrARPES for its user communities.

O 23.13 Mon 18:00 P2

Temporal evolution of surface plasmon polariton skyrmions — •Philipp Gessler, Alexander Neuhaus, Maria Azhar, Pascal Dreher, Frank Meyer zu Heringdorf, and Karin Everschor-Sitte — University of Duisburg-Essen, Germany

In recent years, structures reminiscent of those found in magnets [1] have been predicted and observed in Surface Plasmon Polaritons (SPPs). Of particular interest are topological SPP structures such as skyrmion lattices [2,3] or merons [4]. In particular, these structures have been identified in various quantities related to the electric field, many of which exhibit amplitudes that oscillate over time. Building on insights from micromagnetism, our objective is to explore the dynamic behavior of these novel SPP states beyond mere temporal oscillations.

[1] C. Back et al., J. Phys. D: Appl. Phys. **53**, 36 (2020)
[2] S. Tsesses et al., Science **361**, 6406 (2018)
[3] T. J. Davis et al., Science **368**, 6489 (2020)
[4] Y. Zheng et al., Nanophotonics **13**, 2 (2024)

O 23.14 Mon 18:00 P2

Femtosecond momentum microscopy of field-effect gated bilayer WSe_2 and monolayer graphene — •Bent van Wingerden, Jan Philipp Bange, Jonas Pöhls, Wiebke Bennecke, Paul Werner, Daniel Steil, Matthijs Jansen, R. Thomas Weitz, Marcel Reutzel, and Stefan Mathias — I. Physikalisches Institut, Georg-August Universität Göttingen, Germany

Atomically-thin transition metal dichalcogenides and their respective Moiré heterostructures can host a variety of strongly correlated electronic phases, such as Wigner crystals and Mott insulators. The formation of these phases critically depends on the precise occupation of the corresponding Moiré superlattice states [Regan *et al.* Nature 579, (2020)], and might therefore be controlled by field-

effect doping of charge carriers [Nguyen *et al.* Nature 572 (2019)]. In our work, we realized this in combination with a table-top time-resolved ARPES setup, i.e. our Göttingen femtosecond momentum microscopy experiment [Schmitt *et al.*, Nature 608, (2022)]. Our extension of ARPES experiments on field-effect gated heterostructures into the time domain on a laboratory scale will facilitate the study of non-equilibrium dynamics of strongly correlated phases and charged quasiparticles, e.g. trions. We provide proof-of-principle data on field-effect gated monolayer graphene and present time-resolved photoemission data of a WSe_2 bilayer at different charge carrier densities.

O 23.15 Mon 18:00 P2

Towards ultrafast momentum microscopy of exciton dynamics at ZnO surfaces — •Hashima Marukara, Junde Liu, and Stefan Mathias — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

The semiconductor ZnO, known for its wide band gap and high exciton binding energy, stands out as a promising material among transparent conductive oxides for applications in optoelectronics and catalysis[1,2]. Surface excitons, i.e. bound electron-hole pairs localized at the material's surface, play a crucial role in mediating its optical and electronic properties, significantly influencing energy conversion processes at the surfaces [3]. An ideal tool to study these ultrafast processes is time- and angle-resolved photoelectron spectroscopy, which gives access to the exciton landscape and the relevant excitation and relaxation pathways. In our new project within the CRC1633 "Proton-coupled electron transfer", we aim to study the ultrafast surface exciton dynamics at the ZnO(10-10) surface using our Göttingen time-resolved momentum microscopy setup. By using this technique, which gives us access to full energy and momentum space, we aim to gain detailed information on the ZnO's exciton momentum and real-space properties (localized/delocalized/defect/etc.) and the accompanying exciton dynamics [4].

[1] Gierster et al., Nat Commun 12, 978 (2021)
[2] Foglia et al., Struct. Dyn. 6, 034501 (2019)
[3] Deinert et al., Phys. Rev. Lett. 113 057602 (2014)
[4] Reutzel et al., Advances in Physics X 9, 2378722 (2024)

O 23.16 Mon 18:00 P2

Towards momentum microscopy of plasmon excited WSe_2 — •Mattis Langendorf[1], Paul Werner[1], Marco Merboldt[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Jonas Pöhls[1], Tobias Meyer[2], Thomas R. Weitz[1], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Georg-August-Universität Göttingen, Institut für Materialphysik, Germany

Femtosecond momentum microscopy represents a uni measurement technique that effectively integrates the advantages of angle-resolved photoemission spectroscopy (ARPES) and photoelectron emission microscopy (PEEM) within a single microscope. The capacity to transition between real- and momentum-space imaging in time-resolved photoelectron spectroscopy enables the investigation of quasiparticles in both regimes [Bange et al., Nature Photonics, in press (2024)]. In this contribution, we pursue the characterization of electron-hole pairs, i.e. excitons, which were excited by a collective excitation of charge carriers, i.e. a surface plasmon polariton (SPP). In this approach, the propagating SPPs are imaged with photoemission electron microscopy, and the formation of excitons in the TMD is then visualized with time-resolved dark-field imaging techniques.

O 23.17 Mon 18:00 P2

Control and manipulation of low-energy electrons — •Dennis Epp[1], Frank Long[1,2], Benjamin Schröder[1], and Claus Ropers[1,2] — [1]Max-Planck-Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

In surface science and materials physics, electron pulses are a powerful probe of structural dynamics in time-resolved diffraction and microscopy experiments. A fundamental challenge lies in the Coulomb interaction [1] and initial energy distribution, which negatively affects the electron beam size and pulse duration after propagation towards the sample. Active control of electron pulse properties by compression schemes has proven to enhance temporal resolution [2-4]. This is particularly important for low-energy electrons and their high dispersion due to low propagation velocity [4]. In this paper, we demonstrate longitudinal and transversal phase-space manipulation of low-energy electron pulses using synchronized RF fields in the gigahertz frequency range [4]. Furthermore, novel beam shaping concepts including electron pulse streaking, compression and deflection are discussed.

[1] van Oudheusden, et al., Physical Review Letter 105, 264801 (2010). [2] Kassier, et al., Applied Physics B 109, 249-257 (2012). [3] Epp, et al., Structural Dynamics 11, 024306 (2024). [4] Haindl, et al., Nature Physics 19, 1410*1417 (2023).

O 23.18 Mon 18:00 P2

Band-resolved studies of laser-induced ultrafast dynamics in gold — •Stephanie Roden, Tobias Held, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU in Kaiserslautern

The irradiation of a metal with a short-pulsed optical laser leads to the excitation of electrons, which absorb energy in accordance with their orbital characteristics. To analyze the resulting state of thermodynamic non-equilibrium, the thermalization of the excited electrons and relaxation processes with the phonon system to a joint temperature can be calculated in a kinetic manner by coupled Boltzmann collision integrals.

In this work we extend our existing energy-resolved model based on one effective band for the electrons [1] to a two-band model for a thin metal film that distinguishes between the free sp- and more localized d-electrons [2]. By considering the different electron bands separately, we can investigate the influence of intra- and interband relaxation in the electron system on the dynamics of the entire sample. We are focusing especially on the effect on the band occupation and the coupling strengths between the electron systems and the phonons.

[1] B. Y. Mueller and B. Rethfeld, PRB 87, 035139 (2013)
[2] T. Held, S. T. Weber, and B. Rethfeld, Journal of Physics: Condensed Matter (2025)

O 23.19 Mon 18:00 P2

Ultrafast intra- and interlayer charge transfer at the FePc/WSe_2 interface — •Gregor Zinke[1], Sebastian Hedwig[1], Benito Arnoldi[1], Martin Anstett[1], Lu Lyu[1,2], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern - Landau, Erwin-Schroedinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg

Tailoring the optoelectronic properties of 2D-van-der-Waals materials by material design is a promising approach for functionalizing charge and spin carriers in low-dimensional materials. In this work, we demonstrate how optically excited ultrafast charge carrier dynamics of TMDCs can be altered by the formation of molecule/2D material heterostructures. Here, we focus on an ordered FePc monolayer film deposited on the surface of a bulk WSe_2 crystal. Using time- and angle-resolved photoemission in a VIS-pump, XUV-probe setup, we will elucidate the ultrafast response of the electronic system to an optical excitation on fs-timescales. Of particular interest is the investigation of intra- and interlayer charge carrier dynamics at the FePc / WSe_2 interface, which can be disentangled by the characteristic momentum space signatures of the WSe_2 Bloch-like states and molecular orbitals. We will further illustrate the impact of ultrafast charge separation across the interface on transient changes of the interfacial energy level alignment.

O 23.20 Mon 18:00 P2

Influence of ballistic electrons on temperature equilibration in bulk gold — •Lukas Jonda, Tobias Held, Markus Uehlein, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics andResearch Center OPTIMAS, RPTU Kaiserslautern-Landau

During femtosecond laser irradiation of gold, electrons are excited to a state of non-equilibrium in space and energy. Highly excited electrons transport energy ballistically into the bulk due to their relatively long mean free path. On a picosecond timescale, electrons transfer energy to the crystal lattice via electron-phonon collisions.

The objective of this study is to analyze the influence of non-equilibrium electrons on energy transport. Therefore, a two-temperature model will be coupled with a kinetic Monte Carlo simulation. With the former we describe diffusive transport as well as the electron-phonon equilibration, while the latter describes the primary electron excitation by the laser pulse, secondary electron generation, and transport of non-equilibrium electrons above the Fermi level.

O 23.21 Mon 18:00 P2

Hot carrier dynamics and band gap formation in lead intercalated graphene on Ni(111) — Martin Mitkov[1], Lu Lyu[2], Eva Walther[1], Martin Anstett[1], •Alexander Schmid[2], Christina Schott[1], Gyula Halasi[3], Nikolett Oláh[3], Csaba Vass[3], Zoltán Filus[3], László Óvári[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]RPTU Kaiserslautern-Landau — [2]University of Augsburg — [3]ELI ALPS, Szeged, Hungary

The intercalation of atoms between 2D materials and surfaces offers an intriguing opportunity to tune spin functionalities at surfaces. The combination of heavy metal atoms and magnetic surfaces allows to tune the band structure of 2D materials through the interplay of spin-orbit coupling and magnetic proximity effects. In this poster, we present our recent findings on the band structure and hot electron dynamics of a Pb-intercalated graphene layer on Ni(111).

The highly reactive Ni substrate causes a charge transfer into the graphene layer, which leads to n-doped Dirac cones. Pb intercalation leads to a decoupling of the graphene, resulting in a quasi-free standing graphene layer on Ni.

Our time-resolved momentum microscopy experiment allows us to determine the influence of Pb intercalation on the ultrafast carrier dynamics of the Gr/Ni(111) interface. We discuss the momentum space distribution of the optically excited carriers at the K-point for the bare and Pb intercalated graphene and present indications for a modification of the magnetization dynamics of the Ni substrate by energy and charge transfer from the Pb-intercalated graphene.

O 24: Poster Scanning Probe Techniques: Method Development

Time: Monday 18:00–20:00 Location: P2

O 24.1 Mon 18:00 P2

Comparative Analysis of Work Function Measurements Using STM/AFM Techniques — •Daryoush Nosraty Alamdary, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The engineering of the work functions at the interface of complex materials is sometimes the key [1] for an energy band tuning that supports proximity-induced effects [2]. While there are handful of established methods that allow a precise measurement and determination of the work function, STM-based methods constitute a class of their own since they are based on a local probe. In this work we present a comparative study of 3 different techniques based on a combined STM/AFM setup. For a few well-characterized sample systems we analyze the benefits and difficulties of each method. Finally, we draw a conclusion as to which method is the more precise and reliable method, whereby the special focus lies on the accuracy and the challenges of the interpretation.

[1] P. Rüßmann em et al., Proximity induced superconductivity in a topological insulator, arXiv:2208.14289 (2022)

[2] L. Fu and C. L. Kane, Superconducting Proximity Effect and Majorana Fermions at the Surface of a Topological Insulator, Phys. Rev. Lett. **100**, 096407 (2008)

O 24.2 Mon 18:00 P2

Cryogenic, ultrahigh vacuum sample transfer between electrospray ion beam deposition (ESIBD) and scanning probe microscopy (SPM) — •Alejandro Lynch Gonzalez, Stephan Rauschenbach, Lukas Eriksson, Benjamin Mallada, Tim Esser, and Marko Grabarics — University of Oxford

Electrospray ion beam deposition (ES-IBD) is currently the only viable method for cleanly and selectively depositing large and complex molecules which do not have a vapour pressure while preserving their chemical structure. In our lab, ESIBD[1] and SPM instruments are physically separate and sample transfer between them is performed using a vacuum suitcase system which maintains UHV and cryogenic conditions during transfer, essential for suppressing surface diffusion, conformational changes, and contamination during the transfer. Here, we present the design, implementation, and benchmarking of a cryogenic UHV suitcase and showcase applications.

[1] Fremdling, P. et al. ACS nano 16, 14443-14455 (2022).

O 24.3 Mon 18:00 P2

Ultra-broadband Terahertz Time-Domain Spectroscopy for Space Exploration — •Dominic Azih[1,2], Yookyung Ha[2], Jonas Woeste[1,2], Nikola Stojanovic[2], and Michael Gensch[1,2] — [1]Technical University, Berlin, Germany — [2]DLR Ínstitute of Optical Sensor Systems, Berlin, Germany

Femtosecond lasers have in recent years been shown to be space qualified and with the development of compact femtosecond laser systems [1,2], Terahertz Time-Domain Spectroscopy (THz TDS) allows meanwhile to cover an essential part of the molecular fingerprint spectral range and has several technological advantages over the commonly used Fourier-Transform Infrared techniques (FTIR). The advantages are compactness, replacement of components (cryogenic) spectrally broadband infrared detectors with electro-optic/acousto-optic photonic techniques and the potential to be chip-integrable. Here we show our progress enroute to a THz time-domain spectroscopic setup for space applications with a bandwidth of over 30THz and a resolution of better than 100GHz [3].

O 24.4 Mon 18:00 P2

High-collection efficiency optical scanning probe microscopy with on-axis parabolic mirror — •Aleksander Bogucki[1], Magdalena Grzeszczyk[1], Yeon-ji Kim[1], Yewon Kim[1], German Orlov[1], Lei Fang[1], Wonjun Jang[1,2], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, South Korea — [2]Department of Physics, EWHA Womans University, Seoul, South Korea

Scanning probe microscopy (SPM) techniques are essential for investigating surface physics, from single atoms to complex systems like organic molecules. Combining SPM with optical spectroscopy enhances our ability to explore system dynamics. However, existing setups face photon collection efficiency challenges due to spatial constraints, particularly for systems with long-lived excited states.

We present a homemade optics-integrated scanning probe microscope using a centered on-axis parabolic mirror with a short focal length. The scanning component employs a combined AFM/STM qPlus sensor with a long tip. Free-beam optics maximize photon collection efficiency, reaching an estimated upper limit of 90%. This design eliminates chromatic aberrations, enables polarization measurements, and operates under ultra-high vacuum (UHV) at low temperatures (4K), ensuring high stability and precision.

O 24.5 Mon 18:00 P2

Electron wavefront shaping with light — •martino zanetti[1,2], Tilman Kraeft[1,2], Luis Alfredo Ixquiac Mendez[1,2], Alexandra Pernishova[1,2], and Thomas Juffmann[1,2] — [1]University of Vienna, Faculty of Physics — [2]University of Vienna, Max Perutz Laboratories

Electron Microscopes (EM) are common and fundamental tools in many research fields, as they can image samples with resolutions down to the nanometric scale. The ability to arbitrarily shape the electron beam of an EM with light can help overcome intrinsic limits like electron lens aberrations and pave the way to new EM techniques [1].

For shaping the electron beam, a modified Scanning-EM is coupled to a high-power pulsed laser. The electron-light interaction takes place in the SEM chamber. The electrons are then detected after free propagation to measure their spatial distribution. Here, we present our advancements in applying the electron beam shaping technique to demonstrate single electron wavefront modulation. The intensity profile of a TEM01 laser mode is imprinted on the wavefront of the electron, which thus resembles that of an electron going through a double slit. Adding up the detection of multiple electrons, we expect to see an interference pattern that proves the effective modulation of the electron wavefront. The need for micrometric resolution measurements required us to develop a single-electron detector which outperforms many commercially available ones in the 20-30 keV range, being at the same time more flexible and cheaper.

[1] Mihaila et al., Phys. Rev. X 12, 031043 (2022)

O 24.6 Mon 18:00 P2

Optimizing ESR-STM for mK Temperatures in a Closed-Cycle Dilution Refrigerator — •Luise Renz, Máté Stark, Jonas Arnold, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Using Electron Spin Resonance (ESR) combined with Scanning Tunneling Microscopy (STM), electronic and magnetic properties of single atoms and molecules can be studied. However, the possibility of applying RF voltages to the tip often limits the achievable minimum temperature of the STM. We here describe an ESR-STM setup mounted in ultra-high vacuum (UHV) in a closed-cycle Dilution Refrigerator (DR). The focus here is on the wiring of the STM, the material choice and the filtering of the RF and DC cables with the goal of having a good transmission of the RF lines but nevertheless also mK-temperatures in the STM junction. The resulting bandwidth and transmission of these cables, the noise level of the STM as well as the electronic temperature of the STM junction, is presented. The electronic temperature is estimated on a Pb(111) crystal by evaluating the superconducting gap and the Josephson peak (using a superconducting tip).

O 24.7 Mon 18:00 P2

Detection and Localization of Atoms and Molecules on Different Surfaces Using Computer Vision — •Lovis Hardeweg, Johannes Schwenk, Wantong Huang, Kwan-Ho Au-Yeung, Máté Stark, Paul Greule, Christoph Sügers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Scanning Probe Microscopy (SPM) methods are unparalleled in their ability to image and manipulate structures on the atomic scale. In combination with machine learning techniques, this allowed to automate processes such as removing a molecule from a thin layer [1] or moving an adsorbed molecule to a specific position [2]. However, this often relies on prior human interaction to identify and localize objects of interest, like a thin film or a single adsorbate. Here, we discuss methods that automate several steps in SPM experiments, with the goal of advancing single atomic and molecular spin detection experiments. For that, we employ computer vision techniques to STM topography data and are able to extract information, such as the location of single atoms and molecules or the presence of different sample surfaces, for instance ultra-thin MgO films grown on Ag(001). We believe that these abilities, once sufficiently developed, can lead to a significant reduction in the need for human intervention in the automated use of high-resolution low temperature SPM. [1] P. Leinen et al. Sci. Adv., vol. 6, no. 36, p. eabb6987, Sep. 2020, doi: 10.1126/sciadv.abb6987. [2] B. Ramsauer et al. J. Phys. Chem. A, vol. 127, no. 8, pp. 2041-2050, Mar. 2023, doi: 10.1021/acs.jpca.2c08696.

O 24.8 Mon 18:00 P2

A Closed-Cycle Atomic Force Microscopy Setup for Electron Spin Resonance Measurements at mK Temperatures — •Adrian Seiler, Lovis Hardeweg, Luise Renz, Arian Vosoghi Marand, Kwan Ho Au-Yeung, Wantong Huang, Paul Greule, Máté Stark, Christoph Sürgers, Wolfgang Wernsdorfer, Johannes Schwenk, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Combining scanning probe techniques with electron spin resonance (ESR) provides a unique tool for the investigation as well as the manipulation of individual surface-adsorbed spins. Most experiments up to date are relying on Scanning Tunneling microscopy (STM) and thus conductive samples [1]. As a result, scattering of electrons with the spin system is a major source of decoherence and relaxation. In contrast, atomic force microscopy (AFM) provides the possibility to reduce the scattering intensity with the conducting electrodes. Here, we present the first implementation steps of a commercial AFM head and ultra-high vacuum setup in a compact dilution refrigerator. The final setup is designed to reach milli-Kelvin temperatures (≈ 50 mK) with short cool-down times on the order of several hours. In addition to the dilution unit, the system utilizes a closed-cycle cryocooler allowing longtime stable operation. We further improve the time-consuming sample preparation by automation of the sputter and annealing process to allow for a rapid turnaround of samples in the future.

[1] Y. Chen et al. Adv. Mater. 35, 2107534 (2023).

O 24.9 Mon 18:00 P2

Lightwave driven magnetic field scanning tunneling microscopy — •Leo Ringer, Andreas Rank, Peter Menden, Christian Meineke, Rupert Huber, and Jascha Repp — University of Regensburg, Regensburg, Germany

Lightwave driven scanning tunneling microscopy (LW-STM) is based on the key idea to directly steer electron tunneling in STM by ultrashort light pulses. Combining the development of LW-STM with a tunable magnetic field would allow following spin dynamics - e.g. spin precession - in molecules and other atomistic structures with single-electron sensitivity. To this end, we develop a novel lightwave driven scanning tunneling microscope including an external magnetic field to resolve single-spin dynamics with atomic spatial and ultrafast temporal resolution. Instrumental challenges of this development will be discussed, and we present the resulting instrument design including the head of the scanning tunneling microscope, the laser source as well as the solution to introduce the laser transient from outside the vacuum system to the tip-sample junction.

O 24.10 Mon 18:00 P2

Implementation of radio-frequency magnetic fields for electron spin resonance atomic force microscopy — •Raffael Spachtholz, Lisanne Sellies, Franziska Bruckmann, Sonja Bleher, Philipp Scheuerer, and Jascha Repp — Department of Physics, Universität Regensburg

Implementing electron spin resonance in scanning tunneling microscopy represents a milestone in controlling spin systems at atomic scales [1]. In this emerging research field the required radio-frequency (RF) signal is provided as an electric field, translating to an effective magnetic field.

Here we report the integration of a radio-frequency (RF) magnetic field, in the frequency range of 0.1 to 3 GHz, into a scanning-probe microscope. We utilized a flexible polyimide printed-circuit-board coil to generate the RF magnetic fields. Additionally, an insulating sample, coated with a gold microstructure, was designed to locally enhance the RF magnetic field while mitigating the screening effects caused by a metallic substrate. Up to 3 GHz the transmission only moderately depends on frequency and exhibits no sharp resonances. This development enabled the implementation of electron spin resonance in atomic force microscopy, as demonstrated for individual pentacene molecules [2].

[1] S. Baumann, et al., Science 350, 417-420 (2015)
[2] L. Sellies, et al., Nature 624, 64-68 (2023)

O 24.11 Mon 18:00 P2

Implementation and characterization of all-electronic pump-probe spectroscopy on a low-temperature scanning tunneling microscope — •Guido Hiller, Gaël Reecht, and Manuel Gruber — Universität Duisburg Essen, Duisburg

Pump-probe spectroscopy is a powerful technique for investigating non-equilibrium dynamics, where the time resolution is determined by the duration of the pump and probe pulses rather than the detectors bandwidth. When combined with a scanning tunneling microscope (STM), this method enables dynamic measurements at the level of individual atoms and molecules, achieving both high temporal and spatial resolutions [1].

In this work, we implement an all-electric pump-probe scheme on a low-temperature STM. Cross-correlation measurements on an Au(111) surface reveal a time resolution of 100 ns. This resolution is constrained by the broadening of voltage pulses during transmission to the STM junction [2]. To address this, we conducted a detailed analysis of the frequency-dependent transmission function of the instrument. Funding support from the CRC 1242 is gratefully acknowledged.

[1] Loth et al., Science 329, 1628 (2010)
[2] Herve et al., Applied Physics Letter 107, 093101 (2015)

O 25: Overview Talk Jörg Kröger

Time: Tuesday 9:30–10:15 Location: H24

Topical Talk O 25.1 Tue 9:30 H24

Exploring quantum physics with scanning probe methods — •Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, Germany

It is hardly possible to ignore the importance of scanning probe techniques for the understanding of mechanisms and principles in the quantum behavior of condensed matter. This Overview Talk presents contributions of atomic force microscope experiments to controlling and quantifying interactions involved in bonding processes at the single-atom level. It then demonstrates that scanning tunneling spectroscopy is successfully used in exciting and detecting quantum vibrations and spins as well as in characterizing the charge transport across the metal-superconductor interface. Funding by the DFG through KR 2912/17-1, 18-1, 21-1 and the BMBF through ForLab is acknowledged.

O 26: Focus Session Ultrafast Electron Microscopy at the Space-Time Limit III

Shaping functionalities on the nanoscale is one of the most essential challenges in modern condensed matter research. It requires a comprehensive understanding of the complex interplay of the electronic, spin, and lattice degrees of freedom in materials and requires tailoring energy transfer and dissipation pathways on the smallest length and fastest timescales. Recent instrumentation breakthroughs in different varieties of pump-probe ultrafast electron microscopy have opened the way for accessing electronic and structural dynamics at surfaces, interfaces, and nanostructures with down-to-attosecond resolution in time. While ultrafast photoemission electron microscopy techniques provide supreme sensitivity to spin and electron dynamics in real momentum space, bright ultrashort electron pulses in the ultrafast implementation of more traditional electron microscopes can probe optical states, local magnetization, and lattice dynamics with a nanometer spatial resolution.

This focus session highlights recent advances in ultrafast high-resolution electron probing. These include new instrumentation and techniques, excitations from the THz to X-ray regime, and studying novel phenomena and materials systems. At the same time, it will bring together researchers from the different areas of ultrafast condensed matter physics to foster discussions and new collaborations to explore emergent scientific questions in this field.

Organized by Armin Feist (MPI Göttingen) and Benjamin Stadtmüller (University Augsburg).

Time: Tuesday 10:30–13:00 Location: H2

Invited Talk O 26.1 Tue 10:30 H2

Attosecond Electron Microscopy — •Peter Baum — Universität Konstanz, Germany

All processes in materials, nanostructures and devices are on a fundamental level defined by electronic and atomic motion from initial to final conformations. Our approach for a direct, real-space visualization is pump-probe electron diffraction

and microscopy with single-electron wavepackets under the control of laser light. The resulting few-femtosecond and attosecond time resolution allows to see almost any light-matter interaction or structural dynamics on fundamental scales in space and time. We report selected results on strongly correlated materials, rotational phonons, electronic circuitry, free-electron quantum phenomena and attosecond dynamics in nanomaterials.

O 26.2 Tue 11:00 H2

Steady-State and Time-Resolved Cathodoluminescence of III-Nitride Semiconductors — •Kagiso Loeto, Aidan Flynn Campbell, Domenik Spallelk, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Deutschland

Cathodoluminescence (CL), in steady-state and time-resolved modes, has advanced the study of semiconductor optical properties, crucial for microelectronics and III-nitride optoelectronics. A new state-of-the-art time-resolved CL (TRCL) microscope at the Paul-Drude-Institut features a high-performance SEM with a stable electron source and advanced light collection system, enabling optimized imaging and high spatial resolution at acceleration voltages as low as 0.35 kV. The system features a UV-optimized CCD camera for studying UV-emitting materials like III-nitrides. Time-resolved operation is enabled by an ultrafast beam blanker paired with detectors achieving temporal resolutions of tens of picoseconds, offering new insights into the dynamic optical properties of advanced semiconductors. It will be employed in three focus areas, highlighting its distinct capabilities. First, very-low acceleration voltage operation will enable high-resolution mapping of individual point defects in AlGaN quantum well structures, revealing their impact on AlGaN-based UV LEDs. Second, ultraviolet-optimized photon detectors will study temperature-stable excitonic bands in AlN with high spectral resolution, providing insights into their origins. Lastly, the instrument's time-resolved capabilities combined with spatial mapping will explore the interplay between carrier dynamics and localization in InGaN pseudosubstrates.

O 26.3 Tue 11:15 H2

Spin Resonance Spectroscopy meets Transmission Electron Microscopy — •Philipp Haslinger — Atominstitut, USTEM, Technische Universität Wien, Austria

Coherent spin resonance methods such as nuclear magnetic resonance and electron spin resonance spectroscopy have led to spectrally highly sensitive, non-invasive quantum imaging techniques. Here, we will present a spin resonance spectroscopy approach developed for transmission electron microscopy [1,2] and will explain different techniques to sense with electrons for microwave manipulated spin states of the sample. This could enable state-selective observation of spin dynamics on the nanoscale and indirect measurement of the environment of the spin systems, providing information on, for example, atomic structure, local chemical composition and neighbouring spins.

[1] P. Haslinger, S. Nimmrichter, and D. Rätzel, Spin Resonance Spectroscopy with an Electron Microscope, Quantum Sci. Technol. 9, 035051 (2024). [2] A. Jaroš, J. Toyfl, A. Pupić, B. Czasch, G. Boero, I. C. Bicket, and P. Haslinger, Electron Spin Resonance Spectroscopy in a Transmission Electron Microscope, arXiv:2408.16492 (2024).

O 26.4 Tue 11:30 H2

Observation of Kapitza-Dirac effect with fast electrons — •Kamila Moriová[1], Petr Koutenský[1], Marius Constantin Chirita Mihaila[1], Zbyněk Šobáň[2], Andreas Schertel[3], Jaromír Kopeček[2], and Martin Kozák[1] — [1]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]Carl Zeiss AG, Oberkochen, Germany

Advancing ultrafast electron microscopy relies on coherent control of free electron wavefunctions. While most research focuses on electron interactions with optical near-fields, an all-optical approach using ponderomotive forces offers a promising alternative for manipulating pulsed electron beams. The Kapitza-Dirac effect [1], where free electrons diffract coherently from a standing light wave, enables momentum transfer via stimulated Compton scattering. However, its application has been limited to low-energy electrons due to challenges in resolving small deflection angles of electron beams caused by photon absorption and emission.

We report the observation of the Kapitza-Dirac effect in a scanning electron microscope using high-energy (20 keV) electrons. Photon sidebands in the electron transverse momentum spectrum are detected in a convergent beam diffraction geometry using spatial filtering. This effect can serve as a coherent electron beam splitter or phase plate in various types of electron microscopes and paves the way for exploring fundamental electron-light interactions.

[1] Freimund, D. L. et al. Nature 413, 142 (2001)

O 26.5 Tue 11:45 H2

Recent results of the ultrafast scanning electron microscope in Erlangen — •Stefanie Kraus[1], Tomas Chlouba[1], Roy Shiloh[1], Leon Brückner[1], Julian Litzel[1], Zhexin Zhao[1], Viacheslav Korolev[1], Manuel Konrad[1], Tatsunori Shibuya[1,3], and Peter Hommelhoff[1,2] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen — [2]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München — [3]AIST, Tsukuba, Japan

Ultrafast electron microscopy is revolutionizing the capabilities of electron microscopes, allowing for unprecedented spatial and temporal resolution. Closely related is the coupling of electrons and optical nearfields, which is based on the excellent electron pulse properties an ultrafast scanning electron microscope (USEM) can provide. We have leveraged the interaction of electrons with the near field of a periodic structure to achieve sub-femtosecond electron pulse compression as well as laser acceleration of electrons. This advancement enhances temporal resolution and facilitates large beam energy variations, enabling detailed investigations of ultrafast dynamics. In this talk, we will provide an overview of our recent progress, including electron energy modulation in larger structures illuminated with 10 micrometer light as to enhance the current throughput, electron bunch compression, and the latest experimental results.

O 26.6 Tue 12:00 H2

FEL-based core-cum-conduction momentum microscopy of ultrafast charge-density-wave dynamics — •N. Wind[1,2,3], M. Heber[1,3], D. Kutnyakhov[1], L. Wenthaus[1], J. Dilling[2], L. Bruckmeier[2], S. Chernov[1], O. Tkach[4], A. Mehta[5], J. Koralek[5], G. Dakovski[5], J.A. Sobota[6], P.E. Majchrzak[6], D. Puntel[6], D. Liu[6], G. Schönhense[4], H.J. Elmers[4], Z.X. Shen[6], M. Scholz[1], and K. Rossnagel[1,2] — [1]Deutsches Elektronen Synchrotron DESY, 22607 Hamburg, Germany — [2]Christian-Albrechts-Universität zu Kiel IEAP, 24098 Kiel, Germany — [3]Universität Hamburg, IExP, 22761 Hamburg, Germany — [4]Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany — [5]SLAC National Accelerator Laboratory, Menlo Park, CA 94205, USA — [6]Stanford University, Institute for Materials and Energy Science, CA 94305, USA

Transition-metal dichalcogenides (TMDCs) offer a rich platform for studying novel forms of quantum and nanoelectronics in layered structures approaching the 2D limit. Among them, 1-*T* TaS_2 has been extensively studied due to its various charge-density-wave (CDW) phases. Here, we provide novel insights into the CDW melting in 1-*T* TaS_2, using time- and angle-resolved photoemission spectroscopy with a momentum microscope at the free-electron laser FLASH in Hamburg. Our near-infrared pump–FEL probe experiment uncovers momentum-dependent conduction-band dynamics and core-level responses, advancing our understanding of ultrafast coupled electronic and structural dynamics.

O 26.7 Tue 12:15 H2

Developing a versatile fiber-based cathodoluminescence detection system for an ultrafast scanning electron microscope — •Paul H. Bittorf[1], Filip Majstorovic[1], and Nahid Talebi[1,2] — [1]Institute for Experimental and Applied Physics IEAP, Kiel University, 24118 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Cathodoluminescence (CL) is emitted when a high-energy electron beam interacts with materials like minerals, semiconductors and plasmonic nanoparticles. Depending on the underlying interaction mechanisms of electrons with the sample this radiation can be coherent or incoherent, where both spectral and temporal statistics can be unraveled for material characterization. Thanks to the high spatial resolution and large spectral excitation bandwidth of the electron beams, we could resolve the spatial far-field distribution of locally probed photonic modes by CL microscopy. Moreover, we combined a commercial scanning electron microscope (SEM) with an ultrafast laser system to obtain a pulsed electron beam via the photoemission process. In addition to the excitation by the pulsed electron beam, a time-delayed laser pulse is focused onto the sample to induce an optical near-field and achieve a time-resolved pump-probe measurement. The interaction properties of electrons with nanostructured matter are analyzed through the emitted CL. Here, we report on technical aspects and the implementation of a multimode fiber-based CL detection system inside an ultrafast SEM and highlight its functionality by performing CL spectroscopy and time correlated single-photon counting.

O 26.8 Tue 12:30 H2

Ultrafast Electron Diffraction and Microscopy of Structural Phase Transitions at Megahertz Rates — •Till Domröse[1,2] and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Control over laser-induced structural phase transformations promises tuning of macroscopic materials properties on femtosecond timescales. Ultrafast electron diffraction (UED) elucidates the spatially averaged evolution of lattice symmetries and phonon populations during the transitions. However, resolving nanoscale structural heterogeneity in these measurements remains challenging due to the reduced brightness of pulsed electron beams. Here, we overcome fundamental limitations in the stroboscopic investigation of structural dynamics in thin material films by UED and ultrafast electron microscopy. A high-coherence electron source offers enhanced momentum resolution in collimated electron nanobeams, while thermally-optimized sample supports enable reversible driving of structural transitions at high duty cycles [1]. Utilizing the

associated gain in coherent electron current, we conduct nano-UED investigations of charge-density wave dynamics in layered materials, tomographically reconstructing three-dimensional phase formation kinetics in 1*T*-TaS_2 [2], and revealing a femtosecond structural quench in 1*T*'-$TaTe_2$ cycled at a repetition rate of 2 MHz [3].

[1] T. Domröse, *et al.*, arXiv:2410.02310 (2024)
[2] T. Domröse, *et al.*, Nature Materials **22(11)** (2023)
[3] T. Domröse, C. Ropers, Physical Review B **110(8)** (2024)

O 26.9 Tue 12:45 H2

From Electron-Photon Ghost Imaging Towards Entanglement Certification — •Alexander Preimesberger[1,2], Sergei Bogdanov[1,2], Phila Rembold[1], Santiago Beltrán-Romero[1,2], Dominik Hornof[1,2], Isobel C Bicket[1,2], Nicolai Friis[1], Elizabeth Agudelo[1], Dennis Rätzel[3], and Philipp Haslinger[1,2] — [1]VCQ, Atominstitut, TU Wien, Vienna, Austria — [2]USTEM, TU Wien, Vienna, Austria — [3]ZARM, University of Bremen, Bremen, Germany

Time-resolved detection of single electrons and their associated cathodoluminescence (CL) photons enables the identification of coincident electron-photon pairs. We recently employed this technique to study the tight momentum correlations generated by coherent CL within a transmission electron microscope [1]. In this contribution, we demonstrate ghost imaging using electron-photon pairs in both near-field and far-field configurations. In photonic quantum optics, the ability to produce such images is used to investigate quantum entanglement in photon pairs [2]. We discuss how to translate this concept to electron-photon states and introduce a robust method to certify and quantify their entanglement using measurements in mutually unbiased bases.

[1] A. Preimesberger et al., arXiv:2409.12216 (2024). [2] R. S. Bennink et al., Phys. Rev. Lett. 92 (2004).

O 27: Solid-Liquid Interfaces: Reactions and Electrochemistry I

Time: Tuesday 10:30–13:00 Location: H4

O 27.1 Tue 10:30 H4

Combining electrochemical scanning tunneling microscopy with force microscopy — •Andrea Auer[1,2] and Franz J. Giessibl[2] — [1]Institute of Physical Chemistry, University of Innsbruck, Austria — [2]Institute of Experimental and Applied Physics, University of Regensburg, Germany

Atomic force microscopy (AFM), which can be performed simultaneously with scanning tunneling microscopy (STM) using metal tips attached to self-sensing quartz cantilevers (qPlus sensors) [1], has advanced the field of surface science by providing unprecedented spatial resolution under ultra-high vacuum conditions. The simultaneous performance of AFM and STM with atomic resolution in an electrochemical cell offers new possibilities for local imaging of electrode structures. Here, we present a combined AFM/STM instrument realized with a qPlus sensor and a custom-built potentiostat for electrochemical applications. Graphite was atomically resolved in both STM and AFM channels in acidic electrolytes [2]. The difference in contrast between AFM and STM images demonstrate the ability to measure conductance at the Fermi level (STM) but also the total charge density (AFM) in an electrochemical environment. This allows us to study important electrode processes that involve a change in charge density, such as adsorption, intercalation, or oxidation processes, and their atomic contrasts in more detail.

[1] F.J. Giessibl, Rev. Sci. Instrum. 90, 011101 (2019). [2] A. Auer, B. Eder and F.J. Giessibl, J. Chem. Phys. 159, 174201 (2023).

O 27.2 Tue 10:45 H4

Small change huge effect – Tuning CO2 reduction to Formaldehyde — •Michael Busch — Luleå University of Technology, Luleå, Sweden

CO_2 reduction is a central technology for energy conversion and as access route to basic feedstock for the chemical industry. Unfortunately, its potential is still hindered by high overpotentials and low selectivity towards post-CO products. So far, post-CO products can only be accessed reliably either through Cu catalysts or selected single atom catalysts like metal phthalocyanines. Recent experiments indicate, that Co phthalocyanine is even able to form formaldehyde in good yields.[1]

Building on these experiments, we will explore the underlying origin of this surprising finding using density functional theory (DFT) computations.[1,2] Our results indicate, that the pure Co phthalocyanine complex does not show any unexpected selectivity. However, upon adjusting potential and pH also the catalyst's protonation state is changed. This minor change in turn shifts the selectivity towards formaldehyde. These surprising insights provide an important puzzle piece for the rational design of improved CO_2 reduction catalysts.

[1] A. Singh, M. Busch, M. Robert et al. *J. Am. Chem. Soc.* **146** (2024) 22129.
[2] R. Khakpour, K. Farshadfar, M. Busch et al. *J. Phys. Chem. C.* **128** (2024) 5867.

O 27.3 Tue 11:00 H4

Quantitative Modeling of the Coordination and Solvation Dynamics of Electrically Charged Solvated Systems via Molecular Dynamics Simulations — •Zhenyu Wang, Mira Todorova, Christoph Freysoldt, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials

Chemical and biological processes in water are influenced by the dynamics of the water solvation shell of ions. Despite progress in understanding ion solvation dynamics, the structural changes in the solvation shell with varying charge states remain underexplored. This study uses atomistic molecular dynamics calculations to investigate the solvation shell of a Na ion, as a prototype model, focusing on changes in water molecule arrangement due to charge variations. Gaussian process regression is used to analyze the reorientation of H_2O molecules as the Na-ion charge is changed from negative to positive. Results show significant effects of the ionic charge on the coordination to neighboring water molecules, which form distinct polyhedral structures, such as tetrahedra, triangles, pyramids, and octahedra. These formed patterns can be effectively characterized by using the H_2O-H_2O distance and H_2O-H_2O-H_2O angle. At the highest positive charge, H_2O molecules form an octahedral configuration, transitioning to pyramidal and triangular bipyramidal structures as the charge decreases. At a neutral charge, the solvation shell reveals maximum dispersion, which transitions into a single cluster at negative charges. This study provides valuable insights into ion solvation behavior and significantly enhances the understanding of ion solvation dynamics in aqueous environments.

O 27.4 Tue 11:15 H4

Field-induced water autoionization in two- and three-dimensions — •Yair Litman and Angelos Michaelides — University of Cambridge, Cambridge, U. K.

The behaviour of water under an electric field critically influences the performance of numerous energy conversion and storage devices and remains a subject of active investigation. Recent experiments have shown that at electric field strengths exceeding 10^8V/Å, the water dissociation reaction ($2H_2O \rightleftharpoons H_3O^+ + OH^-$) is significantly accelerated, a phenomenon known as the (secondary) Wien effect [1].

In this work, we employ the modern theory of polarization to perform (periodic) *ab initio* molecular dynamics simulations of water under external electric fields, both in bulk and under nanoconfinement. Our simulations reveal that electric fields facilitate the water dissociation reaction by not only reducing the enthalpy of the reaction but also by increasing the corresponding entropic contribution. Furthermore, we demonstrate that geometric constraints imposed by a 2D confinement can amplify the field-induced reaction rates. These findings highlight the importance of entropy changes in field-induced aqueous reactions and propose nanoconfinement as a promising avenue for enhancing the efficiency of electrocatalytic reactions.

[1] J. Cai. *et al.*, Nat. Commun **13**, 5776 (2022)

O 27.5 Tue 11:30 H4

Predicting Electrocatalytic Urea Synthesis Using a Two-dimensional Descriptor — •Amy Wuttke and Alexander Bagger — Department of Physics, Technical University of Denmark

Electrochemical synthesis routes offer a sustainable alternative to conventional fossil-based processes for producing chemical commodities. An example is the crucial fertiliser urea ($CO(NH_2)_2$), that can be synthesised by co-reducing CO_2 and nitrite (NO_2^-) on transition metal surfaces [1]. This reaction also serves as a model system for studying electrochemical CN-coupling. However, achieving high selectivity toward urea remains a significant challenge due to the complexity of competing reaction pathways.

In this talk, a predictive framework for urea selectivity is presented based on adsorption energies as descriptors without referring to a full reaction mechanism [2]. Using Density Functional Theory, we calculated 10 adsorption energies as potential descriptors on 19 transition metal surfaces. Through Principal Component Analysis, this high-dimensional dataset is reduced to two key descriptors: *H and *O adsorption energies. Our findings demonstrate that these descriptors effectively explain urea selectivity on transition metals, offering a simplified approach to guide catalyst design.

[1] M. Shibata et al., J. Electrochem. Soc., 145(2), 595-600 (1998), doi: [10.1149/1.1838309].
[2] A. Wuttke and A. Bagger, Predicting Electrocatalytic Urea Synthesis Using a Two-Dimensional Descriptor, in review. Research Square Preprint, Jul. 17, 2024, doi: [10.21203/rs.3.rs-4749942/v1].

O 27.6 Tue 11:45 H4

Effect of water on the diffusion barriers of S_{ad} on Cu(100) and Ag(100): DFT-calculations — •Falk Wendorff, Sönke Buttenschön, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Diffusion of adatoms at the electrochemical interface is affected by the electrolyte in various ways. Here we focus on the effect of pure water at the pzc on the diffusion barriers within Transition State Theory. Due to the dynamics of the H_2O molecules in liquid water the process is complicated to simulate. We have investigated the diffusion of a sulfur adatom on Cu(100) and Ag(100) surfaces in the presence of water using explicit water molecules in DFT simulations. The calculations have been carried out with PWscf and PWneb from Quantum ESPRESSO [1]. We have started from initial water layers generated by the Water Structure Creator by Dávila López *et al.* [2] and performed subsequent MD simulations of the water molecules at fixed sulfur and substrate positions. The results show that water lowers the diffusion barriers of sulfur on the metal surfaces compared to the interface versus vacuum.

Funded by the Deutsche Forschungsgemeinschaft project 504552981.

[1] P. Giannozzi *et al.*, J. Phys. Condens. Matter **21**, 395502 (2009), *ibid.* **29**, 465901 (2017).

[2] A. C. Dávila López *et al.*, J. Chem. Phys. **155**, 194702 (2021).

Invited Talk O 27.7 Tue 12:00 H4

Ultrafast electrochemistry beyond the RC time constant — •Yujin Tong — Universität Duisburg-Essen, Duisburg

Electrochemistry relies on charge transfer, which can occur on time scales from femtoseconds to seconds or longer. Traditional electrochemical detection methods are limited in their ability to study ultrafast processes such as solvent reorganization and electron tunneling. This presentation focuses on the advancements and challenges in ultrafast electrochemistry, specifically exploring processes occurring on timescales shorter than the RC time constant. Traditional electrochemical processes have typically been studied over longer timescales, often constrained by limitations in mass diffusion and hardware capabilities. However, recent developments in ultrafast laser technology and femtochemistry have enabled the observation of rapid processes with femto /pico second time resolution at electrochemical interfaces, such as ultrafast potential relaxation in electric double layers and the dynamics of solvated electrons [1-3]. [1] G. Zwaschka, F. Lapointe, R. K. Campen, Y. Tong, Curr. Opin. Electrochem. 29, 100813 (2021) [2] F. Lapointe, M. Wolf, R. K. Campen, Y. Tong, J. Am. Chem. Soc. 142, 18619-18627 (2020) [3] Z. Huang, M. Bridger, O. A. Naranjo-Montoya, A. Tarasevitch, U. Bovensiepen, Y. Tong, R. K. Campen, arXiv preprint, doi: 10.48550/arXiv.2304.06684 (2023)

O 27.8 Tue 12:30 H4

Deciphering the Capacitance of the Pt(111)/Water Interface: A Micro- to Mesoscopic Investigation by AIMD and Implicit Solvation — •Lang Li, Karsten Reuter, and Nicolas Hörmann — Fritz-Haber-Institut der MPG, Berlin

We use *ab initio* molecular dynamics simulations based on density-functional theory to revisit the enigmatic capacitance peak of the electrified Pt(111)/water interface around the potential of zero charge. We demonstrate that counterbalancing the electronic excess charges with partially charged hydrogen atoms constitutes a computationally efficient approach to converged interfacial water structures. The thus enabled detailed analysis of the interfacial water response clarifies that the peak in the capacitance is predominantly due to structural reorientation, although its magnitude is significantly increased by strong internal electronic polarization, also known as charge transfer (CT). We find that CT is more complex than previously thought, resulting from the interplay between chemisorbed water and depolarization effects from surrounding water. Finally, we demonstrate that quantitative agreement with the experimental peak can be achieved through inclusion of the interfacial response into an implicit solvent model for the extended part of the double layer. This suggests that such models can accurately reproduce screened interfacial fields as a function of potential, despite their notoriously small native capacitance. [1] L. Li, K. Reuter, N. G. Hörmann, accepted by ACS Electrochem.

O 27.9 Tue 12:45 H4

Efficient periodic density functional theory calculations of charged molecules and surfaces using Coulomb kernel truncation — •Sudarshan Vijay[1], Martin Schlipf[1], Henrique Miranda[1], Ferenc Karsai[1], Martijn Marsman[1], and Georg Kresse[1,2] — [1]VASP Software GmbH, Berggasse 21, 1090 Vienna, Austria — [2]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

Density functional theory (DFT) calculations of charged molecules and surfaces are critical to applications in electro-catalysis. Periodic DFT implementations such as the Vienna ab-initio Simulation Package (VASP) compute the electrostatic potential under 3D periodic boundary conditions, which necessitates charge neutrality. In this work, I will discuss our recent implementation of 0D and 2D periodic boundary conditions. Unlike 3D boundary conditions, our implementation allows for calculations of charged molecules and surfaces. We implement these boundary conditions using the Coulomb kernel truncation method. We compute the electrostatic potential under 0D and 2D boundary conditions by selectively subtracting unwanted long range interactions from the potential under 3D boundary conditions, removing the need for performing any Fourier transforms in padded supercells. To illustrate the computational efficiency of our method, we perform large supercell calculations of the formation energy of a charged chlorine defect on an NaCl(001) surface and perform long time-scale molecular dynamics simulations on an Au(211) | water electrode-electrolyte interface.

O 28: Graphene: Electronic Structure and Excitations (joint session O/HL)

Time: Tuesday 10:30–12:15 Location: H6

O 28.1 Tue 10:30 H6

Doping of epitaxial graphene by proximitized 2D quantum islands — •Julian Koch[1], Sergii Sologub[1,2], Chitran Ghosal[1], Dorothee Boesler[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainerstr. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The effects of 2D quantum islands on the transport properties of monolayer graphene/SiC(0001) were investigated by magnetotransport. Two types of adsorbates are compared, Bi(110) and Pb(111) islands with average coverages of up to 3.6 bilayers (BL) and 3 monolayers (ML), respectively. The analysis is supported by structural investigations using SPA-LEED and STM. The doping behaviour of both materials is fundamentally different. In the case of Bi, the carrier concentration determined from the SdH oscillations remains at 1×10^{13} cm^{-2} independent of the Bi coverage, although photoemission spectroscopy revealed a strong doping of the graphene by Bi [1]. This strongly indicates a highly anisotropic carrier concentration across the surface and is confirmed by a positive, temperature independent contribution to the magnetoresistivity. The Bi islands rather behave as antidots and reduce the charge carrier mobility slightly from around 2250 cm^2/(Vs) for MLG to 1920 cm^2/(Vs) at 2.4 BL Bi. In contrast, there are no signs of an anisotropic carrier concentration or mobility when Pb is adsorbed. The electron concentration increases uniformly by approximately 5×10^{11} ML^{-1}cm^{-2}. The mobility is reduced from around 1400 cm^2/(Vs) for MLG to 1200 cm^2/(Vs) at 3 ML Pb.

[1] Gierz et al. *Nano Lett.* **8**, 12, 4603 (2008)

O 28.2 Tue 10:45 H6

Photocurrent control in a graphene-based Floquet topological insulator — •Weizhe Li[1], Daniel Lesko[1], Tobias Weitz[1], Simon Wittigschlager[1], Christian Heide[1,2], Ofer Neufeld[3], and Peter Hommelhoff[1,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Haifa, Israel — [4]Department Physik, Ludwig-Maximilians-Universität München (LMU), 80799 München

Topological insulators offer unique opportunities for novel electronics and quantum phenomena. However, intrinsic material limitations often restrict their applications and practical implementation. A circularly-polarized laser pusle can generate topologically non-trivial non-equilibrium states known as Floquet topological insulators (FTIs) which host a variety of topological phenomena. Floquet engineering with strong optical fields opens routes to optically tunable band structures and devices for petahertz electronics.

Here we demonstrate coherent control of photocurrents in light-dressed graphene. Circularly-polarized laser pulses dress the graphene into an FTI, and phase-locked second harmonic pulses drive electrons in the FTI. This approach allows us to measure all-optical anomalous Hall currents and photocurrent circular dichroism, which put FTIs on equal footing with equilibrium topological insulators. The coherent control of photocurrents in graphene-based FTI connects optics tools to condensed matter physics.

O 28.3 Tue 11:00 H6

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], Philip Schädlich[1], Bharti Matta[3], Philipp Rosenzweig[3], Kathrin Küster[3], Ulrich Starke[3], Thomas Seyller[1], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Two-dimensional materials such as graphene are fascinating because they combine unique mechanical and electronic properties. The next level of complexity, however, comprises the assembly of various stacked 2D materials to generate structures with desired properties. Intercalation of epitaxial graphene systems is an effective method to tailor the electronic, optical, and transport properties of graphene while keeping its honeycomb lattice on SiC. Furthermore, intercalation facilitates the synthesis of otherwise unstable 2D layers. A wide range of elements have been used as intercalants below a graphene sheet, forming often well-defined heterobilayers with different functionalities. In particular, intercalation of heavy elements such as Pb and Bi are specially promising since they can introduce additional effects such as spin-orbit coupling to the electron gas of graphene and Rashba spin polarization. Using first-principles methods, we investigate the modifications in the electronic structure of epitaxial graphene due to proximity effects induced by intercalation.

O 28.4 Tue 11:15 H6

Accelerated Exploration of Defective Graphene Superstructures — •Benedict Saunders[1], Lukas Hörmann[1,2], and Reinhard Maurer[1,2] — [1]Department of Chemistry, University of Warwick, Coventry — [2]Department of Physics, University of Warwick, Coventry

Graphene has been meticulously studied due to its remarkable mechanical, electrical, and thermal properties. It is well documented that introducing various dopants and defects to the lattice can be used to tune the material's properties for a specific application, such as in electronics, sensors, or catalysis. In order to design graphene with specific properties, one must achieve precise control over the composition and concentration of defects. This requires a fundamental understanding of the stability of defects and their interaction in a given superstructure. We present a comprehensive method for exploring the configurational space of defective 2D superstructures. We have extended the SAMPLE structure search code to defects in 2D materials. SAMPLE uses Bayesian learning based on sparse Density Functional Theory data for structure exploration. We show the capabilities of our approach for a proof-of-principle application on free-standing graphene with heteroatom defects. Finally, we use the SAMPLE code to gain physical insight into the interactions between these defects, paving the way for effective and rational growth models of topologically designed defective graphene.

O 28.5 Tue 11:30 H6

Polymorphism of a two-dimensional Pb layer underneath charge neutral graphene on SiC — •Markus Gruschwitz, Sergii Sologub, Zamin Mamiyev, Chitran Ghosal, and Christoph Tegenkamp — Institut für Physik, TU Chemnitz, Germany

Since the first studies on graphene, researchers strive to implement its unique properties in industrial relevant processes. The intercalation of epitaxially grown buffer layers on SiC results in high quality, quasi-freestanding graphene, which allows the electronic properties to be modified by varying the intercalants and their arrangement. Pb recently sparked a great interest by reliably providing almost perfectly charge neutral graphene. The Pb layer effectively screens the substrate induced doping. In a novel approach using differential phase contrast in cross-sectional scanning transmission electron microscopy we reveal their vertical charge density distribution. Surprisingly, the charge neutrality is robust against variations in the Pb interface reconstruction. Depending on the preparation, a Pb monolayer often reconstructed in two coexisting phases, the so-called stripe [1] or bubble [2] phase. Intercalated multilayers reveal a similar striped phase arising from two twisted plumbene layers [3]. Here we combine structural investigations by scanning tunneling microscopy and high-resolution low-energy electron diffraction in a model of flexibly arranged grain boundaries releasing lattice mismatch stress.

[1] Materials 14, 7706 (2021), [2] Adv. Mater. Interfaces 10, 2300471 (2023), [3] Phys. Rev. Lett. 129, 116802 (2022)

O 28.6 Tue 11:45 H6

Facet-dependent growth and properties of graphene on Al_2O_3 surfaces from first principles — •Armin Sahinovic and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The direct growth of graphene on functional substrates such as sapphire (Al_2O_3) enables the use in optoelectronic devices without the necessity of sample transfer. We explore the role of the surface orientation of Al_2O_3 on the growth of graphene [1] using density functional theory. The stoichiometric terminations are identified as the most stable surface terminations of the C-, R- and A-plane facets in the framework of *ab initio* thermodynamics. Next, we consider the adsorption of carbon atoms on the different surface facets, varying their position and concentration. The adsorption energy shows the weakest binding at the R-plane and the most favorable at the A-plane. We associate this with the more unsaturated oxygen bonds at the A-plane compared to the R- and C-plane. Furthermore, we explore the graphene - Al_2O_3 interaction and its impact on the electronic properties of graphene. Our results provide a deeper understanding of the role of the surface facets of the substrate in the scalable graphene growth on Al_2O_3.

Funding by GRK2803 2D-MATURE (Project P4) and computational time at the supercomputers MagnitUDE and AmplitUDE are gratefully acknowledged

[1] Y. Ueda et al., Appl. Phys. Lett. 1, 115 (1), 013103 (2019)

O 28.7 Tue 12:00 H6

Enhanced light-matter interactions via Sn nanoislands on epitaxial graphene — •Zamin Mamiyev, Narmina Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Surface-enhanced Raman scattering (SERS) is an advanced technique for coupling light into quasiparticle excitations in low-dimensional materials, offering promising applications in trace detection, enhanced light-matter interactions, photonic energy harvesting, and catalytic processes. Recent studies in this field have focused on integrating noble metal nanostructures with graphene.

In this study, we investigate a novel SERS platform utilizing tin (Sn) nanoislands to enhance graphene Raman signals by up to two orders of magnitude. We examine the SERS performance on Sn-intercalated charge-neutral and intrinsically doped epitaxial monolayer graphene (MLG) on SiC(0001). The increase in the Raman cross-section and enhanced intensity is accompanied by spectral shifts, which may be correlated with the localized surface plasmons (LSPs) of Sn nanoislands as well as dynamic charge transfer between the Sn particles and graphene. This dynamic charge redistribution, primarily determined by the doping concentration and interface interactions, enables control over the SERS response. Additionally, plasmonic and thermalization-induced carrier density propagation across μm ranges indicates efficient coupling between localized and propagating plasmons.

[1] Z. Mamiyev and C. Tegenkamp, 2D Materials. 11, 025013 (2024)
[2] Z. Mamiyev and C. Tegenkamp, Surf. & Int. 34, 102304 (2022)

O 29: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

O 29.1 Tue 10:30 H8

Line-moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) — •Romana Ganser, Muthu P. T. Masilamani, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

We present angle-resolved photoemission spectroscopy (ARPES) measurements on tunable one-dimensional moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) [1]. In this model system, the moiré structure can be tuned almost continuously in contrast to hardly controllable twist angles in bilayer van-der-Waals heterostructures [2]. We experimentally observe moiré minibands and band gaps of 120 - 170 meV suggesting sizable superlattice potentials. By comparing the experimental data to simple model calculations, we analyze the local character of the potential. This provides important information of interface hybridization effects on the band structure, which may not be limited to the system at hand but rather a broad range of moiré interfaces.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020).
[2] Lisi, S. et al. Nat. Phys. 17, 189-193 (2021).

O 29.2 Tue 10:45 H8

Photoemission Time Scale Determination: the Effect of Crystal Dimensionality and Electronic Correlation — •Fei Guo[1], Dmitrii Usanov[2], Eduardo B. Guedes[2], Mauro Fanciulli[3], Arnaud Magrez[1], Michele Puppin[1], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, 95031, France

Spin polarization of photoelectrons from spin-degenerate dispersive initial states originates from the interference of multiple photoemission channels, measuring the spin polarization with spin- and angle-resolved photoemission spectroscopy

(SARPES) allows the estimation of the phases of the interfering channels, and hence the Eisenbud-Wigner-Smith (EWS) time delay of photoemission, which is the amount of time required by the photoelectron to evolve into a free particle final state. While not directly measurable for solid-state photoemission, this time scale has been measured for gaseous photoionization, which is generally in the attosecond (10^-18s) range.

We present investigations with multiple materials of different properties, and by comparing with previous studies, we propose a relationship between the EWS time delay, electronic correlation mechanism, and dimensionality.

O 29.3 Tue 11:00 H8

Disorder effects in the Band Structure of Transition Metal Dichalcogenide alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W) — •Sarath Sasi[1], Aki Pulkkinen[1], Laurent Nicolaï[1], Raphaël Salazar[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

Recent advances in materials synthesis have enabled the creation of 2D TMDC alloys, which offer unique opportunities for tailoring electronic and optoelectronic properties to meet diverse application demands.[1].This study investigates the band structure evolution of $A_xB_{1-x}Se_2$ alloys (A, B = Cr, Mo, W) across varying composition fractions (x). Using the Coherent Potential Approximation (CPA)[2], which accurately models scattering in disordered systems, theoretical calculations were performed with the *SPR-KKR* package[3]. Results reveal that some of the TMDC alloys maintain their band structures without significant disorder effects. Angle-Resolved Photoemission Spectroscopy (ARPES) measurements align closely with one-step model photoemission calculations, confirming theoretical predictions. These insights provide a foundation for tailoring electronic properties, advancing their applicability in next-generation devices.

[1] Zhou, J., Lin, J., Huang, X., et al. Nature, 556, 355-359 (2018).

[2] Soven, P., Phys. Rev., 156, 809(1967).

[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 29.4 Tue 11:15 H8

Unveiling Doping-Induced Electronic Modifications in Antiferromagnetic MPS_3 van der Waals Materials — •Till Willershausen[1], Jonah Elias Nitschke[1], Patrick Merisescu[2], David Janas[1], Lasse Sternemann[1], Michele Capra[1], Mira Arndt[1], Valentin Mischke[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Bath University

Antiferromagnetic van der Waals (vdW) materials, with scalability to monolayer thickness, semiconducting properties, and intrinsic antiferromagnetic ordering, hold promise for spintronic and quantum technology applications. We investigate alkali metal doping effects on the MPS_3 family (M = Mn, Ni, Co, Fe) of 2D antiferromagnetic vdW materials, revealing doping-induced changes in their electronic structure. X-ray Photoelectron Spectroscopy (XPS) shows shifts in oxidation states in $NiPS_3$, $CoPS_3$, and $FePS_3$, while $MnPS_3$ displays no significant changes, indicating distinct charge transfer. Further investigation with Angle-Resolved Photoelectron Spectroscopy (ARPES) reveals new alkali-metal induced bands appearing above the previous valence band maximum. This analysis highlights doping-induced modifications and contrasts in transition metal behavior in MPS_3, providing insights into doping mechanisms and electronic tunability.

O 29.5 Tue 11:30 H8

Enhanced electron-phonon coupling in few-layer $MoTe_2$ from micro-ARPES — •Thomas P. van Waas[1], Julia Issing[2], Marco Gibertini[3], Christophe Berthod[2], Anna Tamai[2], Felix Baumberger[2,4], and Samuel Poncé[1,5] — [1]European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland — [5]WEL Research Institute, Belgium

Bulk orthorhombic T_d-$MoTe_2$ is a type-II Weyl semimetal with a superconducting critical temperature of T_c = 0.1 K. Transport measurements show a monotonic increase in T_c as the thickness of multilayer $MoTe_2$ is reduced, reaching T_c = 7.6 K in the monolayer. We investigate photoemission kinks in the electron pocket of exfoliated mono- bi-, and trilayer $MoTe_2$ from micro-focused angle-resolved photoemission spectroscopy. We use a custom code to quantify the electron self-energy $\Sigma_n(E)$ for a parabolic non-interacting dispersion, and obtain from $\Sigma_n(E)$ the Eliashberg spectral function $\alpha^2F_n(\omega)$ using the maximum entropy method. We find two dominant phonon modes in $\alpha^2F_n(\omega)$ for the mono- and trilayer, with a large enhancement of the lower-frequency phonon mode in the former. We also provide tentative results for the bilayer, where quantification is more challenging due to a small splitting of the electronic bands.

O 29.6 Tue 11:45 H8

Electronic structure of V-doped WSe_2 — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics represents a promising and energy-efficient alternative to conventional electronics, with significant potential applications, e.g., in areas such as classical and quantum computing. The vanadium-doped layered transition metal dichalcogenide 2H-WSe_2 is a promising candidate to fulfill the desired properties as a room-temperature magnetic semiconductor with gating tunability. Here, we present a comprehensive electronic structure study of chemical vapor transport-grown pristine and V-doped WSe_2 by soft X-ray, VUV and 11eV-laser ARPES, highlighting the influence of a low V doping concentration on the electronic structure of WSe_2.

O 29.7 Tue 12:00 H8

Unraveling magnetic ordering in a van der Waals correlated material — Tommaso Pincelli[1,2], •Tania Mukherjee[1,2], Lawson Lloyd[2], Shuo Dong[2,3], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], and Ralph Ernstorfer[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society, 14195 Berlin, Germany — [3]Beijing National Laboratory for Condensed Matter Physics, China

Layered van der Waals (vdW) materials offer a compelling platform to investigate various emergent quantum properties in low dimensions. Fe_3GeTe_2 (FGT), a vdW ferromagnetic metal, is well-known for exhibiting exotic phenomena, ranging from skyrmion formation to heavy fermion behavior. However, an understanding of the magnetic ordering, a key feature for spintronic applications, still remains elusive in this material. In particular, the interplay of both local magnetic moments and an itinerant mechanism in the formation of ferromagnetic ordering in FGT, a non-f-electron correlated system, remains to be clarified. Using time- and angle-resolved photoemission spectroscopy (trARPES) and first-principles calculations, we provide evidence for an ordering mechanism in FGT by observing a pronounced reduction in the Stoner exchange gap. This stands in contrast to earlier temperature-dependent ARPES studies of the electronic structure of FGT, which favored a localized excitation model over the weak-coupling itinerant picture. We also observe the impact of phononic excitations which further confirm our findings.

O 29.8 Tue 12:15 H8

Spin structure of the unoccupied surface state at AgTe/Ag(111) — •Carolin Benfer, Marcel Holtmann, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

The AgTe/Ag(111) surface alloy has recently been investigated as a model system for the role of orbital angular momentum in the formation of spin effects in the electronic structure [1]. Two p-like surface states were detected in ARPES measurements, one shows a Rashba-type spin splitting, while the other one does not. This behavior is attributed to the symmetries of the orbital wave functions of the electrons. For the unoccupied states a third surface state has been predicted. Following the symmetry arguments given in [1], a Rashba-type spin splitting of the state is expected.

We use inverse photoemission (IPE) to directly study the unoccupied state of the surface alloy. Low-energy electron diffraction and scanning tunneling microscopy measurements confirm a homogeneous monolayer film of the surface alloy, which is growing in a honeycomb structure. Angle-resolved IPE measurements detect the predicted surface state with free electron-like dispersion. Spin-resolved IPE measurements reveal a Rashba-type spin structure.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

O 29.9 Tue 12:30 H8

Orbital mixing as key mechanism for ferromagnetism in van der Waals CrI3 — •Alessandro De Vita[1,2], Srdjan Stavrič[3], Roberto Sant[4], Nicholas B. Brookes[4], Giancarlo Panaccione[5], Silvia Picozzi[3], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17 Juni 135, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]Consiglio Nazionale delle Ricerche CNR-SPIN, c/o Università degli Studi G. D'Annunzio, 66100 Chieti, Italy — [4]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [5]Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, km 163.5, I-34149 Trieste, Italy

Van der Waals ferromagnets constitute a versatile platform where exotic quantum states can be realized; among them, CrI3 is a prototypical and widely studied 2D ferromagnet, with promising applications in spin- and orbitronics. Despite that, key information on its electronic occupation and stabilization of the magnetic configuration are missing. By means of complementary absorption and

photoemission spectroscopies, and density functional theory calculations, we give a description of the orbital character of bulk CrI3, and demonstrate that the emergence of ferromagnetism in this material is underpinned by the orbital mixing between I p and Cr eg states. Our results have clear impact on the understanding of how microscopic interactions at the orbital level stabilize ordered states in van der Waals ferromagnets.

O 29.10 Tue 12:45 H8

Resonant Photoemission Studies of Transition Metal Sulfides and Selenides — •Yashasvi Mehra[1,2,3], Samuel Beaulieu[4], Mauro Faniculli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Aki I.O. Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Universite de Bordeaux CNRS CEA, CELIA, UMR5107, F33405 Talence, France

By performing resonant ARPES measurements and SPR-KKR photoemission calculations on Transition Metal Selenide, Sulfide and the Vanadium intercalated NbS2 systems, we study the interplay between different decay mechanisms in resonant conditions, radiation-less Raman Auger and Classical Auger emissions. Through a method proposed by Cini and Sawatzky we can determine the on-site Coulomb interaction per element in some cases. On the theoretical front the calculations are performed using the SPR-KKR method, which is based on one-step model, that incorporates the effect of all matrix elements which accounts for the photoemission process. Furthermore, we analyze calculated ARPES, XAS, element and orbital resolved band structure underlining agreement with experimental results and helping with its interpretation.

O 30: Surface Magnetism

Time: Tuesday 10:30–12:45 Location: H11

O 30.1 Tue 10:30 H11

Spin-polarized chiral edge modes in the topological nodal-point superconductor Mn/Ta(110) — •Felix Zahner[1], Felix Nickel[2], Roberto Lo Conte[3], Tim Drevelow[2], Roland Wiesendanger[1], Stefan Heinze[2], and Kirsten von Bergmann[1] — [1]University of Hamburg, Germany — [2]University of Kiel, Germany — [3]University of Groningen, The Netherlands

Topological superconducting phases in magnet-superconductor hybrid (MSH) - systems have been investigated recently due to their potential applications in quantum devices. Zero-energy states and chiral edge modes have previously been observed in ferromagnetic 1D [1] and 2D [2] MSH systems. In a 2D antiferromagnet (AFM) MSH and a spin spiral MSH system, gapless topological nodal-point superconducting (TNPSC) phases have been observed [3, 4].

Using scanning tunnelling microscopy/spectroscopy (STM/S), we investigate the mono- and bilayers on a Ta(110) surface. Both exhibit local AFM order and tight-binding calculations indicate that both host a TNPSC phase. Interestingly, we observe edge modes not only at the boundaries between the TNPSC and the topologically trivial superconducting substrate, but also at specific boundaries between these two AFM systems of Mn mono- and bilayer. Our spin-polarized STM measurements reveal a significant spin-polarization of this edge mode, which we discuss based on the tight-binding results.

[1] Nadj-Perge, S. et al., Science 346, 602 (2014). [2] Palacio-Morales, A. et al., Sci. Adv. 5, eaav6600 (2019). [3] Bazarnik, M. et al, Nat Commun 14, 614 (2023). [4] Brüning, R. et al., arXiv:2405.14673.

O 30.2 Tue 10:45 H11

Interaction of chiral molecules with magnetic substrates: An ongoing DFT puzzle — •Nicolae Atodiresei — Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich

A challenging puzzle in surface science that has to be solved is the interplay between electron spin and molecular chirality. As an example, the interaction of chiral helical aromatic molecules with magnetic surfaces leads to an enantioselective adsorption, i.e. molecules of opposite handedness would preferentially adsorb to ferromagnetic islands with opposite magnetization [1]. In this talk, I will discuss how state-of-the-art spin-resolved *ab initio* simulations based on density functional theory calculations support and guide the interpretation of scanning tunneling microscopy experiments performed on the adsorption of heptahelicene molecule onto ferromagnetic cobalt islands.

The author acknowledges funding from CRC 1238 of the Deutsche Forschungsgemeinschaft and computing time granted on the supercomputer JURECA at Forschungszentrum Jülich.

[1] Mohammad Reza Safari et al., Adv. Mater. **36**, 2308666 (2024)

O 30.3 Tue 11:00 H11

Spin-lattice relaxation of nitrogen-vacancy centers in nanodiamonds on conducting and non-conducting surfaces — •Izidor Benedičič[1], Yuri Tanuma[1], Bastien Anézo[1,2], Žiga Gosar[1,3], and Denis Arčon[1,3] — [1]Department of Condensed Matter Physics, Jožef Stefan Institute, Ljubljana, Slovenia — [2]Institut des Matériaux de Nantes Jean Rouxel (IMN), Nantes University, Nantes, France — [3]Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia

Nitrogen-vacancy (NV) centers in diamond are versatile probes for the detection of both static magnetic fields and magnetic fluctuations. While single-NV sensors are very capable, they suffer from high cost and experimental complexity. Nanodiamonds with embedded NV ensembles offer a promising low-cost alternative, however, their application in solid-state physics has been largely overlooked. Here, we investigate the use of nanodiamonds for measuring the electrical conductivity of substrates. We measured the temperature dependence of longitudinal relaxation time T_1 of NV centres in nanodiamonds on glass and gold substrates. We find that T_1 is determined both by phononic relaxation processes and the coupling to the magnetic moments at the surface. All samples show a stretched exponential relaxation, hinting at a significant distribution of relaxation processes. The theoretical models show the intrinsic distribution is too wide to reliably detect coupling to electronic states even of very good conductors. Our results hint at the limitations of nanodiamonds for measurements of transport properties in condensed matter systems.

O 30.4 Tue 11:15 H11

Imaging in-plane magnetic domains using magnetic circular dichroism in darkfield laser PEEM — •David Huber[1], Friederike E. Wührl[1], Frank O. Schumann[2], and Wolf Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Max-Planck-Insitut für Mikrostrukturphyisk, Halle

Magnetic circular dichroism (MCD) in threshold photoelectron emission microscopy (PEEM) enables imaging of magnetic domains at the nanoscale. Utilizing femtosecond (fs) laser excitation in a laboratory setting offers a significant advantage in terms of temporal resolution compared to more commonly used X-ray MCD measurements. However, this poses new challenges with respect to in-plane magnetization, given the previously reported low domain contrast [1, 2].

In this contribution we show that symmetry breaking and photoelectron filtering in momentum and energy help to overcome these challenges. Using this methodology, we obtain MCD contrast for in-plane domains of 11 nm Fe(001)-(1 × 1)-O on MgO(001) using both continuous wave and fs laser excitation at normal incidence and compare these results to a Fe(001)-(1 × 1)-O single crystal in PEEM and μARPES.

[1] Marx et al., PRL **84**, 5888 (2000).
[2] Nakagawa et al. PRL **96**, 237402 (2006).

Invited Talk O 30.5 Tue 11:30 H11

Resonant molecular transitions in femtosecond second harmonic generation spectroscopy of Fe-porphyrin/Cu(001) — •Andrea Eschenlohr[1], Rui Shi[2], Jinghao Chen[1], Ping Zhou[1], Uwe Bovensiepen[1], Wolfgang Hübner[2], and Georg Lefkidis[2] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Department of Physics, RPTU, Box 3049, 67653 Kaiserslautern, Germany

Metal-organic molecular adsorbates on metallic surfaces are potential future materials for (spin-)electronics applications, provided that the molecule-substrate interaction can be analyzed and manipulated in a targeted manner. By combining interface-sensitive optical second harmonic generation (SHG) spectroscopy experiments and electronic structure calculations using coupled cluster methods including optical excitations on iron-octaethylporphyrin (FeOEP) adsorbed on Cu(001), we find that the SHG response of FeOEP/Cu(001) is modified at 2.15-2.35 eV fundamental photon energy compared to the bare Cu(001) surface. We conclude a resonantly enhanced SHG by molecular transitions, which results from a strong charge-transfer character of the molecule-substrate interaction [1]. Pump-probe SHG reveals a markedly slower relaxation time at this resonance, indicating an increased lifetime of the optically induced state compared to the bare Cu(001) surface, which will be discussed in the context of charge transfer dynamics.

[1] Eschenlohr et al., arXiv:2409.09801

O 30.6 Tue 12:00 H11

Single-layer magnetism of epitaxial NiBr2 and FeBr2 on NbSe2 — •Sebastien E. Hadjadj[1], Carmen Gonzalez-Orellana[2], Adriana Candia[3], Pierluigi Gargiani[4], Matthias Muntwiler[5], Jan Dreiser[5], Jorge Lobo[3], Celia Rogero[2], and Maxim Ilyn[2] — [1]Materials Physics Center (MPC), Donostia, Spain — [2]Centro de Fisica de Materiales (CSIC/UPV-EHU), Donostia-San Sebastian, Spain — [3]Instituto de Nanociencia y Materiales de Aragon (INMA),Zaragoza, Spain — [4]ALBA Synchrotron Light Source, Barcelona, Spain — [5]Paul Scherrer Institut, Villigen, Switzerland

Two-dimensional metal dihalides exhibit promising magnetic and electronic properties. Over the past years, the research focus on novel 2D magnetic materials has shifted to transition metal di-halides (TMDH). Recent reports have shown that the first layer of Br-based TMDH grown on Au(111) behaves structurally and magnetically differently from the second layer [1-2]. Here we report the first layer growth of NiBr2 and FeBr2 on NbSe2, which shows no signs of decomposition as observed for NiBr2 on Au(111) and shows unaffected stable magnetic properties ranging from monolayer to multilayer. The structural characterization of the samples revealed a strong temperature dependence in the resulting island growth and appearence of the moiré pattern. XMCD measurements probed magnetic ordering down to the 2D limit, which is in agreement with the literature values. In the case of FeBr2 a strong reduction of the spin magnetic moment has been observed. [1] Djuro Bikaljevic et al., ACS Nano, 15, 14985, (2021) [2] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847-9856, (2023)

O 30.7 Tue 12:15 H11

Graphene intercalated Eu on magnetic surfaces a DFT study — •Gustav Bihlmayer[1], Polina M. Sheverdyaeva[2], Matteo Jugovac[3], Luisa Ferrari[4], Frederico Mazzola[5], Paolo Perna[6], Nicolae Atodiresei[1], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich — [2]CNR-ISM, 34149 Trieste, Italy — [3]Elettra Sincrotrone Trieste, 34149 Trieste, Italy — [4]CNR-ISM, 00133 Roma, Italy — [5]CNR-IOM, 34149 Trieste, Italy — [6]IMDEA Nanociencia, Campus de Cantoblanco, 28049, Madrid, Spain

Europium can be intercalated between graphene and magnetic surfaces like Co(0001) or Ni(111) forming a $\sqrt{3} \times \sqrt{3}$ layer [1]. The doping of graphene can create a pronounced flat band at the Fermi level and the interaction of the $4f$ states with the π band of graphene leads to spin-selective hybridization and opening of the Dirac cone with interesting consequences for edge channels [2]. This system can be compared to Eu on-top of a graphene covered Co substrate, that changes the magnetic coupling between the lanthanide and the substrate [3] and modifies the graphene's interaction with the $4f$ states. Further stacking combinations are possible and will be discussed [4].

We acknowledge funding from the FLAG-ERA grant SOgrapMEM and from CRC 1238 of the Deutsche Forschungsgemeinschaft.

[1] F. Huttmann et al., Phys. Rev. B **95**, 075427 (2017) [2] P. M. Sheverdyaeva et al., Phys. Rev. Lett. **132**, 266401 (2024) [3] M. Jugovac et al., Adv. Mater. **35**, 2301441 (2023) [4] M. Jugovac et al., Carbon **230**, 119666 (2024)

O 30.8 Tue 12:30 H11

Emergence of Ferromagnetism in 3d-4f Hetero-Bimetallic Surface-Architectures — •Massine Kelai[1], Serim Jeon[1], Dasom Choi[1], Corina Urdaniz[1], Pierre Josse[1], Jaehyun Lee[1], Stefano Reale[1], Yongwoo Kim[1], Weibin Li[2], Pierluigi Gargiani[2], Woo-Suk Noh[3], Dominik Lungerich[4], Christoph Wolf[1], Fabio Donati[1], and Lucinao Colazzo[1] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]ALBA Synchrotron Light Source, 08290 Catalonia, Spain — [3]MPPC/CPM, Max Planck POSTECH, Pohang 37673, Republic of Korea — [4]Center for Nanomedicine, Institute for Basic Science (IBS), 50 Yonsei-ro, Seodaemun-gu, 03722 Seoul, Republic of Korea

Surface-confined metal-organic coordination networks (SMONs) are emerging platforms for designing tunable low-dimensional nanostructures, with 3d-4f hetero-bimetallic systems being promising candidates for high-density memory and qubit applications. However, the mechanisms underlying their formation and magnetic interactions remain largely unexplored. Here, we investigate a novel 3d-4f SMON, Dy-FeTCPP (TCPP = 5,10,15,20-(tetra-4-cyanophenyl)porphyrin), formed on Au(111) via on-surface chemical reaction pathways. Using X-ray absorption spectroscopy, magnetic circular dichroism, scanning tunneling spectroscopy, and density functional theory, we show that lanthanide insertion induces strong substrate-mediated ferromagnetic coupling between 3d units, driven by porphyrin core deformation upon Dy-cyanophenyl bonding. This work advances the understanding of SMONs, paving the way for scalable quantum devices on surfaces.

O 31: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Tuesday 10:30–13:00 Location: H24

O 31.1 Tue 10:30 H24

AMAN-SPM: Autonomous Molecular and Atomic Nanofabrication via SPM — •Bernhard Ramsauer[1], Qigang Zhong[2], Bettina Könighofer[3], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, 8010, Austria — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, 215006, China — [3]Institute of Applied Information Processing and Communications, Graz University of Technology, Graz, 8010, Austria

The precise manipulation of individual molecules and atoms using scanning probe microscopy (SPM) offers transformative possibilities for nanofabrication. Yet the inherently stochastic nature at the nanoscale and the labour-intensive process of building nanostructures contains significant challenges. In this contribution, we introduce AMAN-SPM, a tool that integrates reinforcement learning and automation to revolutionize the on-surface synthesis process.

AMAN-SPM employs dedicated reinforcement learning agents to optimize the manipulation parameters, which allows for precise positioning, reorientation, and the controlled breaking and formation of molecular bonds. Coupled with machine vision and path-planning algorithms, this system autonomously constructs nanostructures, eliminating the need for human intervention.

Beyond fabrication, AMAN-SPM enhances real-time data acquisition and analysis, providing detailed physical insights into molecular interactions. This establishes a foundation for scalable nanostructures with tailored properties.

O 31.2 Tue 10:45 H24

Sliding friction over covalent bonds increases with bond order — Shinjae Nam[1], Lukas Hörmann[2,3], Oliver Gretz[1], Oliver T. Hofmann[2], Franz J. Giessibl[1], and •Alfred J. Weymouth[1] — [1]Universität Regensburg, Regensburg, Deutschland — [2]TU Graz, Graz, Österreich — [3]The University of Warwick, Warwick, U.K.

Friction is governed by atomic-scale interactions, yet we lack a complete understanding of its working at this length scale. To address this, we reduce one sliding surface to the limit of a single atom and measure sliding friction with lateral force microscopy over single bonds. We examine islands of PTCDA on Cu(111), which present a rich variety of covalent and hydrogen bonds. There is a large

variety in the maximum energy dissipation over different covalent bonds. The maximum energy dissipation over hydrogen bonds has similar values, although energy dissipation over hydrogen bonds is observed at lower heights than over covalent bonds. With DFT-based simulations and a machine-learning model, we determine that larger bond order is correlated to higher sliding friction.

Invited Talk O 31.3 Tue 11:00 H24

Single molecule machines on surface — •Francesca Moresco — TU Dresden. Germany

Scanning tunneling microscopy is a unique experimental technique to control the motion of a single molecule, testing the boundary between classical and quantum movement and making thermodynamics at the scale of a single molecule accessible to experimental investigation. Under the tip of a scanning tunneling microscope, inelastic tunneling electrons or local electric fields can produce controlled rotations or translations of a single adsorbed molecule, while thermal excitation can modify the energy barrier for motion. In this talk, we will discuss the controlled rotation and translation of asymmetric and chiral model structures adsorbed on the Au(111) surface.

O 31.4 Tue 11:30 H24

How to measure cones of reaction for single-molecule collisions — •Matthew J. Timm[1], Stefan Hecht[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Austria — [2]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Collisions between reagents are necessary for bond formation, and hence fundamental to reaction. The collision outcome depends on the collision energy, which must be enough to overcome the reaction barrier, and on the collision geometry, which modifies the height of this barrier. The collision geometry is defined by the relative orientation of reagents at the point of collision and on the miss-distance between their centers of mass (termed the impact parameter). Selection of impact parameter has been demonstrated for on-surface reactions with a 'surface-molecular-beam' of CF2 'projectiles', formed by dissociation of chemisorbed CF3 molecules with a scanning tunneling microscope tip, aimed along Cu-rows of the Cu(110) surface toward chemisorbed 'targets' [1]. However, control over the relative orientation of the target has remained elusive. Here a singly-debrominated molecular species (BTFyl) is chosen as a target, as it adopts many possible adsorption alignments relative to the incoming CF2 projectile. This allows simultaneous control over both the impact parameter and reagent orientation, thus allowing an unprecedented ability to map how collision geometry contributes to collision outcome.

[1] Anggara, K.; Leung, L.; Timm, M. J.; Hu, Z.; Polanyi, J. C.; Faraday Discuss., 2019, 214, 89-103.

O 31.5 Tue 11:45 H24

Friction Anisotropy in the Sliding Motion of PMMA microsphere on Rippled PVS Surface — •Ebru Cihan[1], Hesam Khaksar[2], Kevin Lubig[3], Stephan Gräf[3], Frank A. Müller[3], and Enrico Gnecco[1,2] — [1]TU Dresden — [2]Jagiellonian University — [3]Friedrich Schiller University Jena

The sliding motion of an elastically driven polymethyl methacrylate (PMMA) microsphere on a rippled polyvinyl siloxane (PVS) surface (laser-induced periodic surface structures LIPSS) was investigated for different values of normal load, scan velocity and temperature. The morphologies of the PMMA spheres and modified PVS surfaces were observed to be geometrically convoluted in AFM topographies recorded simultaneously with friction measurements. The spheres were rubbed both parallel and perpendicular to the LIPSS, and the resulting friction was found to be nearly constant, exhibiting a stick-slip behavior over time. This result differs from the reverse stick-slip observed in friction characterizations with similar PMMA microspheres on harder periodic surfaces, such as wedge-shaped silicon gratings [Trib. Lett. 67, 2019] and rippled stainless steel [Appl. Mater. Interfaces 15, 2023]. In both scanning cases, the friction force was found to increase linearly with increasing load, consistent with the increase in contact area expected from Persson contact theory. Furthermore, friction was observed to increase logarithmically with velocity, and to decrease with increasing temperature in accordance with Eyring's reaction rate theory. The stability of this sample system suggests its possible application as a basic unit for artificial tactile sensors.

O 31.6 Tue 12:00 H24

Electronic and phononic frictional dissipation in single-molecule dynamics at CO-decorated tips — •Lukas Hörmann and Reinhard J. Maurer — University of Warwick, Coventry, UK

Friction causes significant energy loss in any moving mechanical device. As the miniaturisation of devices reaches the quantum limit, so do dynamical dissipation processes. Fundamentally quantum mechanical mechanisms govern friction at the nanoscale. We account for all relevant quantum mechanical effects, such as charge transfer, or van der Waals interactions, by employing density functional theory, machine learning, and non-adiabatic molecular dynamics. Using this approach, we investigate friction energy dissipation at the natural limit of singular atoms. This allows us to explore how the local electronic and geometric structure affects the dissipation of mechanical energy, where electron-phonon and phonon-phonon coupling give rise to electronic and phononic excitations. Focusing on the example of CO on various Cu surface geometries, we find that electron-phonon coupling strongly depends on the local electronic density of states, while the geometric structure significantly influences phonon-phonon coupling. Our findings quantitatively agree with experiment. Finally, we present a mechanistic interpretation of our findings that provides insights into the underlying physics of single-molecule dynamics on surfaces.

O 31.7 Tue 12:15 H24

Manipulation of a CO molecule on a copper surface with lateral force microscopy — •Norio Okabayashi[1], Alfred. J. Weymouth[2], Shinjae Nam[2], Sophia Schweiss[2], Thomas Frederiksen[3,4], and Franz J. Giessibl[2] — [1]School of Mathematics and Physics, Kanazawa University — [2]Institute of Experimental and Applied Physics, University of Regensburg — [3]Donostia International Physics Center — [4]IKERBASQUE, Basque Foundation for Science

The manipulation of a single molecule on a surface by scanning tunneling microscopy (STM) and atomic force microscopy (AFM) has been intensively studied because of its relation to friction research. Recently, we have studied the manipulation process for CO on a Cu(110) surface with AFM, STM and density functional theory [1][2]. We found that at the tip height for the beginning of the manipulation, CO is manipulated from the top to the neighboring top site by transiently using the bridge site, but for lower tip heights, the manipulation occurs from the top to the bridge site and then from the bridge to the neighboring top site. Here, we have extended our experimental technique by incorporating lateral force microscopy, where the tip oscillates laterally [3], to directly observe the energy dissipation during manipulation. Indeed, the observation confirms the validity of our previous claim. This result paves the way for quantitative evaluation of dynamic friction during manipulation. [1] N. Okabayashi, T. Frederiksen, A. Liebig, F. J. Giessibl, Phys. Rev. Lett. 131 (2023) 148001, [2] N. Okabayashi, T. Frederiksen, A. Liebig, F. J. Giessibl, Phys. Rev. B 108 (2023) 165401, [3] A. J. Weymouth, J. Phys.: Condens. Matter 29 (2017).

O 31.8 Tue 12:30 H24

Intermediates, reactions and products of cyclocarbons — •Leo Gross[1], Fabian Paschke[1], Florian Albrecht[1], Yueze Gao[2], Igor Roncevic[3], and Harry L. Anderson[2] — [1]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [2]Oxford University, Chemistry Research Laboratory, Oxford, UK — [3]University of Manchester, Department of Chemistry, Manchester, UK

Cyclocarbons, molecular allotropes of carbon in which all carbon atoms are two-fold coordinated, have been synthesized on surface using tip-induced chemistry [1-4], and the formation of larger cyclocarbons by dimerization of precursors was shown [4]. This presentation will focus on products, reactions and intermediates of cyclocarbons, generated by tip-induced chemistry on ultrathin NaCl layers and characterized by STM and AFM with CO-functionalized tips.

[1] K. Kaiser et al., Science, 365, 1299-1301 (2019)
[2] L. Sun et al., Nature, 623, 972-976 (2023)
[3] Y. Gao et al. Nature, 623, 977-981 (2023)
[4] F. Albrecht et al. Science, 384, 677-682 (2024)

O 31.9 Tue 12:45 H24

Temperature Induced Ring-Opening Polymerization Reaction for the Synthesis of Carbon Nanoribbons: Strain Influence on the On-surface Synthesis Using [6], [8]-, and [10]Cycloparaphenylenes — •Miguel Wiche[1], Qigang Zhong[2], Daniel Kohrs[1], Qitang Fan[3], J. Michael Gottfried[4], Daniel Ebeling[1], Hermann A. Wegner[1], and André Schirmeisen[1] — [1]Justus Liebig University Giessen, Germany — [2]Soochow University, Suzhou, China — [3]University of Science and Technology of China, Hefei, China — [4]Philipps University Marburg, Germany

As the on-surface synthesis is an emerging reseach field, there is a lack of general understanding of reaction mechanisms, compared to conven- tional organic synthesis. Therefore, comprehensive research studies are required to figure out basic principles in the on-surface reaction mech- anisms of organic molecules. In this work we investigate the strain influence of a set of Cycloparaphenylenes (CPP) in the temperature in- duced on-surface synthesis of biphenylene and graphene nanoribbons, using a strain induced ring opening polymerization (ROP) reaction. The decisive step of the polymerization, the ring opening, is found to strongly depend on the ring size and strain of the CPP molecules. Our work suggests that using smaller, highly strained rings, instead of rings with increasing number of phenyl units facilitates the ROP and nanoribbon formation.

O 32: Heterogeneous Catalysis I

Time: Tuesday 10:30–12:45 Location: H25

O 32.1 Tue 10:30 H25

Stability and reactivity of metal clusters on rutile TiO_2(110) under near-ambient pressure conditions — •Marina Isabel de la Higuera Domingo, Florian Kraushofer, Matthias Krinninger, Friedrich Esch, and Barbara A. J. Lechner — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, 85748 Garching, Germany

Clusters are widely recognized for their unique performance in heterogeneous catalysis as they exhibit discrete electronic states that lead to strongly size-dependent catalytic properties [1]. However, their application in industrial processes is often limited by their instability under reaction conditions. At elevated temperatures, clusters tend to sinter, which reduces their surface area and alters their catalytic behavior.

Reducible oxides, such as titania (TiO_2), are effective supports to stabilize clusters and tune their activity through encapsulation induced by the strong metal-support interaction (SMSI) [2]. While metal nanoparticles on TiO_2 are well-studied, much less is known about the dynamics of clusters, in particular at high temperatures and pressures. In the present work, we employ near-ambient pressure scanning tunneling microscopy (NAP-STM) to study the effect of reducing and oxidizing atmospheres on metal clusters on rutile TiO_2(110). We will also delve into the influence of the sample stoichiometry on its reactivity at different ambient conditions [3].

[1] A.Beck, et al. Nat.Commun. 2020, 3220.
[2] S.J. Tauster. Acc. Chem. Res. 1987, 389-394
[3] F. Kraushofer, et al. Nanoscale 2024, 17825-17837

O 32.2 Tue 10:45 H25

Structural and chemical analysis of coexisting hexagoal and monoclinic phases of samarium oxide on Cu(111) — •Björn Riedel, lars Buss, Raquel Sanchez-Barquilla, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

The absence of in-depth spectroscopic and structural studies on model systems leads to a knowledge gap in understanding how the structure of samaria influences its chemical behavior. A multi-method approach has been employed to investigate the Cu(111)-supported Sm_2O_3 surface with high structural and chemical sensitivity by using low-energy electron microscopy (LEEM) in combination with X-ray absorption photoemission electron microscopy (XAS-PEEM) and other complementary methods such as micro-spot low-energy electron diffraction (μLEED) and X-ray photoelectron spectroscopy (XPS). Our measurements show the phase coexistence of small hexagonal A-Sm_2O_3(0001) islands and monoclinic B-Sm_2O_3(100) rectangular-shaped islands with different rotated rectangular domains. Furthermore, the redox properties of both Sm_2O_3 phases were studied by exposing the system to reducing (H_2) and oxidizing (CO_2) conditions, indicating a face-dependent reduction and oxidation behavior. Moreover, the monoclinic Sm_2O_3(100) islands appear less stable as they change to the hexagonal phase during annealing. These results indicate a highly dynamic system that can easily be adjusted by adapting the growth conditions, such as growth temperature and oxygen partial pressure.

O 32.3 Tue 11:00 H25

Digital Catalysis: Accelerated Discovery through Human in the Loop — •Charles Pare[1], Aybike Terzi[2], Christian Kunkel[1], Frederik Rüther[2], Frederic Felsen[1], Robert Baumgarten[2], Esteban Gioria[2], Raoul Naumann d'Alnoncourt[2], Christoph Scheurer[1], Frank Rosowski[2,3], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]BasCat - UniCat BASF JointLab, Berlin — [3]BASF SE, Catalysis Research, Ludwigshafen

Catalyst promoters often form key components of stable and well-performing industrial heterogeneous catalysts. Yet, today's industrial catalysts often only benefit from one or two promoters. This can often be traced back to the laborious empirical research required to identify promising formulations that jointly act to improve catalyst performance. To overcome such hurdles, we implemented an accelerated catalyst discovery approach by globally exploring a large catalyst design space using only a limited number of experiments. Its pillars are an efficient Design-of-Experiment (DoE) planning, a fast parallelized testing protocol and an iterative incorporation of experimental feedback. New and competitive promoter chemistries for the non-oxidative propane dehydrogenation to propylene over supported Pt were discovered in a limited experimental campaign. The results show the potential of iterative DoE strategies for the data-efficient knowledge-generation and optimization in complex, academically and industrially relevant catalytic systems.

O 32.4 Tue 11:15 H25

Synergistic effect of oxygen and water on the environmental reactivity of 2D layered GeAs — •Luca Persichetti[1], Giacomo Giorgi[2], Luca Lozzi[3], Maurizio Passacantando[3], Fabrice Bournel[4], Jean-Jacques Gallet[4], and Luca Camilli[1] — [1]University of Rome Tor Vergata, Italy — [2]University of Perugia, Italy; — [3]University of L'Aquila, Italy — [4]Sorbonne Université, CNRS, Paris, France

GeAs is a fascinating 2D material with compelling properties stemming from its intrinsic anisotropy. However, it reacts strongly with air, forming a Ge-oxide layer that affects its optoelectronic properties, such as contact resistance and refractive index. Investigating GeAs reactivity under realistic device conditions, including humid O2 and water exposure, is therefore crucial.

At the TEMPO beamline of Soleil, near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) was employed to study GeAs in the presence of oxygen and water. Results showed minimal reactivity with dry O2 and de-aerated water, while slight humidity (Rw = 0.5%, T = 20°C) in an O2 atmosphere significantly enhanced reactivity. Density functional theory calculations confirmed this synergistic effect, revealing a highly exothermic formation energy for the simultaneous chemisorption of O2 and H2O, compared to the adsorption of each molecule individually.

This research was supported by EU-funded MUR programs PRIN2022 ATYPICAL (2022JW8LHZ) and PRIN 2022-PNRR SPIGA (P2022LXNYN).

O 32.5 Tue 11:30 H25

A comparative DFT+U study of the oxygen evolution reaction at infinite-layer, brownmillerite and perovskite nickelates — •Achim Füngerlings and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen, Duisburg, Germany

We present a detailed DFT+U investigation of rare earth nickelates $R\mathrm{NiO}_x$(001), R = La, Nd; x = 2, 2.5, 3 as anode materials for the oxygen evolution reaction (OER). In these materials the Ni reaction sites at the surface exhibit different coordination, i.e. square-planar in the infinite layer (x = 2, IL), fivefold coordination at the (001) perovskite surface (x = 3) and both fourfold and fivefold coordination at the brownmillerite surface (x = 2.5, BM). Voltammetry measurements find a lower onset potential for the catalytically much more active infinite layer compared to the perovskite counterparts.[1] Moreover, x-ray diffraction measurements suggest that the infinite layer gradually transform into brownmillerite during OER.[1] Our calculations confirm a lower overpotential for both the infinite layer and brownmillerite phases over the respective perovskite phase. The results reveal that the oxidation state of surface Ni has a more profound effect on the catalytic activity than the coordination number, with Ni^{2+} (found at the IL and the fivefold coordinated BM site) leading to lower (0.53, 0.56 V for R=La; x=2, 2.5) and Ni^{3+} (at the fourfold coordinated site in BM and the fivefold coordinated site at the perovskite surface) leading to higher overpotentials (0.67, 0.68 V for R=La; x=2.5, 3).

[1] M. Osada, A. Füngerlings, R. Pentcheva, and H. Y. Hwang, to be submitted.

O 32.6 Tue 11:45 H25

How does lanthanum promote cobalt for ammonia synthesis in Co/La_2O_3 catalysts? — •Clara C. Aletsee, Lau H. Wandall, Ke Zhang, Oliver Christensen, Jens K. Nørskov, and Ib Chorkendorff — Physics, Technical University of Denmark

The interest in developing catalysts for ammonia synthesis, operating under milder reaction conditions than the Haber-Bosch process, has increased in the last decades. Cobalt, typically unreactive, can be activated for ammonia synthesis through the addition of lanthanum in metallic or oxidized form.[1,2] To obtain a comprehensive understanding of the promotion mechanism, we investigate the ammonia formation over Co particles on La_2O_3 by combining experiments with theory. For this, we synthesized defined model catalyst, consisting of mass-selected Co nanoparticles, deposited on La_2O_3 films generated by magnetron sputtering. Their catalytic activity was tested at 1 bar and 350-500°C in a UHV-compatible reaction cell.[3] Catalyst states before and after reaction were analyzed by X-ray photoelectron spectroscopy and low-energy ion scattering. The results, combined with previous findings on the Co/LaN system,[2] suggest that the reaction proceeds on La-promoted Co steps due to spin-mediated effects supported by theoretical calculations.[4] We further demonstrate that the activity of the Co/La_2O_3 can be partially recovered after air exposure.

[1] S. I. Miyahara *et al.*, *ACS Omega* 7, 24452-24460 (2022). [2] K. Zhang *et al.*, *Science* 383, 1357-1363 (2024). [3] K. Zhang *et al.*, *Rev. Sci. Instrum.* 94, 114102 (2023). [4] A. Cao *et al.*, *Nat. Commun.* 13, 2382 (2022).

O 32.7 Tue 12:00 H25

U-Ce charge transfer in epitaxial $Ce_{1-x}U_xO_2$ films grown on Ru(0001): consequences for thermochemical water splitting — •Carlos Morales[1], Rudi Tschammer[1], Thomas Gouder[2], Hicham Idriss[3], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology, Cottbus, Germany — [2]European Commission, Joint Research Centre (JRC), Karlsruhe, Germany — [3]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Reducible metal oxides are crucial in applications like catalysis and solar energy conversion. Among these, cerium oxide (CeO_2) stands out for its stability and activity, yet its reduction requires high energy. Ceria doping or mixing with other elements has been proven successful in increasing the conversion from Ce^{4+} to Ce^{3+}. Uranium cations are the most suitable candidates: substituting a fraction of Ce^{4+} by U^{4+} results in a charge transfer that promotes the formation of Ce^{3+} and U^{5+} states. The fundamental study of the charge transfer process requires model systems, as heat and mass transfer limitations are largely absent compared to polycrystalline powders. By in-situ X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED), we explored the redox properties and structural stability of epitaxial (111)-oriented $Ce_{1-x}U_xO_2$ on Ru(0001). The as-grown films, prepared by reactive direct current sputtering from metallic targets, show a high Ce^{4+} to Ce^{3+} conversion, reversible upon reducing-oxidizing cycles. The experimental results are discussed in the light of density function theory (DFT) calculations.

O 32.8 Tue 12:15 H25

Accelerating Surface Adsorption Energy Prediction with Machine Learning Foundation Models — •Karlo Sovic[1,2] and Johannes T. Margraf[2] — [1]University of Zagreb Faculty of Science — [2]University of Bayreuth

Determining the adsorption energies of molecular adsorbates on surfaces is critically important in heterogeneous catalysis, as well as in many other fields of materials science and chemistry. Understanding the nature and strength of adsorbate-surface interaction leads to a more rational design of efficient catalysts and improvements in their performance. While accurate first-principles calculations have brought about a revolutionary advance in our ability to predict properties and design materials *in silico*, high computational costs and poor scaling limit their application in exploring complex real-world materials. Machine-learning interatomic potentials offer a solution to this materials exploration problem. In particular, the recent emergence of pre-trained foundation models offers a data-efficient route to obtain accurate models via fine-tuning. To showcase their efficiency and performance, extensive computational research has been conducted using a fine-tuned MACE-MP-0 model to study the adsorption of glycerol on various metallic surfaces in the gas phase. This talk will present the methodology for investigating the global minima of complex adsorbate molecules on various metal surfaces, determining their respective adsorption energies, and exploring various reaction mechanisms on adsorbent's surface through computational approaches.

O 32.9 Tue 12:30 H25

Role of Co-Catalyst Loading in the Photoreforming of Tertiary Alcohols at Ambient Pressure on Titania P25 — •Paula Neumann, Clara Aletsee, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Efficient semiconductor photocatalysts are usually modified with a so-called co-catalyst, a metal particle which is commonly assumed to promote charge separation, but whose exact role remains elusive. To elucidate the influence of platinum particles loaded onto a titania powder catalyst we investigated the photoconversion of tertiary alcohols in our gas phase-photoreactor at ambient conditions. Different to its usual interpretation but in accordance with UHV studies we show that the co-catalyst facilitates the recombination of surface hydrogen. Thereby, a second reaction pathway is opened up where a C-C coupling product forms on the titania surface. Hence, identifying the mechanistics of alcohol photochemistry is not only providing insights into hydrogen formation but it also sheds light onto complex alkyl coupling reactions.

O 33: Poster Graphene: Electronic Structure and Excitations

Time: Tuesday 13:30–15:30 Location: P3

O 33.1 Tue 13:30 P3

Reversible transition between (10×10) **and** (11×11) **phases of Pb intercalated EG on 6H/SiC(0001)** — •Sergii Sologub[1,2], Markus Gruschwitz[2], Bharti Matta[3], Andres David Pena Unigarro[2], Philipp Rosenzweig[3], Sibylle Gemming[2], Kathrin Küster[3], Ulrich Starke[3], and Christoph Tegenkamp[2] — [1]Institute of Physics, NAS of Ukraine, Kyiv — [2]Institut für Physik, TU Chemnitz, Chemnitz — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

Epitaxial graphene (EG) obtained by intercalation of a buffer layer on 6H/SiC(0001) with Pb atoms is the subject of intensive experimental and theoretical studies due to its charge neutrality, the band gap opening and proximity superconductivity. The hallmark of Pb-intercalated EG is the formation of diffraction spots with (10×10) or (11×11) periodicity in the high-resolution LEED patterns. The correlation between these phases and corresponding microstructure, i.e. "striped" and "bubble" Pb intercalated phases, were examined by STM and by dark field imaging in a photoemission electron microscope. We have also established a recipe to reversibly switch between the (10×10) and (11×11) structures. In addition, the ratio of areas occupied by these coexisting phases could be estimated from the intensity ratio of second order LEED spots. Importantly, the degree and ease of intercalation strongly depends on the defect density of the initial buffer layer. The transformation between the different phases can be rationalized by the low diffusion barrier of Pb on SiC observed by density functional calculations.

O 33.2 Tue 13:30 P3

Confinement-mediated intercalation of metals in epitaxial graphene: Unlocking room temperature intercalation — •Kathrin Küster[1], Stefan Wundrack[2,3], Markus Gruschwitz[4], Sawani Datta[1], Bharti Matta[1], Teresa Tschirner[2], Marius Eckert[2,3], Rainer Stosch[2], Christoph Tegenkamp[4], Ulrich Starke[1], Klaus Pierz[2], and Andrey Bakin[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Physikalisch-Technische Bundesanstalt, Braunschweig — [3]Institut für Halbleitertechnik - TU-Braunschweig — [4]Institut für Physik, TU Chemnitz

Intercalation of materials underneath epitaxial graphene is an effective way to tune graphene's properties but also to stabilize otherwise unstable 2D materials. Usually, this procedure requires extreme conditions like ultra-high vacuum and elevated temperatures often above 400 °C. Within the DFG research unit FOR 5242 we also investigate alternative routes of intercalation under more accessible conditions. Here, we report on the intercalation of Ga and In under monolayer graphene at ambient conditions. A multi-technique approach combining spectro-microscopy techniques with density functional theory calculations gives detailed insights into the intercalation pathways and the diffusion of the intercalants at the interface between graphene and the SiC substrate. It is evident that the intercalated atoms are strongly bound to the topography of the SiC terraces during their diffusion and exhibit anomalies in their diffusion behavior. The monolayer graphene is transformed into a decoupled bilayer upon intercalation and the intercalated materials develop their own metallic 2D electronic structure.

O 33.3 Tue 13:30 P3

Proximity-effects in epitaxial graphene: recent highlights of our Research Unit FOR5242 — S. Gemming[1], I. Gierz-Pehla[2], K. Küster[3], K. Pierz[4], Th. Seyller[1], U. Starke[3], •C. Tegenkamp[1], T. Wehling[5], and M. Wenderoth[6] — [1]Institut für Physik, TU Chemnitz — [2]Institut für Experimentelle und Angewandte Physik, U Regensburg — [3]Institut für Festkörperforschung, MPI Stuttgart — [4]Physikalisch-Technische Bundesanstalt, Braunschweig — [5]Institut für Theoretische Physik, U Hamburg — [6]IV. Physikalische Institut, U Göttingen

Proximity effects in low dimensional electron gases are essential for the design of new quantum materials with tailored electronic, magnetic and optical properties. A recent example is superconductivity in twisted bilayer graphene. Our Research Unit FOR 5242 studies the influence of proximity-induced spin-orbit interaction (SOI), electronic correlations as well as local electric fields on 2D electron gases, using epitaxial graphene (EG) on SiC substrates as a model system. EG is known for its flexible functionalization schemes including intercalation and adsorption, enabling control of the doping level, hybridization effects, and the strength of the Coulomb interaction. Here, we highlight a few of our recent results including (1) the use of EG for quantum Hall resistance standards, (2) SOI in graphene induced by 2D Pb layers, (3) Mott-Hubbard physics realized by the intercalation of Sn and Si, (4) many-body effects in extremely doped EG and (5) novel 2D interface layers. For further details see www.for5242.de

O 33.4 Tue 13:30 P3

Quasi-freestanding monolayer graphene achieved by Pb intercalation — •S Wolff[1], P Schädlich[1], A D Peña Unigarro[1], B Matta[2], G Ghosal[1], F Schölzel[1], P Richter[1], M Hutter[3], M Stettner[3], K Küster[2], C Kumpf[3], S Gemming[1], U Starke[2], C Tegenkamp[1], and T Seyller[1] — [1]Institute of Physics, TU Chemnitz — [2]MPI für Festkörperforschung, Stuttgart — [3]Peter Grünberg Institut, Forschungszentrum Jülich

Intercalation is a promising approach for tailoring the electronic structure of epitaxial graphene on SiC. Beyond that, it enables the formation of otherwise

unstable 2D phases of elements and opens a route to study the interplay between the two 2D materials and the substrate. We have studied the Pb intercalation process under the buffer layer in detail using low-energy electron microscopy (LEEM), photoelectron spectroscopy (PES), scanning tunneling microscopy (STM), density functional theory calculations (DFT) and X-ray standing wave (XSW). LEEM is used to monitor the intercalation process at different intercalation temperatures, resulting in either a (1 × 1) symmetry or in a (10 × 10) superstructure of the Pb atoms. These findings can be supported by angle-resolved PES and STM. Experiments indicate, in agreement with DFT, different filling of the Pb bands depending on the SiC polytype. Furthermore, XSW was used to determine the interlayer distances, revealing covalent bonding of the intercalant to the substrate and van der Waals bonding to graphene.

O 33.5 Tue 13:30 P3

Liquid metal intercalation of epitaxial graphene Hall bar devices on SiC — •Marc Bothe[1,2], Stefan Wundrack[1,2], Teresa Tschirner[1], Markus Gruschwitz[3], Yefei Yin[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Christoph Tegenkamp[3], Hans Werner Schumacher[1], and Andrey Bakin[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig — [3]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany

Epitaxial graphene grown on SiC is a promising platform for metal intercalation, enabling the investigation of proximity effects. Metal intercalation relies on the controlled introduction of lattice defect densities in monolayer graphene, achieved through plasma treatment. This is followed by liquid metal intercalation, during which atoms diffuse through lattice defects and propagate beneath the graphene. However, the use of metal intercalated graphene samples for device fabrication presents two challenges. First, solvents used for lithography often lead to metal deintercalation. Second, lattice defects in graphene compromise the structural and electronic integrity of the graphene device. We use an alternative strategy that combines lithography with metal intercalation through predefined channels. Initial measurements of Hall bar structures intercalated with gallium show superconducting behavior, demonstrating the potential of this approach for advanced device applications.

O 33.6 Tue 13:30 P3

Mesoscopic Lateral Intercalation Dynamics of Tin Between the Epitaxial Buffer Layer of Graphene and SiC — •Benno Harling[1], Zamin Mamiyev[2], Christoph Tegenkamp[2], and Martin Wenderoth[1] — [1]IV. Physical Institute, Georg-August-University Göttingen, Germany — [2]Analysis of Solid Surfaces, Nanostructures and Quantum Materials, TU Chemnitz, Germany

Within the challenges of modern electronics, the dynamics of intercalation in layered structures is key for pushing the boundaries of technological limits. Fine-tuned control and a deeper understanding of the intercalation process is needed. Our study focuses on the lateral dynamics of this intercalation process. Whereas penetration of the graphene sheet was already often discussed [1], the lateral atom transport processes according to the mesoscopic landscape of the substrate has been less addressed. Kelvin Probe Force Microscopy (KPFM) was used to investigate an epitaxial graphene buffer layer intercalated with tin. A diffusion edge to the pristine buffer layer can be identified with this method down to the mesoscopic scale below 100 nanometers. On a vicinal surface, we find surface steps as a clear barrier for diffusion. Material transfer over the substrate steps is mediated by a local defect, i.e. local pin-holes. Moreover, we do not observe nucleation on the terrace, but the decoration of the next step by tin. Faster diffusion at the step edges leads to directional growth of the intercalated phase.

Financial support by the DFG within research unit FOR5242 is greatly acknowledged.

[1] Wu et al., Prog. Surf. Sci. 96, 100637, 2021

O 33.7 Tue 13:30 P3

Magnetic MnPc molecules adsorbed on epitaxial graphene — •James Oyuga[1], Nhung Nguyen[1], Uwe Gerstmann[2], Eva Rauls[3], Julian Koch[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]Theoretische Physik, Universität Paderborn, Germany — [3]Department of Mathematics and Physics, University of Stavanger, Norway

Phthalocyanines (Pc) are prototype molecules hosting magnetic ions. When adsorbed on surfaces, the spin state of the molecules is influenced by the substrate. In a combined experimental and theoretical study, we investigated this influence for the case of MnPc molecules adsorbed on monolayer graphene/SiC(0001) using STM, magnetotransport and theoretical DFT modeling. The STM measurements showed that the self-assembly of the MnPc molecules results in an almost defect-free monolayer with a (4×2) unit cell accommodating 8 MnPc molecules. The DFT modeling revealed that the structure and thereby the spin states of the molecules are decisively influenced by the substrate. In the gas phase the MnPc molecules are symmetrically bended with a spin state of $S = 3/2$. However, on an epitaxial graphene monolayer this is changed into an even mixture of flat molecules with an $S = 5/2$ spin state and upward bended molecules with an $S = 3/2$ spin state. This mixture allows for a denser arrangement of the molecules in a (4 × 2) unit cell, that is commensurable with both the graphene layer and the underlying SiC substrate. The impact of such molecular structures towards transport in epitaxial monolayer graphene is quantified by magneto transport experiments analyzing the weak (anti) localization.

O 33.8 Tue 13:30 P3

Intercalation of a condensed 2D-Ag phase within the epitaxial graphene/SiC interface — •Sawani Datta[1], Vibha Reddy[1], Bharti Matta[1], Arpit Jain[2], Kathrin Küster[1], Joshua A. Robinson[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalating 2D materials at the epitaxial graphene (EG)/SiC interface improves their environmental stability, facilitating the use of various ex-situ techniques for their fundamental study and application purposes. In a previous study, we showed that Ag atoms intercalated at the EG/SiC interface form a triangular (1×1) lattice with respect to the SiC and the Ag interlayer is semiconducting [1,2]. Interestingly, intercalating Pb into a previously Ag-intercalated sample results in the complete replacement of Ag by Pb. Subsequently, another round of Ag intercalation can entirely replace Pb, forming a new Ag phase characterized by a 4/3 packing of Ag with respect to the underlying Si layer. Theory suggested the existence of two intercalated 2D material phases also for several other materials [3] and Auger electron spectroscopy mapping indeed shows a higher Ag concentration of the latter Ag phase [4]. In this work, we compare the 2 different Ag phases by low-energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES). This ongoing study is supported by DFG through FOR 5242 and by NSF Grant DMR-2011839. [1] Phys. Rev. B 101, 201407(R) (2020). [2] Phys. Rev. B 105, 235428 (2022). [3] arXiv:2011.01914v1 (2020). [4] 2D Materials 8, 41003 (2021).

O 33.9 Tue 13:30 P3

Scanning tunneling potentiometry methods for intercalated graphene systems — •Tim Güldenpfennig[1], Simeon Bode[2], Markus Gruschwitz[1], Martin Wenderoth[2], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]IV. Physikalisches Institut, Universität Göttingen, Germany

Graphene and graphene-based (hetero-)systems were subjects in a wide range of studies in the past decades revealing their intriguing electronic properties. Epitaxially grown graphene on SiC plays a vital role as a base for electronic application. By intercalating such grown buffer layer with different elements the electronic properties of the decoupled graphene layer can be precisely manipulated. Recently a great interest in the two dimensional intercalant layers arose as well. The latest advance towards intercalation of heavy elements (Pb, Bi, etc.) comes along with new challenges due to defect-dependent intercalation paths. Macro- and mesoscopic transport experiments on these percolated but multi-scale defective intercalated phases become impractical [1].

For transport investigations at the nanometer scale we utilize scanning tunneling potentiometry (STP). In combination with finite element simulations the conductivity of the intercalated phase and the influence of defects can be separated precisely. Two different setups to investigate the transport properties of intercalated graphene systems on nanoscopic scale are presented. One is implemented in a 4pp-STM/SEM setup with the ability to locally apply transverse voltages. The other setup uses an home-built STM for measurements at 6 K with micro-Volt resolution. [1] Phys. Rev. B 109, 245430 (2024)

O 33.10 Tue 13:30 P3

Electronic and structural properties of a Sn Mott phase proximitized to graphene — C. Ghosal[1], •H.-T. Ngo[1], S. Ryee[2], Z. Mamiyev[1], N. Witt[2,3], T. Wehling[2,3], and C. Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz — [2]Institute of Theoretical Physics, U Hamburg — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg

Graphene, renowned for its exceptional electronic and optical properties as a robust 2D material, traditionally lacks electronic correlation effects. Proximity coupling offers a promising method to endow quantum materials with novel properties. In this study, we achieved such a proximity coupling by intercalating Sn between the buffer layer of graphene on SiC(0001). In the $\sqrt{3}$-areas, the Sn-p_z electrons exhibit robust correlation effects manifest as characteristic Hubbard bands analyzed by STS and EELS. Thereby, the system revealed a spatially modulated hybridization between the Dirac and the correlated electrons depending on the Sn sites with respect to the graphene lattice. The DFT and DMFT calculations show excellent agreement regarding the spectral properties. The analyses revealed further that besides the hybridization and Coulomb interaction also the charge transfer plays an important role for electronic state that emerges in these artificial correlated systems.

O 33.11 Tue 13:30 P3

Twisted Bilayer Graphene by Hydrogen Intercalation — •Hao Yin[1,2], Andrei Matetskii[1], Frank Stefan Tautz[1,2], François C. Bocquet[1], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), FZ-Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany

Quasi-free-standing twisted bilayer graphene (TBLG) with a 30° twist angle is achieved on a 6H-SiC(0001) surface via hydrogen intercalation of the zeroth-layer graphene (ZLG). Initially, 0°-rotated monolayer graphene is prepared using the surfactant-mediated epitaxial growth method [PRL **125**, 106102 (2020)]. The processes of hydrogen intercalation and deintercalation were investigated using Low Energy Electron Microscopy (LEEM), with intercalation conducted stepwise, while deintercalation was monitored in real time. Our results provide valuable insights into the mechanisms underlying hydrogen intercalation and deintercalation.

A sharp reaction front was observed, aligned parallel to the step edges, suggesting that hydrogen atoms migrate beneath the ZLG from surface discontinuities, such as step edges or defects.

Deintercalation, taking place 200°C above the intercalation temperature, was significantly faster (within one minute) and occurred uniformly, as indicated by the homogeneous brightness changes in deintercalated regions. This implies a much faster diffusion of H under the TBLG at this temperature, or possibly that H atoms are able to penetrate through the graphene layers.

O 33.12 Tue 13:30 P3

Near-Field Optical spectroscopy of few-layer Graphene's interband resonances to study it's gate-tunable band structures — •Dominique Malik, Lina Jäckering, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

The band structure of few-layer graphene (FLG) defined by the crystallographic stacking order determines its electronic and optical properties. Optical spectroscopy of interband resonances - the excitation of electron transitions between two electronic bands - allows to directly probe the gate-tunable band structure. Within one flake FLG can exist in different stacking orders. However, conventional far-field spectroscopy is diffraction limited and cannot resolve stacking domains below this limit [1]. Recently, with scanning near-field optical microscopy (s-SNOM) the interband resonances of bilayer graphene (BLG) and 4LG have been retrieved [2]. Due to the stacking specific resonance energy, s-SNOM spectroscopy allowed for the identification of stacking domains on the nanometer scale [2]. The local effect of the application of a gate voltage to FLG has not been studied. Here, we present the theoretical foundation to perform near-field optical spectroscopy of interband resonances of gated trilayer and BLG over the energy range from 0.28 to 0.54 eV to gain insights into gate-tunable modifications of their band structures. We layout the design and fabrication of a suitable sample and show initial results. We expect high-resolution s-SNOM measurements could reveal local variations in band gap opening, which are unachievable with far-field techniques. [1] Lui et al. Nano Lett. 11, 1 (2011) [2] Wirth et al. ACS Photonics 8.2 (2021)

O 33.13 Tue 13:30 P3

non-equilibrium carrier dynamics of a graphene - 2D Mott insulator interface — Maria-Elisabeth Federl[1], •Franziska Bergmeier[1], Zamin Mamiyev[2], Niklas Witt[3], Tim Wehling[3], Christoph Tegenkamp[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Technical University Chemnitz — [3]University of Hamburg

Hybridization between localized and itinerant electrons is believed to be responsible for the formation of exotic electronic states including heavy-fermion behaviour or unconventional superconductivity. Confinement heteroepitaxy, where novel 2D structures are stabilized at the interface between epitaxial graphene and SiC substrate, provides a pathway to engineer proximity-coupling between the massless carriers in graphene and the carriers in the underlying layer. We intercalated graphene with Sn, where the $(\sqrt{3}\times\sqrt{3})$R30° phase formed on SiC(0001) is believed to be a Mott insulator [1], and used time- and angle-resolved photoemission spectroscopy (trARPES) as well as density functional theory (DFT) to search for indications of interlayer hybridization that might pave the wave towards the realization of exotic electronic phases.

[1] Phys. Rev. Lett. 114, 247602 (2015)

O 33.14 Tue 13:30 P3

Sequential Intercalation of Epitaxial Graphene with Multiple Elements — •Niels Rösch, Mohammad Elkhawaga, Philip Schädlich, Fabian Göhler, and Thomas Seyller — Chemnitz University of Technology, Institute of Physics, 09126 Chemnitz, Germany

The intercalation of epitaxial graphene on SiC(0001) is a field of research that currently attracts attention. On one hand it provides the possibility to fine-tune the properties of the graphene layer. On the other hand it also is a means to fabricate two-dimensional materials in a confined state [1,2].

In this study we test the possibility to synthesize binary compounds by sequential intercalation of two elements. As test cases we have chosen the topological insulator Bi_2Se_3 [3] and the superconductor FeSe [4]. To that end, Bi or Fe is first intercalated using a deposition and annealing approach. This is followed by an exposure to a selenium-rich atmosphere at elevated temperatures. Samples are characterized by photoelectron spectroscopy and electron diffraction.

[1] Z. Y. Al Balushi et al., Nat. Mater (2016) 1166.
[2] N. Briggs et al., Nat. Mater. 19 (2020) 637.
[3] H. Zhang et al., Nat. Phys. 5 (2009) 438.
[4] J.-F. Ge et al., Nat. Mater. 14 (2014) 285.

O 33.15 Tue 13:30 P3

Free-standing graphene films/membranes — •Leon Lasnig, Lukas Kalkhoff, Steffen Franzka, and Marika Schleberger — Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany

Large-area graphene films are usually grown onto a copper sheet via chemical vapor deposition. The transfer of the graphene to another substrate to this date has been done with the help of polymer films, which leads to impurities and residues. These residues can change the properties of graphene. It is therefore necessary to develop new fabrication protocols to prevent or at least minimize contaminations.

Here we present a new technique for fabricating membranes without the requirement of an PMMA layer. The samples were then transferred on hole substrates with a hole diameter of 150 μm. Since a monolayer is not stable enough to cover the hole, samples with multiple layers were prepared. These were characterized using Raman spectroscopy and an optical profilometer. Raman spectroscopy showed that the samples within the holes are very homogeneous in terms of doping and strain. The lack of D mode in the measured Raman spectra indicates a clean sample. The profilometer revealed that the graphene membranes in the holes have an average hight deviation of only 138 nm.

O 33.16 Tue 13:30 P3

Electronic and structural properties of Bi-intercalated epitaxial graphene on SiC(0001) — Niclas Tilgner[1], Susanne Wolff[1], Andres D. Peña Unigarro[1], Philip Schädlich[1], Fabian Göhler[1], Bharti Matta[2], Philipp Rosenzweig[3], Kathrin Küster[2], Mark Hutter[4], Monja Stettner[4], Hao Yin[4], Serguei Soubatch[4], François C. Bocquet[4], Tien-Lin Lee[5], Christian Kumpf[4], Ulrich Starke[2], Sibylle Gemming[1], and •Thomas Seyller[1] — [1]Institut für Physik, TU Chemnitz — [2]Max Planck Institut für Festkörperforschung, Stuttgart — [3]Physikalisches Institut, Universität Stuttgart — [4]Peter Grünberg Institut, Forschungszentrum Jülich — [5]Diamond Light Source, United Kingdom

The intercalation of epitaxial graphene on SiC(0001) is a research area that currently attracts attention. Not only does it provide the possibility to fine-tune the properties of the graphene layer, it also allows fabricating two-dimensional materials in a confined state. Using a variety of experimental (LEED, LEEM, XPS, ARPES, XSW) and theoretical (DFT) approaches we studied the structural and electronic properties of different intercalated Bi phases that are formed depending on the preparation conditions. While a dense phase with a (1×1) periodicity with respect to SiC(0001) shows metallic properties, a diluted $(\sqrt{3}\times\sqrt{3})R30°$ phase appears insulating. Upon annealing in hydrogen, the latter can be transformed into a layer of bismuthene. However, while the bismuthene is arranged with the same periodicity, DFT calculations suggest that the transition is accompanied by a major structural rearrangement.

O 33.17 Tue 13:30 P3

Transport Properties of Epitaxial Graphene on 4H-SiC(0001) and 6H-SiC(0001) on the Local Scale — •Simeon Bode[1], Benno Harling[1], Teresa Tschirner[2], Klaus Pierz[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

Recent experiments on epitaxial graphene on silicon carbide have shown that transport properties strongly depend on the surface termination of the SiC substrate. Here, we study the impact of the polytype of the substrate SiC on various local properties of Polymer Assisted Sublimation Grown (PASG) graphene. Recently, it has been shown that there are two different surface terminations present at 6H-SiC [1], whereas mainly one surface termination was observed on 4H-SiC. The structural properties are investigated by STM and AFM, whereas electronic properties are extracted from STS data. Local transport measurements using Scanning Tunneling Potentiometry (STP) on 6H-SiC reveal variations in the sheet resistance from terrace to terrace when changing the stacking sequence across a step. On the other hand, the local sheet resistances of neighbouring terraces are very similar if the step height is half of a SiC unit cell, i.e., having the same termination on both sides. PASG graphene on 4H-SiC predominantly exhibits steps of half the unit cell. First data on 4H-SiC indicates that also on this system the sheet resistance is only slightly varying across steps. This work was financially supported by the DFG through the FOR5242. [1] Sinterhauf et al., Nat Commun 11, 555, 2020

O 33.18 Tue 13:30 P3

Growth dynamics of the graphene buffer layer on SiC(0001) grown by polymer-assisted sublimation growth (PASG) — •Julia Guse[1], Teresa Tschirner[1], Stefan Wundrack[1], Kathrin Küster[2], Ulrich Starke[2], Philip Schädlich[3], Thomas Seyller[3], Klaus Pierz[1], and Hans Werner Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]Institut für Physik, TU Chemnitz

Fabrication of two-dimensional (2D) heterostructures using epitaxial graphene on SiC is gaining interest for engineering new electronic material systems. Important for the quality of the epigraphene layer is the 0th graphene layer, the buffer layer, being covalently bonded to the SiC substrate. However, there is still conflicting theoretical and experimental evidence of the structural properties of the buffer layer and its influence on epigraphene. Further, the quality of this buffer layer is not well defined and systematic studies are still lacking. We use an advanced growth technique preventing step bunching and large terrace step heights to achieve high quality buffer layer on millimeter scale. The buffer layer is grown by thermal sublimation in an argon atmosphere and by applying the polymer-assisted sublimation growth (PASG) method. By pretreatment of the SiC substrate which supplies additional carbon during the initial nucleation process the SiC surface is stabilized by rapid buffer layer formation which prevents step bunching. We investigate the growth parameters for homogeneous buffer layer formation and systematically study its growth dynamics.

O 33.19 Tue 13:30 P3

Modeling the intercalation of epitaxial graphene with main group elements from first-principles — Andres D. Peña Unigarro[1], Niklas Witt[2,3], Maria-Elisabeth Federl[4], •Alexander Korn[1], Isabella Gierz[4], Tim Wehling[2], Florian S. Günther[5], and Sibylle Gemming[1,6] — [1]Inst. Physik, TU Chemnitz — [2]Inst. Theoretische Physik, U Hamburg — [3]Theoretische Physik, JMU Würzburg — [4]Inst. Experimentelle und Angewandte Physik, U Regensburg — [5]UNESP, Rio Claro, Brazil — [6]MAIN Center, TU Chemnitz.

Intercalation of epitaxial graphene on silicon carbide (EG) with metallic interlayers opens up a plethora of fascinating physical phenomena, rooted in both spatial confinement and proximity coupling effects. A rich variety of exotic electronic states is obtained by the simultaneous presence of flat and Dirac-like bands with intricate splittings of the spins and pseudospins in EG and the intercalant.

Here, we present first-principles calculations for supercell models, which capture the essential structural and electronic properties of thin intercalation layers in EG. Ordered structures with different interlayer coverages have been studied, which provide distinctly tailored degrees of proximity coupling. Comparing interlayers from the experimentally well-studied main group elements Sn, Pb, and Bi allows distinguishing between isovalent and heterovalent intercalants as well as studying the influence of relativistic effects, in particular spin-orbit coupling (https://www.epigraphene.de/).

O 33.20 Tue 13:30 P3

Influence of doping on non-equilibrium carrier dynamics in graphene — •Leonard Weigl[1], Johannes Gradl[1], Peter Richter[2], Thomas Seyller[2], Camilla Coletti[3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Technical University of Chemnitz, Germany — [3]Instituto Italiano di Tecnologia, Pisa, Italy

The understanding of non-equilibrium charge carrier dynamics in the quasi-relativistic dispersion of graphene is a key ingredient for the design of future ultrafast electronic devices. Despite its crucial importance for device operation, the role of the doping level remains controversial. Here, we use time- and angle-resolved photoemission spectroscopy (tr-ARPES) to study the energy-resolved photo-carrier relaxation in epitaxial graphene for different doping levels. In contrast to previous studies on the same material [1], we find the energy-resolved relaxation times to be independent of doping. We attribute this to the fact that - with increasing doping level - the peak electronic temperature is found to decrease, making the phase space for carrier relaxation doping-independent. Therefore, we speculate that the previously observed differences in carrier dynamics between graphene resting on C- and H-terminated SiC substrates, respectively, originate from the different interfaces to the substrate rather than the doping level. [1] J. C. Johannsen et al., Nano Lett. 15, 326-331 (2014)

O 33.21 Tue 13:30 P3

Hexagons on Rectangles: Epitaxial Graphene on Ru$(10\bar{1}0)$ — •Lars Buss[1], Giovanni Zamborlini[2], Cathy Sulaiman[1], Moritz Ewert[1], Mirko Cinchetti[2], Jens Falta[3], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Germany — [2]Department of Physics, TU Dortmund University, Germany — [3]Institute of Solid State Physics, University of Bremen, Germany

The miniaturization of integrated electronics drives the demand for barrierless interconnects, with graphene-ruthenium structures emerging as promising candidates. We present an *in situ* study of the growth and electronic properties of graphene on rectangular Ru$(10\bar{1}0)$ grown by high-temperature carbon segregation. Using low-energy electron microscopy (LEEM), it is shown that graphene grows preferentially along the $[1\bar{2}10]$ direction, forming micrometer-sized rectangular islands. Microspot low-energy electron diffraction (μLEED) reveals two predominant graphene orientations, rotated by 0° (R0) and 30° (R30), with indications for the formation of graphene nanoribbons in bilayer graphene/Ru$(10\bar{1}0)$. Microspot angle-resolved photoemission spectroscopy (μARPES) shows that the Dirac cones remain intact in bilayer graphene with reduced n-type doping compared to graphene/Ru(0001), indicating a weaker interaction with the Ru$(10\bar{1}0)$ surface. These results highlight the influence of substrate symmetry and interactions on graphene properties and provide insights for engineering graphene beyond hexagonal substrates.

O 34: Poster Solid-Liquid Interfaces: Reactions and Electrochemistry

Time: Tuesday 13:30–15:30 Location: P3

O 34.1 Tue 13:30 P3

Free Energy Calculations of Electrolyte Decomposition Reactions on Lithium Battery Electrodes — •Azad Kirsan and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

For the development of lithium metal batteries (LMBs) it is essential to understand how a stable solid electrolyte interphase (SEI) is formed. Ethylene carbonate (EC), a commonly used electrolyte, plays a critical role in SEI formation through its electrochemical decomposition at the electrode surface. Thus, insights into the mechanism of the decomposition reaction are of crucial importance for understanding the processes that govern SEI composition, structure and stability.

In this work, *ab initio* molecular dynamics simulations using state-of-the-art enhanced sampling methods (metadynamics, umbrella sampling, well-sliced metadynamics [1]) including explicitly the liquid electrolyte were performed in order to unravel the reaction mechanisms of the first steps of the EC dissociation on a Li_2O surface. The trajectories, encompassing more than 1 ns of sampling time, were used to reconstruct the free energy surfaces and obtain activation barriers for the decomposition reaction.

[1] S. Awasthi, V. Kapil, N.N. Nair, J. Comput. Chem. **37** (2016) 1413

O 34.2 Tue 13:30 P3

Optimizing Parameters in Metadynamics Simulations for Free Energy Calculations — •Marlene Sell, Azad Kirsan, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg

The calculation of free energy surfaces (FES) is essential for understanding chemical reactions. Especially the free energy differences between educts, products and possible transition states, as well as the structure of the latter, allow insight into the nature of the reactions. Well-sliced metadynamics (WS-MTD) [1] is a novel method to calculate FES. It combines umbrella sampling and metadynamics in order to speed up the simulations. However, it employs several fine-tuning parameters whose exact influence on the efficiency and accuracy of the results is not yet well understood.

In this study, the FES of the reaction of 1,3-butadiene and ethylene to cyclohexene, the simplest Diels-Alder reaction, was calculated by WS-MTD. This reaction is well studied, both experimentally and theoretically, and could thus be used to compare the influence of the studied parameters. Using FES calculated with different values of the relevant parameters, the free energy differences between the educts, transition state and products were determined in the form of the activation barrier and reaction energy. These were compared to literature values from experimental and other theoretical studies.

[1] S. Awasthi, V. Kapil, N.N. Nair, J. Comput. Chem. **37** (2016) 1413

O 34.3 Tue 13:30 P3

Exploration of the Pt(111)-water interface by high-dimensional neural network potentials — •Daniel Trzewik[1,2], Moritz R. Schäfer[1,2], Alexander L. Knoll[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Detailed insights into solid-liquid interfaces are crucial for understanding many processes in catalysis and electrochemistry. Accurately modeling these interfaces using first-principles methods is computationally very demanding, which strongly restricts the complexity of the systems that can be studied. Machine learning potentials now can provide an efficient alternative with almost no loss in accuracy. In this study, high-dimensional neural network potentials (HDNNPs)

are employed to investigate the Pt(111)-water interface in detail. After training to DFT reference data, molecular dynamics simulations are utilized to uncover the structural and dynamical properties of the interfacial water molecules.

O 34.4 Tue 13:30 P3

Studying Tricalcium Silicate-Water Interfaces Using High-Dimensional Neural Network Potentials — •Henry Wang[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

The advent of machine learning potentials (MLP) trained to energies and forces from electronic structure calculations has revolutionized the simulation of solid-liquid interfaces by molecular dynamics (MD). For instance, High-Dimensional Neural Network Potentials (HDNNP) have shown excellent accuracy for describing the interaction of water with numerous solid minerals. In this study, we investigate interfaces of liquid water with alite (Ca_3SiO_5), an important cement mineral exhibiting various polymorphic states. Using large-scale MD simulations, an analysis of the structural and dynamical properties of interfacial water is presented.

O 34.5 Tue 13:30 P3

Electrocatalytic CO_2 Reduction in Ionic Liquid/Nitrile Electrolytes — •Björn Ratschmeier, Arik Geringswald, Alisa Kamaric, and Björn Braunschweig — University Münster, Institute of Physical Chemistry, Münster, Germany

Room-temperature ionic liquids (RTILs) play an important role in CO_2 reduction reactions (CO_2RR), providing a viable alternative to aqueous electrolytes, but face challenges such as high overpotentials and product selectivity. As we have previously shown for 1-butyl-3-methylimidazolium trifluorosulfonylimide ([BMIM][NTf_2]) electrolytes [1], the accessibility of water as a co-reactant at the interface is a limiting factor for CO formation potentials. To modulate the interfacial structure, different concentrations of acetonitrile and benzonitrile were introduced into [BMIM][NTf_2] electrolytes in the presence of 1.5 M H_2O. The resulting mixtures were investigated in terms of CO_2RR at polycrystalline Au electrodes. The presence of 7.5 M benzonitrile resulted in a 20-fold increase in CO formation, and in even higher CO concentrations with acetonitrile compared to the pure ionic liquid. Consequently, we propose that nitrile additives tune the interfacial structure in such a way that the access of water molecules is improved. In order to validate this hypothesis, we aim for an in-depth investigation of the bulk electrolyte as well as of the interfacial structure using *in situ* IR and SFG spectroscopy. [1] Ratschmeier et al. Electrochem. Sci. Adv. 2023, 3, e2100173.

O 34.6 Tue 13:30 P3

Investigating Zinc Oxide-Water Interfaces with High-Dimensional Neural Network Potentials — •Jan Elsner and Jörg Behler — Theoretische Chemie II, Ruhr-Universität Bochum, Germany, and ResearchCenter Chemical Sciences and Sustainability, Research Alliance Ruhr,Germany

Zinc oxide (ZnO) is a promising material for sustainable hydrogen production via catalytic water splitting. The interface of ZnO with water exhibits complex dynamical behavior, including water dissociation and recombination, as well as long-range proton transport. Traditionally, density functional theory (DFT)-based molecular dynamics has been the primary theoretical tool for probing such mechanisms at the atomistic scale. However, the complexity of the interface, requiring large simulation boxes, and the long time scales associated with dynamical processes pose substantial theoretical challenges for any method relying on explicit electronic structure calculations. High-Dimensional Neural Network Potentials (HDNNPs) offer a solution to these challenges, enabling atomistic simulations with DFT-level accuracy at only a fraction of the computational expense. Here, we present HDNNP-based simulations of ZnO-water interfaces, providing insights into their structure and dynamics.

O 35: Poster Solid-Liquid Interfaces: Structure

Time: Tuesday 13:30–15:30 Location: P3

O 35.1 Tue 13:30 P3

Comparision of spin and orbital Rashba effect in Bi_xPb_{1-x}/Ag(111) — •Himanshu Lohani — EP7 University of Wurzburg

Superstructure of heavy elements constructed on the surface of noble metals is one of the most celebrated system in the field of spintronics due to giant Rashba spin splitting found in its surface electronic structure. A new perspective of orbitronics has emerged recently for reinvestigating this system after the uprising of orbital based Rashba effect. Angle resolved photoelectron spectroscopy (ARPES) not only visualizes directly the electronic band dispersion but intensity of the photoemission signal itself carries important information of orbital character of the bands. By using the photoemission intensity calculation which is designed on a tight binding model, we successfully capture evolution of the Rashba surface state bands (SSBs) dispersion and intensity as they are observed in our ARPES data on Bi_xPb_{1-x}/Ag(111). This comparative study hints that buckling of Bi/Pb atoms on Ag(111) surface affects spin polarization of the Rashba SSBs more than their orbital polarization

O 35.2 Tue 13:30 P3

High-Dimensional Neural Network Potentials for Molecular Dynamics Simulations of Mineral-Water Interfaces — •Maite Böhm[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In recent years, High-Dimensional Neural Network Potentials (HDNNP), a frequently used type of machine learning potential, have become a popular tool for simulations of complex systems such as mineral-water interfaces. Here, we present a HDNNP trained to density functional theory energies and forces for tricalcium aluminate ($Ca_3Al_2O_6$, C_3A)-water interfaces, which are of high interest for concrete chemistry. After validation, the obtained HDNNP is applied in large-scale molecular dynamics simulations to unravel the interactions of water with this material by computing a series of structural and dynamical properties.

O 35.3 Tue 13:30 P3

Informed Automated Structure Discovery of Atomic Force Microscopy Images — •Azin Alesafar[1], Joakim Jestilä[1], and Adam Foster[1,2] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

Atomic Force Microscopy (AFM) enables direct imaging of atomic-level features however, the interpretation of non-planar molecules is challenging due to the fact that only the top layers of these systems interact with the microscope tip. This leads to images deviating from structures familiar to us. Recent Advances in machine learning-based image recognition tools have provided a framework suited to tackle this challenge. However, these methods rely heavily on training data and may produce inaccurate results when faced with unfamiliar structures. An alternative approach is to develop an iterative algorithm that generates realistic 3D structures by comparing simulated and experimental AFM images in a fully automated manner. The final workflow enables the generation of candidate structures using different techniques, such as molecular dynamics, minima hopping, or machine learning models. A deeper understanding of the simulated structural information is achieved through feature detection algorithms and image registration. Furthermore, the simulated structures, and consequently their corresponding AFM images, are automatically evaluated for similarity to reference AFM images using image quality metrics. These approaches are tested on water clusters modeled on gold and copper surfaces using the Neural equivariant interatomic potential (NequIP).

O 35.4 Tue 13:30 P3

In situ electrochemical atomic force microscopy studies of a copper surface during lithium plating and dissolution — •Luca Kaufer[1,2], Daniel Ebeling[1], Thomas Göddenhenrich[1], André Schirmeisen[1], and Jürgen Janek[2] — [1]Institute of Applied Physics, Justus-Liebig-University, Gießen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University, Gießen, Germany

This investigation demonstrates the utilisation of atomic force microscopy (AFM) to examine the interactions between liquid electrolytes and copper electrodes. In particular, the focus is on the deposition of lithium on copper surfaces, a crucial process in lithium batteries. Atomic force microscopy (AFM) measurements allow for precise analysis of the surface structure, morphology and dynamic changes during lithium deposition, thereby providing deeper insights into the mechanisms of electrode reactions and the quality of the electrode surface. Such measurements are of great importance to improve the efficiency and lifetime of batteries by helping to understand and control processes such as dendritic growth or non-uniform deposition.[1,2] We will include an examination of the modification of the single-crystal electrode surface, which has been achieved through the utilisation of a bespoke methodology that integrates sputtering, annealing and polishing techniques.

[1] J. Phys. Chem. C 2023, 127, 12492-12501. [2] Faraday Discuss, 2022, 233, 190.

O 36: Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 36.1 Tue 13:30 P3

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

In recent years, the emerging class of non-van der Waals 2D materials has attracted considerable interest due to the unique electronic and magnetic properties of the representatives [1]. We study here the role of spin-orbit coupling (SOC) in these non-van der Waals 2D systems and related effects that might eventually lead to topological properties. With several 2D candidates including heavy elements such as Bi and Tl, significant effects due to SOC are present in the electronic structure. For the initial screening, we employ AFLOW [2] with its standardized workflows. In a second step, we retrieve the metadata using AFLOW and adapt the extracted parameters with an AiiDA-plugin [3] for accurate electronic structure calculations using the full-potential all-electron program FLEUR [4] within AiiDA. We discuss the effect of SOC on the band structures and densities of states and also focus on the topologically protected 1D conduction edge channels [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.
[5] M. Lokamani *et al.*, manuscript in preparation (2024).

O 36.2 Tue 13:30 P3

Influence of surface relaxations on scanning probe microscopy images of the charge density wave material $NbSe_2$ — Nikhil S. Sivakumar[1], Joost Aretz[1], •Sebastian Scherb[1], Marion van Midden Mavric[2], Nora Huijgen[1], Umut Kamber[3], Daniel Wegner[1], Alexander A. Khajetoorians[1], Malte Rösner[1], and Nadine Hauptmann[1] — [1]IMM, Radboud University, Nijmegen, The Netherlands — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, USA

Scanning tunneling microscopy (STM) images of the charge density wave (CDW) in 2H-$NbSe_2$ at voltages around the Fermi level lack a contrast inversion expected for a single-band CDW. Recent works have ascribed this to a multi-band CDW or the displacement of the surface Se atoms. While STM cannot disentangle geometric and electronic structure variations, non-contact atomic force microscopy (nc-AFM) can provide better characterization of the geometric structure due to its sensitivity to the interaction between the charge densities of tip and surface. We employ distance-dependent combined constant-height STM/nc-AFM measurements to characterize the surface relaxations of 2H-$NbSe_2$. Nc-AFM images show different image contrasts depending on distance. Based on ab-initio calculations, we show that the contrast at small distances is dominated by the displacement of the surface Se atoms. For large distances, the contrast is dominated by the interaction of the permanent dipole of the tip with the potential above the surface that is predominantly modulated by the underlying Nb atoms.

O 36.3 Tue 13:30 P3

Investigation of the electronic structure of 1T-$Ta_{1-x}Mo_xS_2$ using 11eV-laser ARPES — •Adina Timm[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The ability to modify the electronic structure of quantum materials by controlling charge density waves (CDWs) offers various possibilities for use in next-generation technologies as electronic and optoelectronic components. A material platform for testing this approach is 1T-TaS_2, which exhibits different temperature-dependent CDWs that we aim to tune by doping. Using 11eV-laser ARPES, we determine the differences in the electronic band structure of both doped and pristine TaS_2 crystals. The dopant molybdenum was introduced into TaS_2 during crystal growth by chemical vapor transport. The photoemission results show that different CDW phases are present at low doping concentrations of less than one percent with modified transition temperatures.

O 36.4 Tue 13:30 P3

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Florian K. Diekmann[1,2], Adina Timm[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a two-dimensional hexagonal 2H structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping, making it a highly attractive candidate for spintronic applications. This assumption is supported by density functional theory calculations and scanning transmission electron microscopy studies, and RKKY interactions are predicted as the driving mechanism. The crystals investigated in this study were synthesized in-house employing the chemical vapor transport method. This process produced as-is vanadium-doped WSe_2 crystals with approximately 2% of the tungsten atoms (presumably) substituted by vanadium. The results reported here were obtained using a Physical Property Measurement System (PPMS) in ACMS configuration and provide valuable insights into the magnetic characteristics of this doped material.

O 36.5 Tue 13:30 P3

Polarons in single-layer MoS_2 via downfolding approach to the coupling of electronic and nuclear degrees of freedom — •Laura Pätzold[1], Camiel van Efferen[2], Arne Schobert[1], Tfyeche Y. Tounsi[2], Michael Winter[1], Mark Georger[2], Affan Safeer[2], Christian Krämer[2], Jeison Fischer[2], Jan Berges[3], Thomas Michely[2], Roberto Mozara[1], Wouter Jolie[2], and Tim O. Wehling[1,4] — [1]U Hamburg — [2]U Köln — [3]U Bremen — [4]The Hamburg Centre for Ultrafast Imaging

A polaron is a quasiparticle describing a localized bound state resulting from the interaction of charge carriers with lattice vibrations. Though they are a well-studied phenomenon, experimental observations of polarons in 2D crystals are sparse. Here, we present the theoretical analysis of polaronic distortions in n-doped single-layer MoS_2 via a downfolding approach with linear electron-lattice coupling based on density functional theory calculations [1]. With this, a multi-polaronic distortion, caused by a renormalized M-point phonon, can be stabilized on supercells of up to 18×18. We compare our results to scanning tunneling microscopy measuremens obtained on n-doped single-layer MoS_2, which support the existence of polarons emerging from the coupling of non-polar zone-boundary phonons to Bloch electrons. This tunneling into the vibrationally coupled polaronic states is visible through evenly spaced peaks around the Fermi energy in the differential conductance, whose spacing matches the frequency of the M-point phonon responsible for the multi-polaronic distortion in our simulations.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 36.6 Tue 13:30 P3

Electronic and phononic characterization of 2H-NbS2 at the atomic scale — •Werner M.J. van Weerdenburg, Margarete Huisinga, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDs) are a class of layered materials that can exhibit a variety of electronic properties, including low-temperature quantum phases such as superconductivity and charge density wave (CDW) formation. These phases may coexist, for instance in 2H-NbSe2, and electron-phonon interactions have been suggested as a common driving factor for the two phases [1]. In contrast, the similar compound 2H-NbS2 has a comparable superconducting critical temperature, but lacks a CDW phase [2], highlighting the importance of subtle differences in electron-phonon interactions.

Here, we apply scanning tunneling microscopy and spectroscopy (STM/STS) to investigate the electronic and phononic properties of 2H-NbS2 at the atomic scale. Based on quasiparticle interference mapping, we probe the spatial variation of the electronic density of states and identify the dispersion of the band structure around the Fermi level. Moreover, inelastic excitation spectroscopy reveals the phononic excitations of the material. By mapping the atomic-scale variation of phononic excitations around intrinsic defects of the material and adatoms, we study how electrons and phonons interact at the atomic scale.

[1] Rossnagel et al., PRB 64, 235119 (2001)
[2] Heil et al., PRL 119, 087003 (2017)

O 36.7 Tue 13:30 P3

Characterization of surficial defect states in Mott insulator 1T-TaS_2 — •Junyoung Sim, Vibhuti Rai, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

The Mott insulating state in 1T-TaS_2, arising from strong correlations among unpaired electrons within its charge density wave superlattice, is distinct from a trivial band insulator and serves as a model system for exploring the dynamics of

exotic many-body states [1]. Here, we investigate bulk 1T-TaS_2 using scanning tunneling microscopy (STM) at 5 K. We find arious nanoscopic defects including vacancies, and domain. Additionally, we adsorb transition metal adatoms on the bare surface. Using tunneling spectroscopy, we map out their electronic signatures and compare them to prior studies [2].

[1] Hellmann et al. Phys. Rev. Lett. 105, 187401 (2010)
[2] Fei et al. AAPPS Bull. 32, 20 (2022)

O 36.8 Tue 13:30 P3

FinEstBeAMS: a multipurpose VUV and soft X-ray beamline at the max iv laboratory — •Weimin Wang, Antti Kivimäki, Kirill Chernenko, Calle Preger, and Stephan Appelfeller — MAX IV Laboratory, Lund University, PO Box 118, SE-22100 Lund, Sweden

The Finnish-Estonian Beamline for Atmospheric and Materials Science (FinEstBeAMS), located at the 1.5 GeV storage ring of the MAX IV Laboratory (Lund, Sweden), is a multidisciplinary beamline that was designed to fulfil the various needs of scientific communities in atomic, molecular and optical research, surface science, and photoluminescence research.

The gas-phase end station is equipped for electron and time-of-flight ion spectroscopies in low-density matter, while the photoluminescence end station focuses on luminescence spectroscopy of solid samples. The solid-state end station is dedicated to photoelectron and X-ray absorption spectroscopy of surfaces and interfaces, utilizing a hemispherical electron energy analyzer (PHOIBOS 150 2D-DLD from SPECS). The sample is positioned via a 5-axis motorized manipulator, offering three linear and two rotational motions (polar and azimuthal). A cryostat integrated into the manipulator enables sample cooling with liquid helium (~50 K) and nitrogen (~90 K). Additionally, a preparation chamber allows for sample treatment and analysis using supplementary techniques.

O 37: Poster 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 37.1 Tue 13:30 P3

Two-dimensional hexagonal β-GeSe on Au(111) — •Dina Wilks, Veronika Blecker, Muhammad Ali Martuza, Marina Hammer, Christoph Schuster, Paulus Aleksa, and Carsten Busse — Walter-Flex-Straße 3, 57072 Siegen, Germany

Two-dimensional (2D) group-IV monochalcogenides (general form MX with M=Sn, Ge; X=S, Se, Te) demonstrate a high degree of polymorphism. While the orthorhombic phase, widely studied for its in-plane ferroelectricity, holds significant promise, experimental studies on other polymorphs remain scarce.

Here, we investigate the growth and structure of 2D hexagonal β-GeSe on Au(111). This phase is predicted to exhibit out-of-plane ferroelectricity, which could be more technologically feasible for device integration. Samples are prepared using molecular beam epitaxy (MBE) with GeSe powder as the source material and analyzed with low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). The degree of structural order was found to depend sensitively on the heat treatment. We observe a (5×5) superstructure relative to Au(111), accompanied by a continuously varying density of states (DOS) across the superstructure's unit cell. Additionally, an intriguing self-similar pattern emerges, which can be attributed to antiphase grain boundaries. These boundaries exhibit metallic behaviour near the Fermi level, highlighting their potential significance in the electronic properties of the system.

O 37.2 Tue 13:30 P3

Scanning Tunneling Microscopy and Spectroscopy of epitaxial grown TaS_2 on GaN (0001) — •Jan-Niclas Schmidt, Constantin Hilbrunner, Georg A. Traeger, Jörg Malindretos, Angela Rizzi, and Martin Wenderoth — University of Göttingen, IV. Physikalisches Institut, Fridrich-Hund-Platz 1, 37077 Göttingen

Tantalum Disulfide crystals are interesting due to its complex phase diagram including the effect of Charge Density Waves. We are interested in how the layer thickness influences properties of Tantalum Disulfide. With Molecular Beam Epitaxy a three monolayer thick film of 2H-Tantalum Disulfide was grown on Gallium Nitride. To gain insight into the growth mechanism, the sample was transferred to a low temperature Scanning Tunneling Microscope (STM) operated at 80 K. To avoid any surface contamination, the transfer was done with a portable ultrahigh vacuum chamber. The constant-current STM-topography show small nanometer-sized, trigonal islands on a rough layer with some holes. The spectroscopy data show metallic behavior for the island as well as for the layer below.

This work is financially supported by the DFG through the SFB1073.

O 37.3 Tue 13:30 P3

Growth dynamics of 2D materials on Ir(111) — •Smruti Ranjan Mohanty, Marko Kriegel, Frank Meyer zu Heringdorf, and Michael Horn- von Hoegen — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

The structure and morphology of 2D materials are profoundly influenced by the choice of growth substrates, with noble metal substrates offering enhanced catalytic activity and complex surface morphology facilitating precise control over the growth of 2D materials. Employing low-energy electron microscopy (LEEM), we investigated the kinetics of graphene island nucleation during the CVD of ethylene on Ir(111) at growth temperatures ranging from 750°C to 1050°C for various dosing pressures. Graphene islands nucleate heterogeneously at Ir(111) step edges, leading to edge decorations, but a transition to homogeneous nucleation occurs at island densities lower than the step density. The strong variation in island density as a function of growth temperature and dosing pressure is explained by Venables nucleation theory, with the near-linear dependence on dosing pressure attributed to a critical nucleus size (i*) of 5. The work presented here also extends to the growth and characterization of other atomically thin 2D materials, including hexagonal boron nitride (hBN), and borophene on Ir(111). The investigation reveals complex growth mechanisms, the emergence of Moiré superlattices, and substrate-influenced interactions, providing insights for designing heterostructures and functional materials with significant potential for next-generation technological applications.

O 37.4 Tue 13:30 P3

Incommensurability and negative thermal expansion of single-layer hexagonal boron nitride — •Marko Kriegel[1], Karim Omambac[1], Steffen Franzka[2], Frank Meyer zu Heringdorf[1,2], and Michael Horn-von Hoegen[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Carl-Benz-Str. 199, 47057 Duisburg, Germany

The emerging field of straintronics, i.e., the control and utilization of the strain state of 2D-materials, is of great importance for their technological development, specifically in view of their future incorporation into van der Waals heterostructures. To gain fundamental insight into structural peculiarities of two-dimensional systems, single-layer hexagonal boron nitride (hBN) grown on Ir(1 1 1) by chemical vapor deposition was used as a prototypical model system: High-resolution reciprocal space mapping reveals the incommensurate nature of the material system by measuring the *h*BN in plane lattice parameter with high precision, facilitated by the moiré magnification effect in electron diffraction. In a growth temperature (T_g) regime of 700 to 1150°C an average lattice parameter of 2.496 ± 0.006 Å was found. Eventually, careful disentanglement of the hBN and substrate behavior for rising T_g allowed the determination of a negative thermal expansion coefficient of $\alpha_{hBN} = 2.4 \pm 1.2 \times 10^{-6}\,K^{-1}$ for free-standing hBN.[1] [1] M. Kriegel et al. Appl. Surf. Sci. 624 (2023) 157156

O 37.5 Tue 13:30 P3

UHV-CVD on Ir(111) for the Growth of 2D Materials — •Niels Ganser[1], Marko Kriegel[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Hexagonal boron nitride (hBN) can be grown by scalable chemical vapor deposition (CVD) from a borazine $B_3N_3H_6$ precursor. Here we show that the hBN quality depends strongly on the growth temperature T_g and the dosing pressure *p*.

Combined SPA-LEED and LEEM measurements show a strong dependence of *n* on *p*. We find that the quality of the hBN layers that can be achieved by increasing T_g is limited by the process of disintegration of the borazine at $T_g > 950$°C resulting in growth of borophene (2D Boron) instead [1]. Thus, it is possible to selectively grow either hBN or borophene from the same precursor [2].

Corroborating SPA-LEED measurements reveal a negative thermal expansion coefficient of $\alpha = (-2.4 \pm 1.2) \times 10^{-6}\,K^{-1}$ for 2D hBN in the temperature regime between 700 and 1100 °C. This finding can be explained by Lifshitz' membrane effect [3].

[1] Lifshitz, I., Zh. Eksp. Teor. Fiz. 22, 475 (1952)
[2] Omambac, K. et al., ACS Nano 15, 7421 (2021)
[3] Omambac, K. et al., ACS Nano 17, 17946 (2023)

O 38: Poster 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

O 38.1 Tue 13:30 P3

Stability and electronic properties of double-layer o-B2N2 in different stacking modes — •Na Li and Claudia Draxl — Department Physics and CSMB, Humboldt-Universit at zu Berlin, D-12489 Berlin, Germany

Two-dimensional orthorhombic boron nitride (o-B2N2) has recently attracted significant attention due to its direct band gap of approximately 1.7eV and excellent visible-light absorption properties. In its layered conformations, the stacking order plays a crucial role in determining the material's stability as well as its electronic and optical properties. In this study, we employ the all-electron full potential code exciting to perform first-principles calculations of four high-symmetry bilayer stacking sequences of o-B2N2, regarding their relative stability and their electronic properties. Our calculations reveal that the AB' stacking sequence has the lowest energy and an optimized interlayer distance of 3.52 Å. The bandgaps of the AA and AA' stacking sequences are reduced relative to the monolayer, where AA' exhibits even semi-metallic behavior. In contrast, the AB and AB' stacking sequences show slightly increased direct bandgaps.

O 38.2 Tue 13:30 P3

In-depth analysis of stratified MoS2 and WS2 2D heterostructures — •Sebastian Klenk, Nikolas Dominik, Cormac Ó Coileáin, Tanja Stimpel-Lindner, and Georg S. Duesberg — University of the Bundeswehr Munich, Institute of Physics, Germany

Starting with graphene roughly two decades ago, two-dimensional (2D) materials have garnered great interest in the scientific community due to their exceptional electrical, mechanical and optical properties. The broad palette of different 2D materials has allowed for the possibility to change and finetune these parameters to one's own liking by combining several 2D materials in one film. Here, we present the metal-organic chemical vapour deposition (MOCVD) synthesis and analysis of MoS2/WS2 heterostructures. We show the ordering of a high-quality 7-layer combination structure of less than 10 nm. The layered nature is confirmed and discussed using XPS, EDX, ToF-SIMS, TEM, AFM and Raman spectroscopy.

O 38.3 Tue 13:30 P3

A Two-dimensional Heterostructure Fabrication System in Ultra-high Vacuum — •Daiyu Geng, Jiabao Yang, Natalie Lehmann, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

We develop an ultra-high vacuum system for the fabrication of two-dimensional heterostructures. The clean transfer and stacking of two dimensional material flakes are realized using a polymer-free method based on SiNx cantilevers coated with Au film (Nature Electronics, 2023, 6(12): 981-990). The system also incorporates multiple surface preparation and characterization techniques like MBE, Plasma sputtering and electron diffraction. All these methods enable us to prepare heterostructures with atomically clean interface, which is important for the spectroscopic investigation of the rich physics effects in two-dimensional heterosystems.

O 38.4 Tue 13:30 P3

Exploring MXenes as Electrodes for Al-ion Batteries: An Ab-initio Study on the Impact of Stacking Configurations and Termination Types — •Amal Raj Veluthedath Nair and Nuala M Caffrey — School of Physics, University College Dublin, Dublin 4, Ireland

MXenes, with their tunable surface chemistry, thin 2D structures, large interlayer spacing, and good conductivity, are promising candidates for battery electrodes. The stacking configuration of MXene layers, determined by their chemistry and surface terminations, influences their electrochemical performance.

This study explores Ti_3C_2 and V_2C MXenes as electrodes for Na, Mg, and Al-ion batteries using density functional theory. We examine four stacking configurations and two coordination sites for intercalated ions. Results reveal that stacking configuration and surface terminations significantly influence change in interlayer distance, with O-terminated octahedral stacking showing the least change in spacing for all intercalants. The smallest interlayer distance change occurs for Al intercalation in V_2C, with a Δd of 0.1 Å, matching experimental findings (Vahidmohammadi et al., 2017). Ion migration studies indicate that prismatic stacking promotes faster ion migration compared to octahedral stacking. O-terminated MXenes significantly enhance the theoretical specific capacity for Al intercalation, reaching a maximum value of 283.48(277.63)mAh/g for $Ti_3C_2O_2(V_2CO_2)$. In contrast, F-terminated MXenes show much lower capacities.

O 38.5 Tue 13:30 P3

Triplet pairing enabled proximity superconductivity in monolayer WTe_2 — •A. Bäder[1,2], T. Wichmann[1,3], J. Martinez-Castro[1,4], P. Rüssmann[5,6], K. Jin[1,4], T. Samuely[7], Z. Lyu[1,3], J. Yan[8], O. Onufriienko[7], P. Szabó[7], F. S. Tautz[1,3], M. Ternes[1,4], S. Lounis[5,9], and F. Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Experimentalphysik IV A, RWTH Aachen — [4]Institut für Experimentalphysik II B, RWTH Aachen — [5]Peter Grünberg Institut (PGI-1), Forschungszentrum Jülich — [6]Julius-Maximilians-Universität Würzburg, Fakultät für Physik und Astronomie — [7]Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University & Institute of Experimental Physics, Slovak Academy of Sciences — [8]Materials Science and Technology Division, Oak Ridge National Laboratory, USA — [9]Fakultät für Physik, Universität zu Duisburg-Essen

We use low-temperature scanning tunneling microscopy to investigate proximity-induced triplet pairing and its role in enabling superconductivity in a monolayer $WTe_2/NbSe_2$ van der Waals heterostructure. Employing the Kohn-Sham Bogoliubov-de Gennes formalism, we find that conventional s-wave pairing fails to induce superconductivity in the WTe_2, in contrast to triplet pairing. Applying an external magnetic field, we examine Abrikosov flux vortices within the heterostructure and exploit them to probe local superconducting properties. Our findings highlight a platform for studying triplet pairing-induced superconductivity with potential topological characteristics.

O 39: Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules I

Time: Tuesday 14:00–15:30 Location: H4

O 39.1 Tue 14:00 H4

Instrumental Innovations for Model Single-Atom Catalysis — •Jiří Pavelec, David Rath, Chunlei Wang, Nail Barama, Panukorn Sombut, Matthias Meier, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — TU Wien, Vienna, Austria

Single-atom catalysts (SACs) reduce reliance on precious materials by using individual atoms as active sites. Infrared spectroscopy of adsorbed CO is widely used to probe these sites, but spectral interpretation and charge-state assignment remain debated. Surface science studies of model SACs could provide valuable benchmarks, but progress has been hindered by a lack of model systems and challenges in detecting low coverages of intermediates.

Here, I introduce a novel approach to infrared reflection absorption spectroscopy (IRAS) that adjusts the incidence angle, which resolves signal-to-noise issues on dielectrics [1]. As a case study, we investigated CO titration of rhodium-based SACs on a $Fe_3O_4(001)$ support. The spectra reveal Rh_1CO monocarbonyls as the dominant species. Meanwhile, the $Rh_1(CO)_2$ gem-dicarbonyl arises solely from the breakup of minority Rh_2 dimers, as confirmed by STM movies and theoretical modeling [2]. Though less prevalent in our UHV study, $Rh_1(CO)_2$ may play a critical role under realistic conditions.

Combining advancements in IRAS with a detailed understanding of model SACs provides valuable benchmarks for theoretical studies and spectral references for researchers working with less-defined, high-surface-area powder catalysts. [1] D. Rath et al., Rev. Sci. Instrum. 95, (2024). [2] C. Wang et al., Angew. Chem. Int. Ed. 63, (2024).

O 39.2 Tue 14:15 H4

Structure and oelic acid adsorption properties of magnetite nanoparticles on $SrTiO_3$ — •mohammad ebrahim haji naghi tehrani[1,2], lucio martinelli[3], daniel silvan dolling[1,2], marcus creutzburg[1], ming chao kao[1,2], alexander meinhardt[1,2], mona kohantorabi[1], heshmat noei[1], and andreas stierle[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Fachbereich Physik Universität Hamburg, Hamburg, Germany — [3]Institut Néel, CNRS, Grenoble INP, Université Grenoble Alpes, Grenoble, France

The underlying explanation for the exceptional mechanical properties of hierarchically arranged magnetite nanoparticle super-crystals is closely linked to understanding the oxide-organic interface between the magnetite nanoparticles (NPs) and the oleic acid (OA) molecules. We studied the shape and surface structure changes of the magnetite NPs induced by crosslinking the OA molecules. In this regard, magnetite NPs were grown by reactive physical vapor deposition on a strontium titanate single crystalline surface (STO(001)). The structural and morphological changes in the NPs were monitored under ultra-high

vacuum (UHV) conditions employing synchrotron-based grazing incidence X-ray diffraction (GIXRD). We evidenced the growth of (001) oriented magnetite NPs with predominant (111) side facets. Additionally, our results indicate an increase in the NP lattice constant after OA adsorption, which may be attributed to the incorporation of oxygen vacancies.

O 39.3 Tue 14:30 H4

Towards Understanding the Photoreactivity of $SrTiO_3$ through Studies in Ultra-High Vacuum — •Anna Lemperle, Philip Petzoldt, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Heterogeneous photocatalysis offers the prospect of utilising solar energy for the zero-carbon production of hydrogen from water. The most prominent photocatalytic materials currently employ $SrTiO_3$ as the light harvesting semiconductor. While these catalysts have been shown to promote a stoichiometric reaction, their photocatalytic performance is still insufficient for economically viable application. As their structural complexity impedes mechanistic studies, model systems are necessary to elucidate individual reaction steps and connect catalytic results to distinct catalyst properties. This approach aims to attain a molecular understanding of the reaction mechanisms involved in water splitting in order to enable a more targeted design of photocatalysts. In this contribution, we discuss first results on the reactivity of water and oxygen on the bare $SrTiO_3(110)$ surface. Results obtained by combining temperature programmed desorption and studies under illumination highlight the importance of bulk and surface oxygen for the reactivity of $SrTiO_3$.

O 39.4 Tue 14:45 H4

Effect of Mn and V Doping on the OER activity of $Co_3O_4(001)$: insights from DFT+U calculations — •Palani Muthu Kumar and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Using density functional theory calculations with a Hubbard U term (DFT+U), we study the effect of Mn and V doping on the oxygen evolution reaction (OER) at the $Co_3O_4(001)$ surface. In bulk, both dopants favor the octahedral over the tetrahedral site, providing a foundation for understanding the incorporation at the surface. Both at the A and the B-terminations of $Co_3O_4(001)$, Mn doping at a surface octahedral site enhances the overpotential, reducing overall the OER efficiency. In contrast, at the B-layer, V doping at a surface octahedral site reduces the overpotential from 0.48V (pristine) to 0.43 V, retaining the Co_{oct} reaction site. At the pristine A-surface, η is higher for a tetrahedral (0.74 V) vs. octahedral surface Co site (0.55 V). This trend is reversed for V-doping in the subsurface octahedral site which leads to the lowest overpotential of 0.18 V at the Co_{tet} reaction site. In all studied cases, the potential determining step is the deprotonation of *OH to *O. The improved catalytic activity due to V doping is attributed to a modified charge redistribution on the surface, leading to favorable binding energies of the intermediates. Funding by DFG within CRC247 and computational time at the Leibniz Rechenzentrum are gratefully acknowledged.

O 39.5 Tue 15:00 H4

Complex structural arrangements at the $CO_2/In_2O_3(111)$ interface — Sarah Tobisch[1], Andreas Ziegler[2], Marco Knapp[1], Michael Schmid[1], Ulrike Diebold[1], Bernd Meyer[2], and •Margareta Wagner[1] — [1]Institut für Angewandte Physik, TU Wien — [2]ICMM & CCC, FAU-Erlangen-Nürnberg

Promising catalysts for the hydrogenation of CO_2 to methanol are highly desired to address the pressing issue of rising carbon emissions. Since reactions take place at the interface, understanding the fundamental properties and behavior of molecular species on well-defined surfaces is crucial for designing model catalysts.

In_2O_3 has gained attention as catalytic material due to its high selectivity for methanol synthesis via CO_2 reduction. In this work, the adsorption and interaction of CO_2 molecules on $In_2O_3(111)$ were investigated in detail at the atomic scale and under UHV conditions. We employ non-contact atomic force microscopy (AFM) and compared our findings with results from temperature programmed desorption (TPD) and x-ray photoelectron spectroscopy (XPS) measurements, as well as density functional theory (DFT) calculations. AFM images of the $In_2O_3(111)$ surface show 10 molecular features per surface unit cell arranged in a systematic and uniform order, albeit breaking the threefold symmetry of the substrate surface. The adsorption sites of all individual molecules were identified; some of them are carbonate species, in agreement to XPS showing a mixture of CO_2 molecules and CO_3^{2-}. Moreover, the desorption and structural evolution with increasing temperature was studied.

O 39.6 Tue 15:15 H4

Adsorption and activation of CO_2 on CeO_2 surfaces — •Zairan Yu, Shuang Chen, Wangtao Li, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

CO_2 activation and its subsequent transformation into valuable chemicals pose significant challenges in heterogeneous catalysis. Most studies have focused on powdered catalysts with various facets and unknown defect densities, whereas much less is known about the surface chemistry of CO_2 on well-defined oxide surfaces. Here, we investigate CO_2 adsorption and activation on fully oxidized $CeO_2(111)$ single-crystal surfaces using polarization-resolved IR reflection absorption spectroscopy (IRRAS). The comprehensive IRRAS data reveal that CO_2 is weakly bound to $CeO_2(111)$ at 117 K in a linear, physisorbed state. At elevated temperatures (300 K) and pressures, CO_2 undergoes activation forming an unusual horizontal carbonate. Additionally, in the presence of surface hydroxyl groups, formate and HCO_3 species are identified. These experimental findings are supported by complementary theoretical analysis. Furthermore, the IRRAS results are in excellent agreement with the in situ transmission IR data obtained for CO adsorption on octahedral ceria nanoparticles, which predominantly expose (111) facets. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) -Project-ID 426888090- SFB 1441.

O 40: Surface Dynamics

Time: Tuesday 14:00–15:30 Location: H6

O 40.1 Tue 14:00 H6

Manipulation of Optical Phonons in Strained Bi/Si(001) Heterostructures — •Fabian Thiemann and Michael Horn-von Hoegen — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Intentionally manipulating phononic properties in materials can cause dramatic changes in their dynamic behavior. A system that responds especially strong to structural changes is Bi due to its strong electron-phonon coupling and its inherent Peierls distortion. This renders the optical A_{1g} mode – oscillating along the [111] direction – sensitive to changes in the electronic system and coherently excitable upon photoexcitation. When grown on Si(001) bismuths lattice matches in the $[1\bar{1}0]$ direction, resulting in a compressive strain in the [110] direction, whereas the films are [111] oriented. The strain is relieved rapidly while increasing the thickness from 10 to 16 BL. This is predicted to influence the Peierls distortion heavily. In this work we extensively studied the impact of strain and confinement on the photoexcited coherent A_{1g} mode's frequency and dephasing in Bi/Si(001) heterostructures by in-situ transient-reflectivity spectroscopy. We observe a dramatic blueshift up to 0.2 THz, that can be preciesely tuned by the film thickness. The frequency however does not follow exactly the strain parameter and behaves differently in two regiemes. We attribute this discrepancy to the confinement in the [111] direction and the influence of the strongly shifting electron surface state.

O 40.2 Tue 14:15 H6

Coherent modulation of the charge density wave gap in 1T-$TiSe_2$ probed by tr-ARPES — •Jan Böhnke, Stephan Schmutzler, Mehul Jotshi, Cornelius Gahl, and Martin Weinelt — Freie Universität Berlin, Fachbereich Physik, Germany

Tuning the charge density wave (CDW) gap in 1T-$TiSe_2$ allows for the de/stabilization of the phase transition. An optical excitation breaks long-range order of the CDW state and results in a semi-metallic state on an ultrafast timescale as free carriers near the Fermi-level enhance Coulomb screening [1,2]. By employing time-resolved ARPES with 1.55 eV pump and 6.2 eV probe pulses, we discover for the first time fluence-dependent coherent modulations of the charge-density wave gap (closing and opening) in 1T-$TiSe_2$ at the Brillouin zone center. While for low excitation fluences, we mainly observe signatures of the CDW connected A_{1g}^* mode (3.45 THz), the optical A_{1g} phonon mode (6.1 THz) modulates the electronic structure near the gap for the high fluence regime. For an intermediate fluence we detect the transition from the A_{1g}^* to the A_{1g} mode. As we additionally find three image-potential states on the surface of 1T-$TiSe_2$, we can confirm the samples' low defect density at the surface after in-vacuum cleavage.

[1] T. Rohwer et al., Nature 471, 490–493 (2011)
[2] M. Huber et al., Sci. Adv. 10, eadl4481(2024)

O 40.3 Tue 14:30 H6

Impact of Coherent Phonons on Time-Resolved Optical Properties of WTe_2 — •Francesco Sammartino[1], Manuel Tuniz[1], Wibke Bronsch[2], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Università degli Studi di Trieste — [2]Elettra - Sinctrotrone Trieste

We study the ultrafast dynamics of tungsten ditelluride (WTe_2) along both its in-plane axes, by time-resolved reflectivity (TR-R) and time-resolved second-harmonic generation (TR-SHG) experiments with a varying pump fluence.

We identify two phonon modes: the shear phonon mode at 0.24 THz, indicative of uniform in-plane atomic shifts and detected in both TR-R and TR-SHG signals, and one at 2.4 THz, detected solely in the TR-R signal. We observe a large, fluence-dependent shift of up to ≈90° in the initial phase of the shear mode coherent oscillation, obtained in a narrow fluence range.

This evidence suggests that the excitation density can be used as a powerful knob to control the initial phase of the atomic displacements in a layered material.

O 40.4 Tue 14:45 H6

Controlled formation of thermodynamically unaccessible surface structures — •Simon B. Hollweger, Anna Werkovits, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

It is well known that organic molecules adsorbed on surfaces can form a variety of different surface structures. Which structure is the most favored one at a given temperature and pressure is determined by thermodynamics. However, in this study, we propose the idea of a mechanism with which we can control the formation of a specific metastable surface polymorph that can not be reached thermodynamically. With targeted temperature and pressure changes, a rearrangement process of the adsorbed molecules out of thermodynamic equilibrium is triggered. For specifically designed systems, this rearrangement of the adsorbed molecules leads to a kinetically trapped metastable surface polymorph. As a proof of principle for this proposed mechanism, kinetic Monte Carlo simulations of planar molecules adsorbing on a square lattice are conducted. We show that a metastable upright-standing structure of the planar molecules can be reached with a specific temperature and pressure profile applied to the system.

O 40.5 Tue 15:00 H6

Out of the Crystalline Comfort Zone: Sampling the Initial Oxide Formation at Cu(111) — •Felix Riccius, Nicolas Bergmann, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The oxidation of transition metal surfaces is widely recognized as a complex process that still bears many open questions, specifically at the microscopic level. Atomistic simulations could potentially uncover crucial insights, but state-of-the-art approaches are predominantly guided by human chemical intuition, leading to highly idealized surface representations. Here we demonstrate a systematic approach to model high-quality surface-phase diagrams, using the early oxidation of the Cu(111) surface as an example. To this end, we train a MACE machine learning interatomic potential (MLIP) to density functional theory calculations and combine its fast and accurate energetics with replica exchange molecular dynamics. We extensively explore the vast, thermodynamically relevant phase space and further develop surface phase diagrams based on increasingly involved theoretical frameworks. Our approach yields a comprehensive structural ensemble that predicts early Cu(111) oxidation to be characterized by O-Cu-O ring patterns, bearing significant disorder. Within the computed surface evolution, we recover trends in O-Cu-O ring distribution as a function of reaction conditions in line with scanning tunneling microscopy data. Our study illustrates how MLIPs and extensive sampling can be leveraged to rationalize metal surface oxidation fully *in silico* without the need to rely on experimental guidance.

O 40.6 Tue 15:15 H6

Photo-induced carrier and structural dynamics in anatase TiO_2 nanosheets — •Zhipeng Huang[1,2], Yan Yan[2], Xinxin Cheng[2,3], R. J. Dwayne Miller[4], and R. Kramer Campen[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen — [2]Max Planck Institute for the Structure and Dynamics of Matter — [3]SLAC National Accelerator Laboratory — [4]Departments of Chemistry and Physics, University of Toronto

Ultrathin anatase TiO_2 nanosheets with {001} facets have significantly higher activity for light-induced H_2 evolution than other TiO_2-based materials. The mechanism of this enhancement is not understood. Gaining such insight requires understanding the dynamics of charge carriers and their interactions with lattices after optical excitation. Here we characterize structural and charge carrier dynamics in these materials following UV excitation using ultrafast electron diffraction and transient absorption spectroscopy.

We observed an ultrafast lattice expansion and distortion in the nanosheets, occurring earlier than the Debye-Waller effect. Density Functional Theory (DFT) calculations suggest that the lattice expansion and distortion are induced by the trapping of charge carriers and the formation of large electron polarons. Compared to TiO_2 nanoparticles, the nanosheets exhibit significantly higher polaron populations, which explains their enhanced photocatalytic properties.

O 41: Heterogeneous Catalysis II

Time: Tuesday 14:00–15:15 Location: H8

O 41.1 Tue 14:00 H8

Oxide growth and oxide/metal interaction in CeO_x/Ni(111) — •Dominic Guttmann, Raquel Sánchez-Barquilla, Carlos Morales, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Cottbus 03046, Germany

Ni/ceria catalysts exhibit a high activity and selectivity for CO_2 methanation, making them very promising candidates for applications within a sustainable economy. The redox properties of cerium oxide allow it to readily switch between Ce^{4+} and Ce^{3+} states, facilitating CO_2 activation and conversion. We have studied the so-called strong metal-metal oxide interactions in the inverse catalyst configuration CeO_x/Ni(111) prepared by reactive molecular beam epitaxy in an oxygen atmosphere. Under specific growth conditions, the CeO_x (111)-oriented islands of different heights preferentially align in registry with the Ni(111) surface or are rotated azimuthally by ±10°, as observed by low-energy electron diffraction. Analysis by X-ray photoelectron spectroscopy reveals that during growth, partial oxidation of the Ni(111) surface leads to the formation of a NiO interface layer between the CeO_x islands and Ni substrate, resulting in a complex CeO_x(111)/NiO(111)/Ni(111) system with significant oxide-metal interactions. Finally, when we expose the system to H_2, O_2, and CO_2 atmospheres, we observe a complex behavior of the cerium and nickel oxidation states, which correlate with morphological changes in the oxide islands.

O 41.2 Tue 14:15 H8

Size-dependent nanoparticle sintering under catalytic reaction conditions — •Thomas Florian Keller[1,2], Christoph Seitz[1], Henning Runge[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Department of Physics, Hamburg, Germany

Catalytic metal nanoparticles applied in heterogeneous gas phase catalysis are known to change their shape during the conversion. We elucidate the evolution of the height to diameter aspect ratios of a substantial number of PtRh alloy nanoparticles exposed to mild and harsh catalytic CO oxidation reaction conditions by correlative atomic force- and scanning electron-microscopy. The preferentially (111) oriented Pt rich nanoparticles supported on a (0001) Al_2O_3 single crystal surface were imaged as grown and after the exposure to the catalytic conditions. We utilized an image-registration based approach combined with one-by-one nanoparticle correlation to overcome single nanoparticle studies and ensemble averages. This approach permitted us to shed light onto the active size dependent sintering mechanism as e.g., particle migration and coalescence, and Ostwald ripening. While for mild catalytic conditions the aspect ratio is rather independent of the lateral nanoparticle size, for harsh conditions particles above an initial threshold diameter of around 45 nm tend to extraordinary grow on the cost of the surrounding smaller particles.

O 41.3 Tue 14:30 H8

High-throughput photocatalytic screening of lead-free halide perovskites with bayesian optimization for surface photovoltage — •Astita Dubey[1,2], Mahshid Ahmadi[2], Vladimir Shvartsman[1], Sergei Kalinin[2], and Doru Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany — [2]Institute for Advanced Materials and Manufacturing, Department of Materials Science and Engineering, The University of Tennessee Knoxville, Knoxville, TN 37996, USA

The development of lead-free, stable, and efficient catalysts for energy conversion necessitates rapid materials discovery. In this study, we employed Bayesian optimization (BO) to investigate a one-dimensional binary combinatorial library of zero-dimensional lead-free halide perovskites (A3Bi2I9 types) synthesized using a high-throughput automated pipetting robot. Structural analysis revealed hexagonal P6*/mmc symmetry throughout the library with pronounced variations in the lattice parameter c. Gaussian process-based BO identified the optimal composition featuring 49% cesium substitution, which demonstrated the best photocatalytic activity and stability attributed to the enhanced surface photovoltage and optimized anion vacancies. This composition achieved complete degradation of rhodamine B and methylene blue dyes within 15 and 20 minutes,

respectively. The identified composition's stability, defect management and the most efficient photocatalytic activity among 96 compositions is promising for its further use in water splitting.

O 41.4 Tue 14:45 H8

Automatic Exploration of Catalytic Reaction Networks — •Hyunwook Jung, Johannes T. Margraf, Hendrik H. Heenen, and Karsten Reuter — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin

The reaction network is a crucial element of first-principles microkinetics simulations, representing the connection between surface species and elementary reactions. Lacking systematic exploration methods, the reaction network is presently typically set up by human intuition. Especially for complicated processes such as syngas conversion, this is error prone and the absence of important species and reaction steps can be a source of sizable discrepancy between theoretical modeling and experiment. To address this problem, we introduce an automatic reaction network exploration scheme that starts with a fully enumerated, yet redundant reaction network, in which a reaction pathway is refined iteratively. The associated computational cost for extensive sampling of structures for both adsorption and activation energy calculations along the pathway is circumvented by simultaneously fine-tuning a MACE foundation model. Each trial reaction pathway is coupled with corresponding mean-field microkinetics and a detouring operation is attempted for the identified rate-limiting step. This procedure is repeated until user-defined criteria are reached. We demonstrate this automatic scheme on methanol synthesis at a Cu(111) surface.

O 41.5 Tue 15:00 H8

Functionalization of atomically defined Au step edges with N-heterocyclic carbenes for the electrocatalytic reduction of carbon dioxide — •Philipp Wiesener[1], Duong Tran[1], Ankita Das[2], Ying Pan[3], Nieves Lopez Salas[3], Frank Glorius[2], and Harry Mönig[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]Organisch-Chemisches Institut, Universität Münster, Münster, Germany — [3]Institut für Chemie, Universität Paderborn, Paderborn, Germany

N-Heterocyclic carbenes (NHCs) are versatile ligands allowing to tune the catalytic performance of metal surfaces and nanoparticles. In recent years, the understanding of molecular adsorption of a variety of NHC compounds on flat single crystalline surfaces has significantly advanced the knowledge about their extraordinary properties. In the present work, we use scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) to investigate the adsorption of various NHCs on a Au(788) surface, featuring a high density of atomically defined step edges. Our results reveal that NHC nucleation is significantly more stable at the step edges than on flat terraces. Correlating sub-molecular imaging techniques with voltammetry, we demonstrate the formation of a macroscopically defined and catalytically active nanostructure for the CO_2 reduction reaction. Our results spotlight the important role and opportunities of step edge functionalization by NHC compounds to design highly efficient and selective catalysts with defined active sites.

O 42: Electron-driven Processes

Time: Tuesday 14:00–15:30 Location: H11

O 42.1 Tue 14:00 H11

A simple model of nonadiabatic energy loss during hydrogen scattering from a semiconductor — •Xuexun Lu, Nils Hertl, and Reinhard J. Maurer — University of Warwick, Coventry, UK

Experiments on hydrogen atom scattering from Ge(111) show bimodal energy loss distributions with two peaks. The first peak corresponds to low energy loss and can be quantitatively reproduced with classical molecular dynamics (MD) simulations. The second peak lies at energy losses equivalent to or above the band gap of Ge and arises from electronic transitions between the valence band and the conduction band. Here, we develop a simple and interpretable model for H/Ge(111) scattering to inform the development of new mixed quantum-classical dynamics simulation methods suitable for the description of such nonadiabatic effects in gas-surface scattering. Using density functional theory data and experimental quantities, we parametrize an effective one-dimensional analytical model based on the Newns-Anderson Hamiltonian. The model allows us to study the coupled electron-nuclear dynamics and their conjugate energy transfer using nonadiabatic molecular dynamics methods such as independent electron surface hopping (IESH), molecular dynamics with electronic friction (MDEF), and the Ehrenfest method. In particular, IESH dynamics qualitatively reproduce the nonadiabatic energy transfer channel observed in the experiment.

O 42.2 Tue 14:15 H11

Shaping Polarons in Hematite Fe_2O_3: From Creation to Charge Dynamics — •Sreehari Sreekumar[1], Llorenc Albons Caldentey[1], Jesus Redondo Redondo[1], Aji Alexander[1], Sarah Tobisch[2], Michele Riva[2], and Martin Setvin[1] — [1]Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Applied Physics, Vienna University of Technology, Austria

The non-contact Atomic Force Microscopy (nc-AFM) technique has enabled breakthroughs in single-electron charge manipulation [1]. Here we use this capability to study polaron dynamics. Polarons are self-localized electrons or holes in ionic lattices that are crucial to material properties like conductivity, catalysis, and exotic phenomena such as high-temperature superconductivity and colossal magnetoresistance [2]. Polarons are studied in hematite at the single quasiparticle limit, focusing on the fundamental mechanisms involved in their injection, formation, migration, and interaction with defects [3].

1. Gross, L., et al., Science, 2009. 324(5933).
2. Franchini, C., et al., Nature Reviews Materials, 2021. 6(7).
3. Redondo, J., et al., Science Advances, 2024. 10(44).

The work was supported by project MSMT LL2324 *PoTr*

O 42.3 Tue 14:30 H11

Observing the directed motion of a single molecule after dissociation on a surface — •Ilias Gazizullin[1], Matthew Timm[1], Matthias Krinninger[2], Friedrich Esch[2], and Leonhard Grill[1] — [1]Physical Chemistry Department, University of Graz, Austria — [2]Faculty of Chemistry, TU München, Germany

Unidirectional motion of single molecules on surface can be achieved via a rare interplay between the surface and the intramolecular chemical reaction [1]. An alternative approach to achieve controllable molecular motion on surface is to induce dissociation of a molecule, resulting in the recoiling motion of the products [2, 3].

Here, we show how orientation of functional groups of an adsorbed molecule can steer its motion after controlled dissociation of these groups. We study single organic molecules with azido groups adsorbed on Au(111) surface by low temperature scanning tunneling microscopy (STM). The azido group of the adsorbed molecule can be oriented in two possible directions. We applied voltage pulses from the STM tip onto the azido group to induce its dissociation and found that the molecule rotates after dissociation in a specific direction. This directionality clearly depends on the initial orientation of the dissociating azido group, opening new possibilities to induce controlled motion of single molecules on surfaces.

[1] Simpson et al., Nature, 621, 82-87 (2023)
[2] Anggara et al., Sci. Adv., 4 (2018)
[3] Anggara et al., J. Am. Chem. Soc., 138, 7377-7385 (2016)

O 42.4 Tue 14:45 H11

Nonadiabatic quantum dynamics of molecules scattering from metal surfaces — •Riley Preston[1], Yaling Ke[2], Samuel Rudge[1], Nils Hertl[3], Raffaele Borrelli[4], Reinhard Maurer[3], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg — [2]Department of Chemistry and Applied Biosciences, ETH Zürich — [3]Department of Chemistry and Department of Physics, University of Warwick — [4]DISAFA, University of Torino

Nonadiabatic coupling between electrons and molecular motion at metal surfaces can strongly impact the dynamics of a scattering molecule [1]. We present a theoretical approach based on hierarchical equations of motion (HEOM) [2], which models the scattering of molecules from metal surfaces and incorporates all nonadiabatic and quantum nuclear effects due to the coupling of the molecular degrees of freedom to the electrons in the metal. The approach is exemplified by its application to NO scattering from Au(111), where we observe multi-quantum relaxation of the bond vibrational state due to coupling to electron hole pairs in the surface, in accordance with experiment. The data obtained by the HEOM approach is also used as a rigorous benchmark to assess various mixed quantum-classical methods, from which we derive insights into the validity range of each method [3].

[1] A. M. Wodtke, Chem. Soc. Rev. 45, 3641-3657 (2016).
[2] Y. Ke, R. Borrelli, and M. Thoss, J. Chem. Phys. 156, 194102 (2022).
[3] R. J. Preston, Y. Ke, S. L. Rudge, N. Hertl, R. Borrelli, R. J. Maurer, and M. Thoss, arXiv preprint arXiv:2410.05142 (2024).

O 42.5 Tue 15:00 H11

Nonthermal phonon distributions induced by hot electrons — •Tobias Held, Christopher Seibel, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau

When an ultrashort laser pulse irradiates a metal, the electrons initially absorb the energy and rapidly establish a hot Fermi distribution. Subsequently, on a

picosecond timescale, the electrons transfer energy to the phonon system. Electrons exhibit a stronger coupling to high-wavenumber phonons, leading to non-thermal phonon distributions induced by electron-phonon scattering.

In this study, we use the Boltzmann equation to examine the formation and subsequent relaxation of nonequilibrium phonon distributions. For our model system, we find that the majority of the energy is transferred within 10 ps, while a pronounced phonon nonequilibrium is induced. We observe "hot phonons" at the edge of the Brillouin zone, leading to a collapse of the electron-phonon energy transfer rate. Consequently, a finite temperature difference between electrons and phonons may persist significantly longer than the widely used two-temperature model would predict.

O 42.6 Tue 15:15 H11

Electronic friction simulations of laser-driven hydrogen evolution from copper. Just thermal desorption in a hurry? — •Alexander Spears, Wojciech G Stark, and Reinhard J. Maurer — University of Warwick, Coventry, UK

Ultrafast light pulses can induce energy transfer between light, electrons, and phonons at interfaces, leading to ultrafast dynamics such as light-driven hydrogen evolution from metal surfaces. Whether this energy transfer can drive photocatalysis through selective energy transfer into certain degrees of freedom remains an open question. Molecular dynamics simulations with electronic friction (MDEF) offer a quantum-classical description of electron-phonon coupling and have previously been used to model ultrafast surface dynamics. However, the effect of different electronic friction approximations on the final energy distributions has not been thoroughly investigated. We present MDEF simulations of light-driven hydrogen evolution from different copper surface facets, enabled by machine-learning surrogate models. For various laser fluences, we study desorption probabilities and final state distributions of desorbed molecules. Our results reveal that the choice of electronic friction approximation significantly affects desorption probabilities. However, the magnitude and nature of friction do not seem to affect the final vibrational, rotational, and translational energy distribution of molecular adsorbates. Within the electronic friction approximation, only the shape of the energy landscape determines these properties and no selective energy transfer occurs. This suggests that thermal and laser-driven desorption may yield similar outcomes.

O 43: Scanning Probe Microscopy: Light-Matter Interactions at the Atomic Scale II

Time: Tuesday 14:00–15:45 Location: H24

O 43.1 Tue 14:00 H24

Kinetics of nucleation and crystallization of sodium chloride based on frozen solution sample preparation apparatus — •Xinmeng Liu[1], Jiadong Guo[1], Yunzhe Jia[2], Sheng Meng[2], Enge Wang[1], and Ying Jiang[1] — [1]International Center for Quantum Materials, School of Physics, Peking University, Beijing, People's Republic of China — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, People's Republic of China

Solution environment is ubiquitous and plays a vital role in various fields, especially in the nucleation and crystallization process. Here, we designed and built a new frozen solution sample preparation apparatus compatible with UHV environment, allowing atomic-scale SPM experiments. By utilization of this apparatus, we successfully transferred NaCl solution in glassy states onto the Au(111) substrate. The qPlus-based AFM with CO tip characterized the kinetics of ions nucleation and crystallization after annealing. We found that the ions tend to form disordered networks with water molecules at the initial stage of nucleation, and then adjust to ordered crystals. Furthermore, ions continue to crystallize on the formed island surface by way of chain growth. This is different from the previous view that NaCl nucleation follows the classical nucleation theory. In addition, we also captured the existence of a small crystal nucleus composed of several ions, which is surrounded by water molecules that help the nucleus to further grow. Our results provide new insights into solution process and will have significant effect on the mechanism of material synthesis.

O 43.2 Tue 14:15 H24

Wavefunction Reconstruction of Excitonic Edge States using Machine Learning — •Aritra Mishra, Sidhartha Nayak, and Alexander Eisfeld — Max Planck Institute for the Physics of Complex Systems

A typical problem in quantum mechanics is to reconstruct the eigenstate wave functions from measured data. In the case of molecular aggregates, the information about the excitonic eigenstates is important to understand the optical and transport properties [1]. The reconstruction of the wavefunction coefficients from the near field absorption spectra is shown for a linear and a 2D molecular arrangement [2].

Here, we consider the aggregates arranged in two sublattices in a 2D arrangement, each sublattice having a particular orientation of the molecular transition dipole moment, that shows topological edge states as described in [3]. We show the reconstruction of the excitonic wave function for $N = 50$ molecules and move to $N = 200$, in the presence of disorder in the molecular dipole orientations and noise in the spectra. We observe a better reconstruction for higher noises considering all the input spectra for the electric field polarisation of the nanotip along the x, y and z axes.

[1] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018)
[2] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019)
[3] J. Yuen-Zhou, S. K. Saikin, N. Y. Yao and A. Aspuru-Guzik, Nature Materials 13, 1026 (2014)

O 43.3 Tue 14:30 H24

Probing topological Floquet states in graphene with ultrafast STM — •Nils Jacobsen[1,2], Melanie Müller[3], Michael Schüler[4,5], Martin Wolf[3], Angel Rubio[2,6], and Michael Sentef[1,2] — [1]ITP, University of Bremen, Bremen, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Fritz Haber Institute, Berlin, Germany — [4]Laboratory for Materials Simulations, Paul Scherrer Institut, Villigen, Switzerland — [5]Department of Physics, University of Fribourg, Fribourg, Switzerland — [6]Center for Computational Quantum Physics The Flatiron Institute, New York, USA

Floquet band engineering enables the control of solids via periodic laser driving. The light-induced quantum anomalous Hall effect (QAHE) in graphene with circularly polarized light [1] has been measured in ultrafast transport [2] and recently, Floquet replica bands under linearly polarized light have been reported in time-resolved photoemission spectroscopy [3]. Here, we explore the possibility of probing (topological) Floquet states in graphene with ultrafast scanning tunneling microscopy (USTM) as a complementary experimental technique [4]. Being highly sensitive to gap openings in the local density of states and the formation of edge states, USTM is a promising and versatile tool for probing light-induced topological states in quantum materials.

[1] Oka et al. PRB 79, 081406(R) (2009) [2] McIver et al. Nat. Phys. 16, 38-41 (2020) [3] Merboldt et al. arXiv:2404.12791 (2024) , Choi et al. arXiv:2404:14392 (2024) [4] Müller Prog. Surf Sci. 99, 100727 (2024)

O 43.4 Tue 14:45 H24

Theoretical Study of Electronic and Optical Properties in Edge-Modified Graphene Nanoribbons — •Jian Cheng Wong[1], Song Jiang[2], Sofia Canola[1], Alex Boeglin[2], Guillaume Schull[2], and Tomáš Neuman[1] — [1]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague, Czech Republic — [2]Université de Strasbourg, IPCMS, CNRS, UMR 7504, F-67000 Strasbourg, France

Graphene nanoribbon (GNR) exhibits electronic and optical properties tunable by its geometry. One such approach is to introduce localized electronic states by modifying the edge structure. A previous study [1] using scanning tunneling microscopy-induced luminescence (STML) revealed that the presence of localized single-particle end states in GNR contributed to the formation of localized optical excitations. Here we provide an extensive theoretical description of such excitations on the modified edge structure of GNRs, and how it interacts with the end states. To that end, we develop a many body model that incorporates ab initio electronic structure methods and elucidate the sequence of events involved that leads to the eventual light emission under STML. From this model, we compare the electroluminescence maps obtained with experimental results and show the microscopic details of the localized states probed by STML.

[1] Song et al., Science, 379(6636), 1049-1054 (2023).

O 43.5 Tue 15:00 H24

Correlations between noise and electroluminescence in graphene nanojunctions — •Sascha Korn, Michael Krieger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Light emission in scanning tunneling microscopy is often explained by the granularity of charge and should be therefore correlated with shot noise. Also, hot electrons may create both noise and thermal luminescence [1,2]. Using planar graphene nanojunctions, we study the phenomenon of electroluminescence in the point contact regime in a simple and well controlled electromagnetic environment. A spectral analysis of such measurements perfectly follows Planck's law and unambiguously supports the thermal picture. We present experimental data that correlate electrical noise measurements and optical spectroscopy, providing an in-depth view into the microscopic processes.

[1] Ott, C., Götzinger, S. & Weber, H. B. Thermal origin of light emission in nonresonant and resonant nanojunctions. Phys. Rev. Res. 2, 042019 (2020)

[2] Korn, S., Popp, M.A. & Weber, H.B. A point-like thermal light source as a probe for sensing light-matter interaction. Sci Rep 12, 4881 (2022)

O 43.6 Tue 15:15 H24

Photon blockade in current-driven single-molecule emitters — Andrés Bejarano[1,2], •Moritz Frankerl[1], Rémi Avriller[2], Fabio Pistolesi[2], and Thomas Frederiksen[1,3] — [1]Donostia International Physics Center, Spain — [2]Univ. Bordeaux, CNRS, LOMA, France — [3]Ikerbasque, Bilbao, Spain

We consider photon emission from a single electronic level embedded in a strongly damped cavity, where photon emission is driven by electronic tunneling events. Using a Lindblad master equation approach we investigate the system dynamics, photon emission spectrum as well as the second-order coherence function $g^{(2)}(\tau)$ [1]. We demonstrate that many features observed in scanning tunneling microscopy light-emission experiments can be explained with this simple model. Specifically, restricting the applied bias to the first emission threshold, we find antibunching in the photon statistics irrespective of the coupling strength to the cavity [2]. Employing a higher bias leads to a excitation of states with a photon number greater than one and thus the system shows bunching behavior as well as an emergence of two distinct time scales in the dynamics of $g^{(2)}(\tau)$. [1] Q. Schaeverbeke, R. Avriller, T. Frederiksen, F. Pistolesi, PRL 123, 246601 (2019) [2] P.Merino, C. Große, A. Roslawska, K. Kuhnke, K. Kern, Nat. Comm. 6, 8461 (2015)

O 43.7 Tue 15:30 H24

Attosecond charge transfer in atomic-resolution scanning tunnelling microscopy — •Katharina Glöckl[1], Simon Maier[1], Raffael Spachtholz[1], Carlos Bustamante[2], Korbinian Pürckhauer[1], Franz J. Giessibl[1], Franco Bonafé[2], Markus A. Huber[1], Angel Rubio[2], Jascha Repp[1], and Rupert Huber[1] — [1]Department of Physics & Regensburg Center for Ultrafast Nanoscopy (RUN), Universität Regensburg — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Scanning tunnelling microscopy (STM) driven with single-cycle terahertz pulses has afforded atomic-scale slow motion videos of single molecular orbitals. Driving tunnel currents with the carrier field of near-infrared light could improve the temporal resolution from ~100 fs down to attoseconds. Yet, competing multiphoton processes and thermal effects pose severe challenges in this spectral domain.

Here, we introduce an attosecond STM concept that is largely immune against thermal artifacts. By pulse synthesis, we periodically vary the waveform of single-cycle near-infrared pulses to drive tunnelling currents while keeping the thermal load on the tip constant. In a non-degenerate pump-probe scheme, we observe clear attosecond features in the sub-cycle currents and demonstrate atomic resolution by taking snapshot images of a single Cu adatom on a silver surface. Our results pave the way to recording the fastest relevant dynamics of electrons within atoms, molecules and quantum materials in actual attosecond atomic videography.

O 44: Poster Oxides and Insulator Surfaces: Structure, Epitaxy and Growth

Time: Tuesday 18:00–20:00 Location: P2

O 44.1 Tue 18:00 P2

The dynamic interaction of size-selected Pt clusters with CeO_2/Rh(111) — •Mina Soltanmohammadi, Johanna Reich, Barbara A.J. Lechner, and Friedrich Esch — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Germany

Recent studies on Pt clusters supported on ceria have revealed interesting cluster formation and redispersion processes that can be induced by cyclic redox treatments [1]. These catalysts' activity for combustion is linked to the verge of cluster formation. Here, we investigate the dynamic interaction of size-selected Pt clusters with CeO_2(111) thin films at the atomic scale, using a combination of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). We present a preparation protocol to obtain highly clean, crystalline and stochiometric CeO_2(111) thin films with extended terraces and well-defined monoatomic steps. Distinct oxygen vacancy distributions are obtained by either annealing in vacuum or reducing in a methanol atmosphere. We then systematically explore the interaction of Pt clusters with the support, particularly the mobility and sintering in dependence of the defect state. The influence of support stoichiometry and the parameters controlling the resulting cluster dispersion are presented. Finally, we present first studies of the Pt dispersion under cyclic oxidizing (O_2) and reducing (methanol) conditions at elevated temperatures, focusing on the resulting cluster configurations at the atomic scale.

[1] Farnesi Camellone et al., ACS Catal. 2022, 4859.

O 44.2 Tue 18:00 P2

Search for crystalline SiO_2 on the wet chemically treated 6H-SiC(0001) surface — •Paul Schöngrundner[1], Igor Sokolovic[2], and Ulrike Diebold[2] — [1]Department of Physical Chemistry, University of Graz, 8010, Austria — [2]Department of Applied Physics, Technical University of Vienna, 1040, Austria

A 6H-SiC(0001) surface was found to host a crystalline superstructure consisting of SiO_2 after wet chemical treatment. This surface was envisioned as a model system for surface chemistry studies. In order to replicate and optimize this film, chemical and thermal treatments were investigated systematically. Using atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED), an improved cleaning methodology was established, resulting in contaminant-free surfaces (except adventitious C), but they were terminated with amorphous SiO_2 instead of a crystalline film. If the sample was treated by repeating the original cleaning technique, which was finished with Extran and milliQ sonication, without subsequent boiling in H_2O, the original surface termination could be re-prepared. However, this was accompanied by P and Cr contamination. It is hypothesized that P and/or Cr contamination were ultimately responsible for the crystalline silicon oxide overlayer.

O 44.3 Tue 18:00 P2

Pulsed laser deposition of epitaxial hematite α-Fe_2O_3 thin films on $Al_2O_3(1\bar{1}02)$ — •Sarah Tobisch, Giada Franceschi, Michael Schmid, Gareth Parkinson, Ulrike Diebold, and Michele Riva — Institute of Applied Physics, TU Wien, Vienna, Austria

Hematite α-Fe_2O_3 is a widely used support material for catalysis due to its abundance and high stability at ambient pressures. However, the insulating nature of the material poses major challenges, as it makes it difficult to achieve sufficient conductivity for techniques such as scanning tunnelling microscopy (STM). Samples commonly consist of natural crystals that can contain a variety of impurities as well as structural defects. The former problem is hardly controllable while the latter can lead to mechanical instabilities. While the conductivity can be improved by growing Ti-doped epitaxial films, the synthesis of hematite single crystals is still in its infancy and the size of these crystals is insufficient for many surface-analysis techniques. Therefore, new strategies to ensure the growth of flat and atomically defined doped films without the need of natural-crystal substrates are highly desired.

In this work, epitaxial growth of Ti-doped Fe_2O_3 on $Al_2O_3(1\bar{1}02)$ was investigated using a pulsed-laser-deposition (PLD) system with high-pressure reflection high-energy electron diffraction (RHEED) to optimize the growth conditions and monitor the growth behavior. The morphology and composition of the film's surface was characterized using x-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and STM.

O 45: Poster Spins on Surfaces at the Atomic Scale

Time: Tuesday 18:00–20:00 Location: P2

O 45.1 Tue 18:00 P2

Scanning Tunneling Microscopy and Spectroscopy of YbPc2 Molecules — •Jonas Arnold[1], Kwan Ho Au-Yeung[1], Wantong Huang[1], Paul Greule[1], Christoph Sürgers[1], Wofgang Wernsdorfer[1], Mario Ruben[2], and Philip Willke[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Individual molecules constitute excellent building blocks for quantum technologies thanks to their small size, reproducibility and the benefit of self assembly. A promising class are rare-earth bis-phythalocyanine complexes [1]. In this investigation, YbPc2 molecules are studied using scanning tunneling microscopy (STM) and spectroscopy (STS) to identify potential indicators of a magnetic signature. In the gas phase, the YbPc2 molecule is expected to exhibit a radical spin localized at its ligands as well as an f-shell electron spin S = 1/2 and a nuclear spin (I = 1/2 and 5/2) for certain isotopes. Thus, this system is a potential candidate for a spin cascade [1]. We perform measurements on self-assembled multilayer islands of YbPc2 on Ag(100) that reveal distinct orbital features which vary for the first, second and third molecular layer. Similarly, the orbital signatures

change when introducing a thin dielectric decoupling layer of MgO between the molecule islands and the electron bath. We discuss these results in the context of charge transfer between the molecular film and the underlying substrate [2].
[1] Wernsdorfer, W. et al., Advanced Materials 31, 1806687 (2019). [2] Hollerer, M. et al., ACS nano 11, 6252-6260 (2017).

O 45.2 Tue 18:00 P2

Magnetic adatom manipulation on monolayer transition metal dichalcogenides — •Daniel Jansen[1], Katharina Offermann[1], Tfyeche Tounsi[1], Affan Safeer[1], Jeison Fischer[1], Arkady Krasheninnikov[2], Nicolae Atodiresei[3], Thomas Michely[1], Hannu-Pekka Komsa[4], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Jülich, Germany — [4]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Two-dimensional materials are found to host a large variety of correlated phases. A promising approach towards understanding and controlling these phases is by means of atomic manipulation.
Here we compare two systems for atomic manipulation experiments: Fe on 1H-MoS_2 and Fe on 1H-TaS_2. We find that manipulation of Fe on 1H-MoS_2 results in point defects (sulfur vacancies) [1], which we investigate using scanning tunneling microscopy and spectroscopy. In contrast, we find that single Fe adatoms can be laterally moved on 1H-TaS_2, enabling construction of lattices consisting of tens of adatoms. We additionally report on the observation of two inequivalent adsorption sites for Fe, hollow and Ta-top sites, which manifest as differences in the adatom's apparent height.
[1] Jansen et al., Phys. Rev. B, **109**, 195430, 2024

O 45.3 Tue 18:00 P2

Investigating the origins of spin-polarization in Au(111) : experiments vs theory — •Sourour Ayari[1], Laurent Nicolaï[1], Aki pulkkinen[1], Ridha Eddhib[1], Saleem Khan[1], Trung Phuc[1], Ján Minár[1], and Mauro Fanciulli[2,3] — [1]New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic. — [2]CY Cergy Paris University, France — [3]CEA Paris Saclay, France

This study explores the origins of spin polarization in semi-infinite Au(111), examining whether the observed spin polarization arises primarily from the system's initial states or solely through the Photoemission process. To address this, we will integrate both experimental and theoretical results to provide an understanding of this spin-polarization origins, we calculate the electronic band structure with and without the influence of Mott-Scattering, while isolating additional factors, such as the Rashba effect[1]. On the theoretical side the calculations are performed using the SPRKKR method [2,3] which is based on DFT calculations, which will account for fundamental effects, while the additional one-step model will account for the photoemission process.

[1]E. E. Krasovskii and E. V. Chulkov Phys. Rev. B 83, 155401 (2011) [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011) [3] J. Braun et al., Phys. Rev. B 88, 205409 (2013)

O 45.4 Tue 18:00 P2

Coherent driving of interacting spins in single molecules — •Maria Steiner and Andrea Donarini — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

The low energy spectrum of neutral closed shell molecules generically exhibits a set of singlet and triplet excited levels. The latter arises due to the exchange interaction between the unpaired electrons in singly occupied frontier orbitals. Moreover, the spatial anisotropy of these molecular states, combined with the spin-dipolar interaction, induces a zero-field splitting of the triplet. In recent AFM-ESR experiments on pentacene [1] Rabi oscillations between two of the split triplet states have been demonstrated. We now extend this concept to the full triplet space. By means of multiple frequency coherent driving, we investigate theoretically the rich dynamics of this molecular qutrit in search, for example, of the analogue of the dark states observed for Λ-systems in atomic physics.
[1] Sellies et al., Nature **624**, 64-68 (2023).

O 45.5 Tue 18:00 P2

A molecular spin on a scanning probe tip enables quantum sensing at the atomic scale — Taner Esat[1,2], Dmitriy Borodin[3,4], •Jeongmin Oh[1,2], Andreas Heinrich[3,4], Stefan Tautz[1,2,5], Yujeong Bae[3,4], and Ruslan Temirov[1,2,6] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich; Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology; Jülich, Germany — [3]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS); Seoul, South Korea — [4]Department of Physics, Ewha Womans University; Seoul, South Korea — [5]Experimentalphysik IV A, RWTH Aachen University; Aachen, Germany — [6]Faculty of Mathematics and Natural Sciences, Institute of Physics II, University of Cologne; Cologne, Germany

In this work, we fabricate a single-molecule quantum sensor on a scanning tunneling microscope (STM) tip by attaching Fe atoms and a PTCDA (3,4,9,10-perylenetetracarboxylic-dianhydride) molecule to the tip apex. The PTCDA molecule is a spin-1/2 system on the STM tip and serves as a two-level quantum system in a magnetic field. We probe this molecular spin system by electron spin resonance and achieve about 100 neV resolution in energy. The functionality of the quantum sensor we demonstrate by measuring the magnetic and electric dipole fields emanating from a single Fe atom and an Ag dimer on an Ag(111) surface with sub-angstrom spatial resolution [T. Esat, D. Borodin, J. Oh et al. Nat. Nanotechnol. 19, 1466 (2024)].

O 45.6 Tue 18:00 P2

Thermometry of a millikelvin scanning probe junction with spin-flip inelastic electron tunnelling spectroscopy — •Emilio Scontrino[1,3], Stefan Schulte[2,3], Taner Esat[3], Markus Ternes[1,3], Stefan Tautz[1,3], and Ruslan Temirov[2,3] — [1]RWTH Aachen — [2]Universität zu Köln — [3]Forschungszentrum Jülich, PGI-3, Germany

Organic molecules attached to the apex of a scanning probe tip have recently emerged as promising sensors for electric and magnetic fields at atomic scales [1, 2, 3]. Here, we functionalize the tip of a millikelvin scanning tunnelling microscope (STM) [4] with a 1,4,5,8-naphthalene tetracarboxylic dianhydride (NTCDA) molecule. We measure the inelastic spin-flip excitations of this molecular spin 1/2 system in an out-of-plane magnetic field of 7 T varying the temperature of the adiabatic demagnetization cryostat between 30 mK and 1.2 K. To perform thermometry of the STM junction we fit the temperature-dependent smearing of the spin-flip excitation spectra using the third-order perturbation theory in the Appelbaum-Anderson-Kondo framework [5].

[1] C. Wagner et al., Phys. Rev. Lett. 115, 026101 (2015) [2] B. Verlhac et al., Science 366 , 623 (2019) [3] T. Esat et al., Nat. Nano. 19, 1466 (2024) [4] T. Esat et al., Rev. of Sci. Instr. 92 (6) (2021) [5] M. Ternes, New J. Phys. 17, 063016 (2015)

O 45.7 Tue 18:00 P2

Investigation of the Kondo effect in complex, artificially built, single molecule structures — •Lars Pütz[1], Daria Sostina[1], Taner Esat[1,2], Stefan Tautz[1,2,3], Ruslan Temirov[1,4], and Markus Ternes[1,2,5] — [1]Peter-Grünberg-Institute for Quantum Nanoscience, Research Center Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Institute of Physics IV, RWTH Aachen University, 52074 Aachen, Germany — [4]Institute of Physics II, University of Cologne, 50937 Cologne, Germany — [5]Institute of Physics IIB, RWTH Aachen University, 52074 Aachen, Germany

In engineered spin systems, strongly correlated many-body phenomena such as nontrivial topology, Kondo screening and highly correlated long-range states can be constructed and studied by site-selective measurements with scanning tunneling microscope (STM) tips [C. Zhao et al., Nat. Nanotech. 2024]. Here we show how many-body phenomena evolve by controlled manipulation of NTCDA molecules on Ag(111) using the tip of an STM. Building small clusters of 2-5 molecules and tuning their spatial geometry reveals complexly patterned Kondo resonances and, in addition, an electric field-dependent strong increase in conductance, which we attribute to the collapse of Kondo correlations [S. Arabi et al., arXiv 2022]. Single NTCDA molecules on the other hand show no detectable spin signature, despite the clear formation of Kondo resonances in clusters where their high symmetry with respect to the surface is broken.

O 45.8 Tue 18:00 P2

Investigation of the Yu-Shiba-Rusinov states arising from single Fe atoms on superconducting $2H$-NbS_2 — •Margarete Huisinga, Werner M.J. van Weerdenburg, Lisa M. Rütten, and Katharina J. Franke — Fachbereich-Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Magnetic adatoms on a superconductor give rise to states within the superconducting gap due to the interaction of the unpaired spin(s) with the Cooper pairs of the substrate. These so-called Yu-Shiba-Rusinov (YSR) states are therefore isolated from the rest of the electronic structure of the system, which makes them interesting building blocks for artificial molecules or the design of band structures, if the YSR states of multiple atoms hybridize. The YSR states are especially long range on 2D materials, which enables hybridization over a large spacing. Previous experiments on the hybridization of YSR states performed on $NbSe_2$ were limited by a charge density wave [1], which is not present in $2H$-NbS_2.
Using scanning tunneling microscopy and spectroscopy, we investigate single Fe atoms on superconducting $2H$-NbS_2. We find that Fe adsorbs in two different adsorption sites on the substrate, each with a distinct set of YSR states. We map the spatial distribution of these YSR states to determine their symmetry and find long-ranged YSR features extending up to 4 nm. Additionally, we observe a tip-induced shift in the energy of the YSR states for one adsorption site species.
[1] Liebhaber et al. Nat Commun 13, 2160 (2022).

O 45.9 Tue 18:00 P2

Hybridization of Yu-Shiba-Rusinov states in magnetic clusters on Pb(111) — •Katharina Biel, Bharti Mahendru, Werner M. J. van Weerdenburg, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The unpaired spin of a magnetic impurity on a superconducting substrate interacts with the Cooper pairs via potential and exchange scattering. This leads to local in-gap bound states, so-called Yu-Shiba-Rusinov (YSR) states. The hybridization of close-by atoms can be described by linear combinations of the YSR states [1,2].

We investigated self-assembled manganese (Mn) and iron (Fe) clusters on superconducting lead (Pb(111)) by scanning tunneling microscopy and spectroscopy. While the topography essentially shows featureless protrusions, the differential conductance maps reflect characteristic shapes of the YSR states. We employ a phenomenological hybridization model [3] to simulate the observed shapes. In particular, we show atomic configurations which lead to chiral YSR patterns.

[1] Ruby, M., et al., PRL 120, 156803 (2018); [2] Amann, S., et al., PRB 108, 195403 (2023); [3] Rütten, L., et al., ACS Nano 18, 30798 (2024)

O 45.10 Tue 18:00 P2

Investigation of impurity states on the high-temperature superconductor $Bi_2Sr_2Ca_1Cu_2O_{8+x}$ via scanning tunneling microscopy — •Melvin Grumser, Verena Caspari, Werner M. J. van Weerdenburg, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

The interaction of magnetic impurities and superconductors gives rise to impurity states in the superconducting gap, which have been widely studied for s-wave superconductors [1]. For d-wave superconductors however, only few experiments addressing the interplay of local spins and Cooper pairs, governed by an anisotropic order parameter and non-vanishing density of states (DOS) in the superconducting gap have been reported [2,3].

Here, we investigated the interaction between the high-temperature d-wave superconductor $Bi_2Sr_2Ca_1Cu_2O_{8+x}$ and magnetic adatoms on the atomic scale using scanning tunneling microscopy. We present measurements conducted on scandium, iron and manganese adatoms, expected to display different amounts of in-gap states due to the different number of unpaired electrons. We find strong variations in the spectra that we ascribe to different adsorption sites and variations of the density of states across the substrate.

[1] W. Heinrich, I. Pascual, K. J. Franke, Progress in Surface Science 93 (2018)
[2]U. Erdenemunkh, M. C. Boyer, Physical review letters 117 (2016)
[3] J. Davis, Nature 411 (2001)

O 45.11 Tue 18:00 P2

Atomic-scale Josephson spectroscopy performed over magnetic clusters on Pb(111) — •Bharti Mahendru[1], Martina Trahms[1,2], Katharina Biel[1], Werner M. J. van Weerdenburg[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Université Grenoble Alpes, CNRS, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

When two superconducting leads are brought in close proximity, they form a Josephson junction (JJ). In a JJ, quantum tunnelling of Cooper pairs occurs without an applied voltage between the two superconductors with a phase difference. To study the properties of Cooper-pair tunneling at the atomic scale, a scanning tunneling microscope is a powerful tool. A JJ forms by approaching the tip to the sample. Previously, it has been shown that a Josephson junction including a single magnetic adatom shows non-reciprocity in the retrapping current [1]. This expression of the Josephson-diode effect was ascribed to the broken particle-hole symmetry induced by the Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap. Here, we investigate the effect of hybridized YSR states of self-assembled Fe clusters on Pb(111). We find non-reciprocal retrapping currents that we correlate with the asymmetry in the YSR states and their spatial distribution. [1] Martina Trahms et al., *Nature* 615, (2023)

O 45.12 Tue 18:00 P2

Driving nuclear spin transitions on a single atom using ESR-STM — •Hester Vennema, Cristina Mier Gonzalez, Evert Stolte, Rik Broekhoven, Jinwon Lee, and Sander Otte — Delft University of Technology, The Netherlands

The spin of a single nucleus is a prime candidate for quantum information applications due to its weak coupling to the environment and subsequently longer coherence times [1]. Using the high energy resolution of electron spin resonance (ESR) in combination with the high spatial resolution of scanning tunneling microscopy (STM), it is possible to measure the hyperfine interaction between the nucleus and an electron for single atoms on a surface [2].

A recent effort has successfully resolved the coherent dynamics of a hyperfine-driven interaction between nuclear and electron spin [3]. Moreover, the lifetime of the nuclear spin has been measured to be in the order of seconds [4].

In this study we use a double resonance measurement scheme to resolve nuclear spin transitions of a single 47Ti isotope with a spin of I=5/2. Additionally, we are able to selectively drive multiple transitions directly.

[1] Pla et al. (2013), Nature 496, 334-338
[2] Willke et al. (2018), Science 362, 336-339
[3] Veldman et al. (2024), Nat. Comm. 15, 7951
[4] E. Stolte et al. (2024), arXiv:2410.0870

O 45.13 Tue 18:00 P2

Nanoscale Control of Quantum States in Radical Molecules on Superconducting Pb(111) — •Chao Li, Jung-Ching Liu, Outhmane Chahib, Thilo Glatzel, Rémy Pawlak, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland.

Superconducting surfaces hosting magnetic impurities provide a promising framework for applications in quantum technology. Here, we demonstrate the manipulation of magnetic states in the radical molecule 4,5,9,10-tetrabromo-1,3,6,8-tetraazapyrene (TBTAP) deposited on a Pb(111) superconducting surface, utilizing low-temperature scanning tunneling microscopy. Tunneling spectroscopy reveals the presence of Yu-Shiba-Rusinov (YSR) states near the Fermi level for isolated TBTAP molecules. By varying the tip-molecule distance, we induce a quantum phase transition between singlet and doublet ground states. Furthermore, introducing a second TBTAP molecule enables tuning of the YSR state position through modifications in relative distance and orientation, with specific configurations leading to the splitting of YSR states. Extended molecular chains, up to pentamers, exhibit periodic patterns of charged and neutral molecules, where even-numbered chains form a distinct charged dimer structure at one terminus. This dimer position can be manipulated, allowing for information encoding within the chain.

O 45.14 Tue 18:00 P2

Exchange interactions of spin states in coupled triangular nanographenes — •Suyash Singh[1], Nils Krane[1], Elia Turco[1], Roman Fasel[1,2], and Pascal Ruffieux[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf (Switzerland) — [2]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland

Zigzag-edged triangular nanographenes (triangulenes) are promising realizations of spin qubits at a molecular level, with a total spin S scaling with the length of their edges. Chemical design and on-surface synthesis methods allow atomically precise engineering of carbon-based π–systems with strong spin-spin interactions, using triangulene units as building blocks. Exploiting the rules governing the exchange interactions, functional groups and spacer molecules, such as phenyl rings, can be used to tune the sign and magnitude of the exchange coupling between the triangulene units. We present the bottom-up fabrication of correlated spin platforms using the two smallest members of the triangulene family, the spin S=1/2 phenalenyl and S=1 [3]triangulene. We analyze the origin of spin-polarized states and spin excitations using a tight-binding and mean-field Hubbard Model for the π–orbital network. With an estimate of the couplings within the spin cluster, we describe it using an effective Heisenberg model. The spin excitations are then investigated experimentally using inelastic electron tunneling spectroscopy. Specifically, we summarize the results on dimers and trimers, where the exchange mechanisms can be investigated systematically by hydrogenation and selective re-activation of single spins.

O 45.15 Tue 18:00 P2

Properties of magnetic atoms on a hexagonal insulating lattice — •Johannes Schust, Henrik Lichtl, Julian Zeitler, Lukas Arnhold, Sebastian Loth, and Susanne Baumann — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

The symmetry of the immediate surrounding of an atom heavily influences its static properties and also governs its dynamics. For the exploration of atomic-scale systems by scanning tunneling microscopy (STM), the choice of a suitable thin film is thus key. While most preceding works take advantage of two- or four-fold underlying symmetries, we focus on the hexagonal surface of zinc oxide (ZnO) monolayers. Hexagonal substrates bear the potential for exploring spin frustration effects on a surface, realized by the assembly of magnetic nanostructures built atom-by-atom. ZnO, as a wide bandgap semiconductor [1], is employed to mitigate electron scattering between the Ag(111) substrate and the adsorbed species on the sample. We develop a reliable method to prepare the aforementioned substrate and carry out comprehensive characterization of cobalt (Co) and manganese (Mn) atoms in the present environment. These efforts provide the foundation for investigating novel dynamical aspects of frustrated systems on the atomic scale.

[1] A. Shiotari et al. J. Phys. Chem. (2014)

O 45.16 Tue 18:00 P2

Multiplet calculations of magnetic atoms on a hexagonal insulator — •Julian Zeitler[1], Johannes Schust[1], Henrik Lichtl[1], Lukas Arnhold[1], Sebastian Loth[1,2], and Susanne Baumann[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany

Novel designs for computational devices may offer improvements in energy efficiency, especially if they include a combination of storing and processing parts

in one unit. In such designs, the building blocks should enable slow and fast dynamics, and allow for precise control over the system. Atomic-scale frustrated spin systems combined with atom manipulation capabilities of a scanning tunneling microscope (STM) are a promising prospect in this field. Magnetic atoms placed on a thin hexagonal insulator, such as zinc oxide (ZnO), can potentially be used to realize such systems. As the magnetic atoms interact with their substrate, it is important to understand the substrate's influence on the atoms' characteristics. We use multiplet calculations to study the interactions of individual magnetic atoms with the ZnO substrate. With these calculations, we can make predictions about the magnetic characteristics of different atoms placed on top of this hexagonal substrate, in particular their orbital and spin moments. We are particularly interested in finding atomic-scale systems that, combined with atom manipulation capabilities of an STM, allow for further advancements in the field of atomic-scale frustrated spin systems.

O 45.17 Tue 18:00 P2

Exploiting YSR States for Driving Spin Transitions in a Magnetic Field — •Maneesha Ismail[1], Juan Carlos Cuevas[2], and Christian R. Ast[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Universidad Autónoma de Madrid, Madrid, Spain

In recent years, advances in the field of atomic scale electron spin resonance (ESR-STM) have made it possible to manipulate single spins and observe their interaction [1,2]. In this work, we exploit the tip confinement of superconductivity in a magnetic field to explore a new candidate system, namely Yu-Shiba-Rusinov states. We present how the Zeeman-split states behave under microwave irradiation. Our theory, which is based on a Green's function approach, corroborates the idea that the presence of the YSR state can be used to detect a change in the spin population. A new sample system could open the path to observing new phenomena in the field of spintronics and quantum computing.

1. K. Yang et al., Science 366 (6464), 509-512
2. L. Sellies et al., Nature 624, 64, 2023.

O 45.18 Tue 18:00 P2

Tuning the interaction between spin triplet states at the single-molecule level — Lorenz Meyer, •Maximilian Kögler, Robert Henninger, Nicolas Néel, and Jörg Kröger — Technische Universität Ilmenau, Ilmenau, Germany

In a scanning tunneling microscope junction, two molecular spins - one nickelocene (Nc) decorating the tip and another adsorbed on Pb(111) - are approached toward each other. Simultaneously, inelastic electron tunneling spectra reveal the evolution of spin excitations with increasing magnetic exchange interaction. An avoided energy level crossing occurs at the verge of the Nc-Nc contact. Modeling of the spectra hints at the exchange coupling of tunneling electrons to the Nc spins as the origin. Funding by the DFG through KR 2912/18-1 and KR 2912/21-1 and the BMBF through the ForLab initiative is acknowledged.

O 46: Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties

Time: Tuesday 18:00–20:00 Location: P2

O 46.1 Tue 18:00 P2

Electronic Properties of Interfaces between N-Heterotriangulene Donors and Strong Tetracyanoquinodimethane Acceptors — •Mohsen Ajdari[1], Jakob Roth[1], Ronja Pappenberger[1], Christian Walla[2], Ina Michalsky[3], Friedrich Maass[1], Milan Kivala[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Heidelberg University

N-Heterotriangulenes (N-HTAs) are promising functional molecules with significant potential for optoelectronic applications, in particular, as electron donors in donor/acceptor (D/A) systems. This study explores the electron-donating properties of two N-HTAs, N-HTA 550 and N-HTA 557, at interfaces with well-known tetracyanoquinodimethane acceptors, TCNQ and F4TCNQ. Using high-resolution electron energy loss spectroscopy (HREELS) combined with quantum chemical calculations, we investigated the electronic properties of D/A interfaces adsorbed on Au(111) [1]. For all D/A combinations, low-energy electronic transitions (E<2.5 eV) associated with charge transfer (CT) states are identified. Quantum chemical calculations rule out the formation of ground-state CT complexes. Instead, CT in the excited state, in which an electron-stimulated CT from the N-HTAs to TCNQs is the underlying process, is proposed. The energies of the CT states are determined by the values of the ionization potential and electron affinity of the involved donor and acceptor.

[1] M. Ajdari et al., J. Phys. Chem. C, 128, 14399-14406 (2024)

O 46.2 Tue 18:00 P2

Self-assembly of magnetic complex on Cu (111) using scanning tunneling spectroscopy: probing Kondo resonance and decomposition effects — •Behzad Mortezapour[1], Torben Adam[2], Eike Kuhlemann[2], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Germany

The spin-crossover complex bis-(hydro-tris-(3-methyl-pyrazolyl)-borat)-Iron(II) on Cu (111) at ambient temperature was investigated with a scanning tunneling microscope (STM) under ultrahigh-vacuum conditions at a temperature of 4.6 K. The three-dimensional molecules self-assemble into ordered two dimensional arrays while some decomposition also occurs. The STM images of the intact molecules exhibit a significant dependence on the bias voltage and spectra of the differential conductance (dI/dV) show a zero-bias resonance that we tentatively attribute to the Kondo effect. Time series of the current reveal abrupt transitions that possibly are linked to spin switching. In addition, negative differential resistance is observed from decomposed molecules.

O 46.3 Tue 18:00 P2

stochastic spin-state switching of a Fe(II) complex on Cu (111) — •jasmeen jasmeen[1], sujoy karan[1], karl ridier[2], gaël reecht[1], and manuel gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]LCC, CNRS and Université de Toulouse, UPS, INP, 31077 Toulouse, France

Spin-crossover (SCO) molecules exhibit different spin states that make them attractive for nanoscale memory applications. Using scanning tunneling microscopy (STM) at 4.5 K, we studied the [Fe(HB(1,2,4-triazolyl)3)2] complex adsorbed on a Cu (111) surface, focusing on the spin-state switching dynamics. Time traces of the tunneling current revealed switching in the order of milliseconds, which we investigated under a range of bias voltages and currents, providing insights into the stochastic response of this system.

Controlled switching of individual molecules induced by voltage pulses was successful, but also drove a pronounced neighborhood effect: switching a target molecule simultaneously influenced adjacent ones. These events suggest an intermolecular interaction acting on the neighboring molecules due to the conformational changes of the target molecule.

These findings help improving the understanding of electron-induced switching of SCO molecules. Funding from the CRC 1242 is acknowledged.

O 46.4 Tue 18:00 P2

STM Investigation of Molecular Double Motors — •Ken Kolar[1], Grant Simpson[1], Ben Feringa[2], and Leonhard Grill[1] — [1]Dept. of Physical Chemistry, University of Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, Netherlands

A molecular motor is a molecule with stator and rotor chemical groups which undergo directional motion relative to each other. They represent potential building blocks for nanoscale machinery and their motion on surfaces is of particular interest. With high-resolution imaging from a scanning tunnelling microscope (STM), we revealed distinct appearances of different conformers of a molecule containing two motor units. Furthermore, motion induced by voltage pulses from the STM tip was studied in detail, investigating unidirectionality. Finally, double motors with additional alkane chains attached to them were deposited, showing distinguishable appearances. The experiments showed that the alkane chain conformation can impact the motion of the molecules.

O 46.5 Tue 18:00 P2

Excited state alignment of molecular orbitals on the ferroelectric WTe2 bulk crystal — •Jannis Lessmeister[1], Ralf Hemm[1], Joohyung Park[2], Martin Aeschlimann[1], Oliver L.A. Monti[2], and Benjamin Stadtmüller[3] — [1]Rheinland-Pfälzische technische Universität Kaiserslautern-Landau and Research center OPTIMAS, Kaiserslautern, Germany — [2]University of Arizona, Tucson, USA — [3]Universität Augsburg, Augsburg, Germany

The interaction between organic molecules and ferroelectric domains on WTe_2 offers a promising pathway for tuning the electronic properties of hybrid systems. WTe_2, a layered transition metal dichalcogenide, exhibits ferroelectricity in its few-layer form due to broken inversion symmetry, resulting in switchable polarization domains. When organic molecules are deposited onto the surface, the local electronic environment created by these ferroelectric domains significantly influences molecular adsorption and electronic coupling.

Utilizing real- and momentum-space photoemission electron microscopy, we investigate how the ferroelectric properties of WTe_2 modulate the alignment of excited state energy levels at the FePc/WTe_2 interface. Our study elucidates the charge transfer behavior and interaction strength, exploring the role of local electric polarizations for tuning the energy level alignment in molecule-2D material heterostructures.

O 46.6 Tue 18:00 P2

Momentum space signatures of molecular orbitals on a ferromagnetic surface — •Martin Anstett[1], Lu Lyu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The integration of organic molecules with ferromagnetic surfaces is a promising approach to advance spintronic applications. The spin functionalities depend not only on the molecular properties, but also on the energetics and spin polarization of so-called hybrid interface states, which arise due to the hybridization between molecular orbitals and substrate states.

This work focuses on momentum space imaging of the adsorption-induced modification of molecular orbitals on ferromagnetic surfaces at room temperature. This is challenging due to the lack of ordered or aligned molecules on highly reactive magnetic substrates, which is required for momentum space imaging using ARPES. This limitation can be overcome by using ultrathin cobalt films on Au(111) as a ferromagnetic platform. On this surface, we prepare long-range ordered superstructures using iron phthalocyanine molecules. We combine spin- and momentum-resolved photoemission spectroscopy with photoemission orbital tomography to study the characteristic emission pattern of the orbitals of the adsorbed molecules. Our analysis reveals how the molecules arrange on the cobalt surface, producing distinct photoemission signatures associated with individual molecular orbitals.

O 46.7 Tue 18:00 P2

Thermal-Driven Coordination Effect for Structural and Electronic Tailoring of a Metal-Organic Network — •Jonas Gödde[1], Lu Lyu[1,2], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany

Two-dimensional metal-organic porous networks (2D-MOPNs) have emerged as a unique material platform for designing structural tessellations and emergent electronic states on surfaces. The metal centre in a 2D-MOPN plays a vital role in bridging network and substrate. In this study, we investigate the cobalt-coordination effects in cyano-functionalized hexaaza-triphenylene-hexacarbonitrile (HATCN) on Ag(111). Scanning tunnelling microscopy (STM) reveals that HATCN self-assembles into a well-ordered porous network. A partially occupied LUMO state observed by angle-resolved photoemission spectroscopy (ARPES), indicates charge transfer from the substrate to the molecules. After cobalt deposition, the robust equilibrium, between intermolecular and substrate interactions, preserves the porous structure and molecular orbital states of HATCN, while trapping cobalt in the low-potential pores. Upon post-annealing the molecules coordinate with cobalt atoms, inducing a structural transition and creating distinct energy and momentum states. These results provide insights into tailoring 2D-MOPNs for applications in electronics and spintronics.

O 46.8 Tue 18:00 P2

Spectroscopic study of the interface between organic molecules and platinum telluride thin films — •Lorenz Klein, Hibiki Orio, Romana Ganser, Muthu P. T. Masilamani, Maximilian Ünzelmann, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik VII & Würzburg-Dresden Cluster of Excellence, Würzburg, Germany

Van der Waals heterostructures of organic molecules and transition metal chalcogenides (TMCs) represent excellent model systems for the study of weak molecule-substrate interactions.

Here, we use two phases of metallic platinum telluride, which both host spin-polarized surface states in their electronic surface band structures. Using those as substrates, we deposit copper phthalocyanine (CuPc) and study the resulting atomic and electronic interface structure by means of x-ray (XPS) and angle-resolved photoemission spectroscopy (ARPES) as well as low-energy electron diffraction (LEED). On that basis, we discuss the differences in surface ordering, work function, and the binding energies of the observed molecular features.

O 46.9 Tue 18:00 P2

Fluorescence spectroscopy of linear trans-quinacridone (QA) on KCl/Ag(100): The influence of KCl layer thickness — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

The organic dye-molecule linear QA has attracted interest as a fluorescent probe molecule in STM luminescence (STM-LE) experiments [1]. We have performed fluorescence spectroscopy of multilayers on the bare Ag(100) surface and highly diluted layers of QA on an epitaxially grown thin KCl film on Ag(100) under UHV.

We find spectra that are reminiscent of solid state spectra for multilayers of QA on Ag(100). In addition, we see blue-shifted spectra for highly dilute QA layers (0.0005 ML – 0.1 ML) with a multitude of spectral features. We find that the stability of these spectral features under laser illumination varies depending on the thickness of the underlying KCl layer. Spectra are stable at 13 K for QA on 3-4 layers of KCl. However, on 6-8 layers of KCl, a spectral red-shift and a loss of FL-intensity is induced upon laser illumination at 13 K. We attribute these findings to a diffusion barrier of QA on KCl films that is dependent on the KCl-film thicknesses because the long-range interactions with the Ag(100) substrate are relevant [2].

[1] Phys. Rev. Lett. 2023, **130** (12), 126202.
[2] J. Phys. Chem. C 2023, **127** (49), 23814-23826.

This work was supported by the DFG through the research training group 2591.

O 46.10 Tue 18:00 P2

Field driven crossover of bonding and antibonding states in excitonic aggregates — •Amandeep Sagwal[1,2], Rodrigo Cezar De Campos Ferreira[1,3], Petr Kahan[1], Tomáš Neuman[1], and Martin Švec[1,3] — [1]Institute of Physics, Czech Academy of Sciences — [2]Faculty of Mathematics and Physics, Charles University; Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The present study aims to examine the effect of an electric field on the excitonic states of chromophore aggregates confined in optical nanocavity of a low-temperature SPM. Utilizing an optical configuration intended for near-field spectroscopies, tip-enhanced photoluminescence (TEPL) is used to investigate PTCDA molecules, deposited on a thin decoupling layer of NaCl on Ag(111) surface. A different energy shift is observed consistently between the bonding and antibonding excitonic emission lines in the spectra of dimer, trimer, and tetramer aggregates, in some cases even leading to a crossover. Typically, the antibonding states manifest a larger blue shift with increasing positive bias voltage applied on the gate electrode (substrate). We discuss the phenomenon using TD-DFT simulations and many-body state diagrams.

O 46.11 Tue 18:00 P2

Near-field spectroscopy of vibronic states of molecular aggregates — •Sidhartha Nayak[1], Fulu Zheng[2], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Department of Physics, Ningbo University, Ningbo, China

Strong dipole-dipole interactions between molecules give rise to delocalized electronic excited states in molecular aggregates, which determine their optical properties such as absorption. In near-field spectroscopy, the absorption spectrum of an aggregate is obtained when the molecules interact with electromagnetic radiation that is inhomogeneous across the length of the aggregate. Theoretically, by considering the near-field radiation from the apex of a metallic tip as a source of a localized field, it has been shown that the spectra of the aggregate reveal it's purely electronic states that are inaccessible through traditional far-field methods [1, 2]. In this contribution, we study aggregates composed of molecules with internal vibrational modes that are strongly coupled to electronic excitations, leading to non-Markovian phenomena. Using a local field method, which is numerically inexpensive, we observe that the vibronic states of aggregates are revealed in the near-field spectra and the spectra are comparable to those obtained by using a more accurate but computationally intensive method [3].

[1] X. Gao and A. Eisfeld, *J. Phys. Chem. Lett.* 9, 6003 (2018)
[2] S. Nayak, F. Zheng and A. Eisfeld, *J. Chem. Phys.* 155, 134701 (2021)
[3] D. Suess, A. Eisfeld and W. T. Strunz, *Phys. Rev. Lett.* 113, 150403 (2014)

O 46.12 Tue 18:00 P2

The Luminescence of Rylene Derivatives — •Petr Kahan[1], Rodrigo Ferreira[1,2], Amandeep Sagwal[1], Jiří Doležal[2], and Martin Švec[1,2] — [1]Institute of Physics, Czech Academy of Sciences — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The exploration of single-molecule luminescence using scanning tunneling microscopy (STM) is a vividly developing area of research. A number of works using STM-PL/EL and TERS techniques addressing the photophysics at the true single-molecule limit have employed rylene dyes for their known luminescent properties [1,2]. However, up to this point, a thorough comparison investigating the absorption and luminescent characteristics of molecules that share similar rylene-based configurations has not been carried out. This study presents a comparative analysis with the tip-enhanced spectromicroscopy in STM nanocavity on isolated molecules such as NTCDA, PTCDA, and DBP [3]. The findings reveal surprisingly distinct characteristics of each species; notably of their photoluminescence (PL) fingerprints and photocurrent maps. This shows the versatility of chemically related species, which holds promise for tailoring custom opto-electronic functionality in molecular aggregates.

[1] Doležal, J. et al. ACS Nano 16, 1082*1088 (2022). [2] Kimura, K. et al. Nature 570, 210*213 (2019). [3] Kröger, J. et al. Nano Lett. 18, 3407*3413 (2018).

O 46.13 Tue 18:00 P2

Spin Hall Magnetoresistance as a Probe for Chiral-Induced Spin Selectivity — •Simon Sochiera[1], Ashish Moharana[1], Yael Kapon[2], David Anthofer[1], Fabian Kammerbauer[1], Akashdeep Akashdeep[1], Shira Yochelis[2], Mathias Kläui[1], Yossi Paltiel[2], and Angela Wittmann[1] — [1]Institute for Physics JGU, Mainz, Germany — [2]Hebrew University of Jerusalem, Jerusalem, Israel

Chiral molecules have gained significant attention in the spintronics community due to their ability to polarize electron spin angular momentum without any heavy metal atoms via the chiral-induced spin selectivity (CISS) [1] effect. Several optical and electrical methods confirmed the CISS effect. However, despite numerous theoretical approaches, the fundamental mechanisms of the CISS effect are still an open question. A recent experiment [2] reported a significant modulation of spin-to-charge conversion with chiral molecules in a spin-pumping experiment. Building on this result, we create a hybrid structure by combining a well-established spin Hall magnetoresistance (SMR) experiment with chiral molecules. The SMR relies on the reflection and absorption of spin currents at interfaces adjacent to a layer exhibiting an (inverse) spin Hall effect, such as a heavy metal. This allows for direct probing of the spin-to-charge conversion modulation by chiral molecules. Combined with the results established in the spin-pumping experiment, this paves the path toward designing new chiral-molecule-based spin-torque devices.

[1]: R. Naaman et al., Nat. Rev. Chem. 3, 250 (2019)
[2]: A. Moharana et al., arXiv:2402.19246 (2024)

O 47: Poster Electron-driven Processes

Time: Tuesday 18:00–20:00 Location: P2

O 47.1 Tue 18:00 P2

Non-equilibrium electron distribution effects in ultrafast light-driven desorption dynamics — •Matthew Larkin, Henry Snowden, and Reinhard J. Maurer — University of Warwick, Coventry, UK

At metal surfaces, light excitation drives electronic states out of the (thermal) Fermi-Dirac distribution. The resulting non-equilibrium electronic distribution can induce coupled electron-nuclear dynamics that lead to ultrafast structural processes such as light-driven desorption of molecules. As non-equilibrium electron distributions in metals are short-lived, their role in the mechanics of light-driven surface dynamics remains insufficiently understood. In this work, we perform mixed quantum-classical dynamics simulations using a variant of the trajectory surface hopping method where electrons and nuclei are propagated simultaneously and electronic transitions between hundreds of electronic states can be captured. We describe light-generated non-thermal electron distributions as initial conditions to those dynamics. For simple 1D and 2D model systems of atomic and molecular desorption from metal surfaces, we study the role of non-thermal electrons by simulating light-driven desorption probabilities for comparable thermal and non-thermal electronic distributions and discuss the future applicability of this approach for high-dimensional dynamics.

O 47.2 Tue 18:00 P2

Spin effects in ultrafast non-equilibrium dynamics at surfaces — •Ash Baldwin and Reinhard J. Maurer — University of Warwick, Coventry, United Kingdom

Energy, charge, and spin transfer are important factors in modelling ultrafast gas-surface dynamics such as hyperthermal scattering and light-driven dynamics at surfaces. In particular, on metal surfaces, nonadiabatic energy dissipation is an important energy transfer channel in atomic and molecular dynamics at surfaces. In cases of adsorbates with unpaired spin, an additional question arises if and under which conditions the spin moment of the adsorbate survives the scattering event. The challenge lies in capturing the explicit electron correlation in the electronic structure and its effect on the coupled electron-nuclear motion, which mean-field dynamics methods cannot fully capture.

Here, we model the fate of adsorbate spin during scattering from a metal surface using the Newns-Anderson model. We go beyond previous works by simulating the nuclear dynamics beyond mean-field Ehrenfest dynamics, using stochastic trajectory surface hopping methods. Our model is applied to study the spin survival probability of hydrogen atoms on copper and platinum as a function of various model parameters and initial conditions such as the adsorbate kinetic energy and the adsorbate-metal coupling strength to identify the regime in which a finite spin survival probability can be measured.

O 47.3 Tue 18:00 P2

Adsorbate motors: toward tuning unidirectionality by chemical functionalisation — •Grant J Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]University of Liverpool, UK

The purpose of a molecular motor is to convert external energy into unidirectional motion. Feringa-type molecular motors, in which double-bond isomerisation leads to large geometric changes in the molecule, are known to undergo rapid unidirectional motion in solution but often have a reduced function when adsorbed on a surface. In contrast, recently discovered adsorbate motors [1] do not exhibit large structural changes and thus their motion is efficient and unidirectional when adsorbed on a metal surface. Using a scanning tunnelling microscope (STM), we track such motion at the single-molecule scale. The motion is triggered by an internal proton transfer reaction. We further show that, by altering the local chemical structure, this tautomerisation can be affected and may result in modulation of the unidirectional molecular translation.

[1] G. J. Simpson, M. Persson, L. Grill, Nature, 621, 82-86 (2023)

O 47.4 Tue 18:00 P2

Creation, Displacement, and Dynamics of Individual Phasons on Si(001) — •Gaël Reecht, Michael Horn-von Hoegen, and Manuel Gruber — Universität Duisburg-Essen, Duisburg, Germany

The Si(001) surface, characterized by buckled dimers resulting from dangling bond pairing, exhibits a variety of structural configurations. The energetically favorable c(4x2) reconstruction can be manipulated into the p(2x2) configuration, differing by a glide of adjacent rows. The interface between these two phases is known as a phason [1]. Despite its significance in structural phase transitions, the mechanisms driving phason propagation remain poorly understood.

In this study, we employ low-temperature scanning tunneling microscopy to explore the diffusion of individual phasons under tip-induced excitation. We systematically examine the effects of tunneling current, bias voltage, and electric field on the formation and displacement of these structural defects. Phason motion below the STM tip results in stochastic jumps in tunneling current, which we analyze through time-resolved measurements. These findings shed light on the displacement dynamics of phasons and enhance our understanding of the underlying processes. We gratefully acknowledge funding from the CRC1242.
[1] Y. Pennec et al., Phys. Rev. Lett., 96, 026102 (2006).

O 47.5 Tue 18:00 P2

Triplet exciton dynamics at the tetracene/a-Si/c-Si(111) interface — •Marvin Krenz[1,2], Simone Sanna[1], Wolf Gero Schmidt[2], and Uwe Gerstmann[2] — [1]Institut für Theoretische Physik, Justus-Liebig Universität Gießen, 35392 Gießen, Germany — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Exciton transfer is highly relevant for many physical, chemical, and biological processes. The transfer of triplet excitons across the tetracene-silicon interface in sensitized solar cells is a recent example in this context [1]: The excitons, generated by singlet fission in tetracene (Tc), promise to increase the cell efficiency from the single-junction limit of 29% to values as high as 35% [2]. In a previous work, we showed the significance of dangling bond (db) defects for the triplet transfer [3] at a model interface, where tetracene was bonded to an ideal c-Si(111) surface. Here, we present ab initio calculations for a more realistic structure, with a thin film of amorphous silicon (a-Si:H) in-between, resulting in a Tc/a-Si/c-Si model structure. We find that dbs are vital for the exciton transfer also in this case. Dbs at the a-Si/c-Si interface or in the a-Si interlayer itself affect the exciton transfer differently. Generally, it is found that the a-Si layer is energetically favourable for excitation transfer. However, the exciton electron tends to be trapped in a-Si conduction band tail states. Thus, the exciton transfer requires an external field to be completed. [1] M. Einzinger et al. Nature 571, 90*94 (2019). [2] A. Rao et al., Nat. Rev. Mater. 2, 17063 (2017). [3] M. Krenz et al., Phys. Rev. Lett. 132, 076201 (2024)

O 48: Poster Surface Dynamics

Time: Tuesday 18:00–20:00 Location: P2

O 48.1 Tue 18:00 P2

Atomistic modeling of ultrafast laser induced structural changes in Bismuth — •Sahar Bakhshi Sangari, Jimiben Patel, Bernd Bauerhenne, and Martin Garcia — Institute of Physics, University of Kassel, Kassel, Germany

We present a temperature-dependent interatomic potential for laser-excited bismuth, $\Phi_{Bi}(Te)$, developed using a database of temperature-dependent density functional theory (DFT) calculations. Bismuth is a widely studied material in experiments, yet theoretical studies exploring its atomic dynamics following femtosecond laser excitation remain scarce. Our work compares the physical properties predicted by $\Phi_{Bi}(Te)$ with those obtained from ab initio simulations, demonstrating its reliability. We use $\Phi_{Bi}(Te)$ to describe, in the framework of a generalized two-temperature-model molecular dynamics (TTM-MD) method, laser induced thermal and nonthermal ultrafast structural changes in Bi. We compute the time evolution of selected Bragg peaks and directly compare them with experimental observations. This approach enables efficient and accurate modeling of complex material behaviors, providing a valuable alternative to computationally intensive temperature-dependent DFT simulations.

O 48.2 Tue 18:00 P2

Design and Characterization of Optical Cavities for Light-Induced Phase Transitions in Indium-Based Peierls Insulators — •Florian Spickmann[1,2], Sierra Randall Heinrich[1,2], Sebastian Zafra Koch[1,2], Murat Sivis[1,2], Hannes Boeckmann-Clemens[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

The integration of quantum materials into optical cavities enables active control of their properties through enhanced light-matter interactions. Low-dimensional materials, such as Peierls insulators, are particularly sensitive to external stimuli, making them ideal candidates for such studies [1]. This work focuses on designing and fabricating optical resonators on (111) silicon membranes, including slab waveguides, ridge waveguides, and ring resonators. The structures are created using focused ion beam (FIB) milling and electron beam lithography (e-beam), with light coupling achieved via integrated gratings. Characterization of the resonators is performed using Fabry-Pérot interferometry. Future studies will employ ultrafast low-energy electron diffraction (ULEED) to visualize light-driven phase changes in indium wires localized on these optical resonators, representing a promising model system for cavity-controlled light-matter interaction in condensed matter.

[1] Böckmann, Hannes, et al., Structural Dynamics 9.4 (2022)

O 48.3 Tue 18:00 P2

Ultrafast LEED Study of Bismuth Thin Films on Silicon (001) — •Nandana V Uday[1], Felix Kurtz[1], Jonas Fortmann[3], Alp Akbiyik[1], Michael Horn-von-Hoegen[3,4], and Claus Ropers[1,2] — [1])Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany — [2]4th Physical Institute ,Solids and Nanostructures, University of Göttingen, 37077 Göttingen, Germany — [3]University of Duisburg-Essen, 47057 Duisburg, Germany — [4]Center for Nanointegration (CENIDE), 47057 Duisburg, Germany

The interface between two materials in a heterostructure serves as a barrier to the diffusion of thermal energy, thereby hindering heat flow across the boundary. On the nanoscale, heat transport may further be modified. Recently, it was shown that the thermal transport from Bi film into a Si substrate is reduced for films thinner than the phonon mean free path, due to phonon trapping by total internal reflection [1]. To study the non-equilibrium phonon dynamics in this process, ultrafast low-energy electron diffraction (ULEED) is suitable and direct means providing ultrafast temporal and high momentum resolutions. By analyzing the momentum-resolved map of a transient inelastic scattering background [2], we aim to identify phonon trapping, depopulation, and thermalization. As a first step, we monitor the heat transfer by phonons through the thin film-substrate interface, extracting cooling times from the transient lattice temperature of the bismuth film.

O 48.4 Tue 18:00 P2

Predicting and modelling incommensurate charge density waves in 1H-$TaSe_2$ via downfolding approach — •Clara Pfister[1,2], Laura Pätzold[1], and Tim O. Wehling[1,2] — [1]I. Institute of Theoretical Physics, U Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg

Studying the emergence and thermodynamic behaviour of symmetry-broken phases such as charge density waves (CDWs) in solids is of great interest to deepen our understanding of collective phenomena and interactions between electrons and the crystal lattice. Incommensurate CDWs (ICCDWs) are especially intriguing because a realistic and efficient computational method to predict them has not been developed yet. To model ICCDW phases in the exemplary transition metal dichalcogenide material 1H-$TaSe_2$, we employed a downfolding approach that reduces the electronic degrees of freedom by retaining only the low-energy subspace relevant to CDW formation. This method achieves a computational speed-up of approximately five orders of magnitude compared to purely ab initio calculations [1], making it possible to simulate sufficiently large supercells efficiently. Our approach allows for modelling the ICCDW with reasonable accuracy, with the predicted temperature range for its occurrence agreeing well with experimental results of the ICCDW in undoped 2H-TaSe2 [2]. This suggests that our approach is applicable for the description of other materials exhibiting ICCDWs.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)
[2] X. Shen et al., *Nat. Commun.* **14**, 7282 (2023)

O 49: Poster Nanostructures at Surfaces

Time: Tuesday 18:00–20:00 Location: P2

O 49.1 Tue 18:00 P2

Au induced nanostructures on Si(110) — •Stephan Appelfeller — MAX IV Laboratory, Lund University, Sweden

The deposition and annealing of small amounts of Au on clean Si substrates often lead to enticing nanostructures showing, e. g., spin ordering on vicinal Si(111) substrates or self-doping by adatoms on planar Si(111). A curious case are Au induced nanostructures on Si(110) for which the phase diagram is known in the submonolayer to monolayer regime, but for which few detailed studies exist, although, quasi-1D metallicity has been proposed for one of the nanostructures.

Here, the various nanostructures and their evolution are studied in real space using scanning tunnelling microscopy measured in MAX IVs SPM Support Lab, with core-level and angle-resolved photoemission spectroscopy obtained at the FlexPES beamline of the MAX IV Laboratory. For lowest Au coverages, a 2x1 superstruture showing a distinct Au 4f core-level component forms. With increasing Au coverage, rows of 2x3 subunits develop leading to the formation of the 2x5 reconstruction with quasi 1D-metallicity and the two-domain (4,0)x(±1,3) high coverage phase, which shows a high stability and recoverability in UHV. This stability is shared with Au silicide nanowires, which grow in the mono- to multilayer Au coverage regime. Since there are no stable bulk Au silicides, the observation of Au silicide nanowires is a beautiful reminder that surfaces and interfaces in general are different and often deviate from bulk expectations.

O 49.2 Tue 18:00 P2

XPS study of CuO, WO3 and CuWO nanoparticles-based films — •Michal Procházka[1], Kalyani Shaji[2], Stanislav Haviar[2], Eliška Benediktová[2], Radomír Čerstvý[2], Ján Minár[1], Petr Zeman[2], and Jiří Čapek[2] — [1]New Technologies - Research Centre, University of West Bohemia, Univerzitní 8, Plzeň, 301 00, Czech Republic — [2]Department of Physics and NTIS - European Centre of Excellence, University of West Bohemia, Univerzitní 8, Plzeň, 301 00, Czech Republic

Interest in clean and sustainable technologies is rapidly growing and hydrogen is widely used in this field. With this development, more emphasis is placed on hydrogen gas sensors as hydrogen poses significant risks due to its explosive nature and flammability [1]. Structural parameters and surface properties plays a significant role in interaction of gas with sensor material [2]. Therefore, the nanoparticles of various materials are more and more explored. To understand the surface evolution after annealing in the air we measured XRD, SEM and XPS of CuO, WO3 and CuWO nanoparticles-based films prepared by magnetron-based gas aggregation technique.

[1] P. S. Chauhan, S. Bhattacharya, Hydrogen gas sensing methods, materials, and approach to achieve parts per billion level detection: A review, Int. J. Hydrogen Energy. 44 (2019) 26076-26099.

[2] H. Zhao, Y. Wang, Y. Zhou, Accelerating the Gas-Solid Interactions for Conductometric Gas Sensors: Impacting Factors and Improvement Strategies, Materials. 16 (2023).

O 49.3 Tue 18:00 P2

Hydroxyl Groups on Different Metal Doped Co_3O_4 Particle Catalysts Observed by Sum Frequency Generation Vibrational Spectroscopy — •Furong Yan[1], Carsten Placke-Yan[2], Zhipeng Huang[1], Yujin Tong[1], and R. Kramer Campen[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen — [2]Faculty of Chemistry and Institute of Inorganic Chemistry, University of Duisburg-Essen

Metal-doped Co_3O_4 nanoparticles are promising catalysts for the electrochemical oxygen evolution reaction (OER), with surface Co-OH groups playing a critical role in the water oxidation cycle. However, the influence of metal doping on the behavior of surface OH groups and its subsequent effect on OER activity remains uncertain.

Here, we investigate the effects of metal doping (Mn and V) on the bonding of OH groups using sum frequency generation (SFG) vibrational spectroscopy. Our results reveal that Mn-doped Co_3O_4 exhibits stronger bonding between OH groups and the surface compared to both pristine Co_3O_4 and V-doped Co_3O_4, leading to a reduction in OER activity. We propose two mechanisms: (1) an excess of OH groups can block active sites and increase charge transfer resistance, and (2) the stronger Co-OH bonds in Mn-doped Co_3O_4 may hinder the cleavage of Co-OH bonds, thereby impeding the OER process. These findings provide valuable insights into how surface interactions with OH groups can be tailored to optimize OER catalytic performance.

O 49.4 Tue 18:00 P2

Coral-like structures on nickel surfaces obtained by nitrogen plasma treatment — •Christina Meinert, Timo Wagner, Felix Schaumburg, Moritz Sünner, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics, University Duisburg-Essen

For electrochemical processes, nickel sheets are commonly used as electrode material because of their low cost and easy handling. Here we report on the use of a microwave induced remote nitrogen plasma to change the surface of the nickel, improving the electrochemical and mechanical properties of the nickel electrode. During this process the surface obtains coral-like nanostructures and a nitridation of the nickel can be detected. AFM is employed to characterize these evolved nanostructures. Furthermore, EDX, Raman Spectroscopy and XPS are used to identify the chemical composition of the surface. In addition, wettability is probed as this is important for the efficiency of electrolysis. The plasma process is also applied to more complex surfaces than nickel plates such as wires and meshes. This allows to investigate the feasibility and limitations of treating these substrates.

O 49.5 Tue 18:00 P2

Exploring Topological Boundary Modes in Atomically Assembled Quantum Structures — •Adrian Weindl, Christoph Setescak, and Franz J. Giessibl — Faculty of Physics, University of Regensburg, D-93053 Regensburg, Germany

Single-atom and single-molecule manipulation enables the construction of quantum simulators: artificial structures assembled atom-by-atom or molecule-by-molecule to emulate key properties of complex systems that are challenging or impossible to fabricate directly. Using scanning tunneling microscopy (STM) and atomic force microscopy (AFM), we create two atomic-scale structures from individual CO molecules on Cu(111): a 1D Su-Schrieffer-Heeger (SSH) chain and a 2D Kagome lattice.

The 1D SSH chain represents a fundamental system capable of hosting topological boundary modes. We investigate the interaction between these boundary modes and the AFM tip. As the boundary modes are spatially localized and pinned in energy, they are not expected to undergo chemical bonding, unlike the bulk states of the chain, which may exhibit such interactions.

The 2D Kagome lattice on Cu(111) was initially proposed as a higher-order topological insulator, a classification that remains under debate. Through STM and AFM measurements, we aim to contribute to this ongoing discussion by introducing defects and analyzing the bonding behavior of the purported topological corner modes.

O 49.6 Tue 18:00 P2

Au vs. Ag: How Does the Choice of Substrate Influence the Formation of SAMs with Carboxylic Head Groups? — •Verena Müller[1], Julian Picker[1], Daniel Hüger[1], Christof Neumann[1], Marco Gruenewald[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]Friedrich Schiller University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Self-assembled monolayers (SAMs) enable modification of various solid substrates at the molecular level, providing a wide range of applications in nanoscience and nanotechnology, *e.g.*, photonics, organic electronics and biochemical sensing.

In this contribution, we present a systematic investigation of the formation of SAMs with carboxylic head groups (–COOH) on Ag and Au substrates. To this end, we analyze the results for three molecular precursors: a Ru^{II}-polypyridine complex photosensitizer, hexadecanoic acid and *p*-terphenyl-4-carboxylic acid. Complementary surface science characterization methods - including X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), scanning tunneling microscopy (STM) and polarization-modulation infrared reflection absorption spectroscopy (PM-IRRAS) - were employed to confirm the successful SAM formations. The obtained results are utilized to gain insight into the nature of the chemical interaction between the carboxylate and the metal surface.

O 49.7 Tue 18:00 P2

Phase Transitions of Naphthalene-2,3-carbonitride Steered by Solvent Effects and Metal Ion Concentration Variation — •Longnan Yu[1], Li Wang[2], and Xiaoqing Liu[3] — [1]KIT, Karlsruhe, Germany — [2]Nanchang University, Nanchang, China — [3]Nanchang University, Nanchang, China

This study explores the structural phase transitions of naphthalene-2,3-carbonitride (2,3-DCN) on highly oriented pyrolytic graphite (HOPG) influenced by varying solvents and Cu2+ ion concentrations. By combining scanning tunneling microscopy and density functional theory, it is revealed that in 1-nonanoic acid,Cu2+ ions coordinate with 2,3-DCN and other ligands (Cl- or 1-nonanoic acid), forming structures with a coordination number of 4 that depend on the 2,3-DCN to Cu2+ molar ratio. In contrast, in 1-heptanoic acid,Cu2+ ions do not coordinate with 2,3-DCN, and phase transitions occur solely through altered hydrogen bonding. This work highlights solvent-dependent metal organic coordination as a novel strategy for tailoring nanoarchitectures.

O 49.8 Tue 18:00 P2

Bottom-up realization of quasi-1D electronic states from Cs atoms on InSb(110) — •Niek Aarts, Annique Krieg, Emil Sierda, Danis Badrtdinov, Brian Kiraly, Elze Knol, Gerrit Groenenboom, Mikhail Katsnelson, Malte Rösner, Daniel Wegner, and Alexander Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

1D-electronic systems are predicted to exhibit very different physical phenomena compared to 2D and 3D systems. Scanning tunnelling microscopy (STM) and spectroscopy (STS) provide a way to study 1D electronic systems on surfaces in a bottom-up approach with atomic-scale precision by utilising atomic manipulation.

Here, we study the electronic states of quasi-1D structures that result from coupling individual Cs atoms adsorbed on InSb(110) using low-temperature STM and STS. When constructing chains of Cs atoms, we observe the formation of quantized electronic states in energy with a modulated charge density along the chain. We can tune these electronic states by changing the length and Cs density of the chain. Modifying the chain length, changes the spacing of the electronic states. Changing the density of Cs atoms, changes the onset energy of the electronic states. We ascribe these observations to a 1D-particle in a box behavior for the lowest electronic states. For the electronic states at higher energy, we observe deviations from the simple particle in a box description. These deviations could be due to the onset of states with a higher order orbital symmetry or due to a coupling of these states to a bath.

O 49.9 Tue 18:00 P2

Investigation of onset field variations in annealed and as-deposited NbTiN samples through field emission scanning microscopy — •Frederic Braun[1], Isabel Díaz-Palacio[2], Lea Preece[2], Florian Brockner[1], Robert Zierold[2], Marc Wenskat[2], Wolfgang Hillert[2], and Dirk Lützenkirchen-Hecht[1] — [1]Bergische Universtiät Wuppertal — [2]Universität Hamburg

Current superconducting radio frequency (SRF) cavities are predominantly constructed from high purity Niobium which is pushed to its theoretical limit. To enhance future cavity performance by minimizing operational power losses and increasing accelerating field strength, the focus of research must shift to alternative cavity materials. An effective strategy involves depositing superconducting thin films like NbTiN or Nb3Sn on the cavity inner walls. Heat treating NbTiN may further optimize film properties. In this study various samples, including as deposited NbTiN and annealed NbTiN are analyzed via a Field Emission Scanning Microscopy (FESM). Current-voltage-curves allow the determination of onset-fields for parasitic field emission . Mapping these fields at e.g., 1 nA reveals lateral variations due to thin film inhomogeneities, defects or surface contaminations Additionally, assessing long term surface stability through constant current measurements over an extended period is crucial for practical cavity applications.

O 49.10 Tue 18:00 P2

Surface Reconstructions and Photocatalysis of Thermally Reduced $LiNbO_3$ and $BaTiO_3$ Single Crystals — •Marta Macyk[1], Andrzej Jasicki[1], Llorenç Albons[2], Konrad Szajna[1], Martin Setvin[2], Dominik Wrana[1], and Franciszek Krok[1] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Perovskite oxides, such as $BaTiO_3$ (BTO) and $LiNbO_3$ (LNO), exhibit a wide range of different stoichiometries and crystal structures that make them ideal candidates for applications in optoelectronics and catalysis. Their properties can be tuned by the change of stoichiometry and the introduction of oxygen vacancies achieved by annealing under Ultra High Vacuum (UHV).

This poster presents a comparative study of surface reconstructions for tetragonal $BaTiO_3$(001) and hexagonal $LiNbO_3$(0001) after UHV annealing under low oxygen partial pressure. LEED analysis reveals a (1×1) to ($\sqrt{5}\times\sqrt{5}$)R26.6° transition for BTO, while LNO undergoes a (1×1) to ($\sqrt{3}\times6$)R30° transition, ending with (3 × 3) structure at temperatures near 1200°C. Morphological studies using SEM, STM, and AFM show the formation of nanowire structures aligned with the substrates' crystallographic directions, offering insights into controlled surface engineering. Furthermore, photocurrent measurements at variable temperature were performed on the thermally modified crystals to evaluate their photocatalytic and pyrocatalytic activity under ambient conditions.

O 49.11 Tue 18:00 P2

Freestanding thin film cryo-EM samples for electrospray ion beam deposition and molecular imaging — •Stephanie Stankard, Stephan Rauschenbach, Lukas Eriksson, and Jingjin Fan — Department of Chemistry, University of Oxford

Over the past decade, cryogenic electron microscopy (cryo-EM) has become the dominating method for imaging in structural biology, a method in which samples are conventionally made by plunge freezing.

Combining cryo-EM with soft landing, electrospray ion beam deposition (ESIBD) is a novel approach where intact, folded protein gas phase ions are landed onto the cryo-EM samples. For this, supported grids are required, which also need to be electron-transparent, and conductive. Often also ice needs to be grown on them after protein deposition.

Here, we present an analysis and optimisation of various thin, freestanding, amorphous carbon films for the purpose of application as a ESIBD and cryo-EM substrates.

O 50: Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Tuesday 18:00–20:00 Location: P2

O 50.1 Tue 18:00 P2

Polymorphism of Naphthalene on Ag(111) in and out of thermodynamic equilibrium — •Lorenz Brill[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich-Schiller-Universität, Jena, Germany — [2]Technische Universität, Graz, Austria

Even with a seemingly simple molecule like naphthalene, a rich polymorphism has been observed on Cu(111). Additionally, calculated phase diagrams predict multiple different structures of naphthalene on Ag(111), depending on the pressure and temperature during naphthalene deposition. In this poster, we present first experimental results of naphthalene structures formed in thermodynamic equilibrium obtained in our custom chamber specially designed to enable molecular growth in thermodynamic equilibrium. We compare our results to naphthalene structures grown using a conventional setup.

O 50.2 Tue 18:00 P2

Coverage-dependent assembly of functionalized helicenes — •Elise Fürch[1], Jonas Brandhoff[1], Fumi Nishino[2,3], Keisuke Fukutani[2,3], Marco Gruenewald[1], Maximilian Schaal[1], Felix Otto[1], Roman Forker[1], Takashi Hirose[4], Satoshi Kera[2,3], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Okazaki, Japan — [3]The Graduate University of Advanced Studies, Hayama-cho, 240-193 Kanagawa, Japan — [4]Institute of Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan

Recently, the interest in chiral molecules has spiked. The chirality-induced spin selectivity (CISS) promises a high spin-polarizability for electrons traversing a chiral molecule. However, the CISS effect is yet not fully understood. To be able to probe the CISS effect with area averaging methods like photoelectron spectroscopy a well-defined chiral thin film, consisting of helical molecules, is needed. In this study the chiral molecule thiadiazole[9]helicene (TD[9]H) is investigated on Au(111) and Ag(111) surfaces. To understand how chirality from one single molecule evolves into a fully chiral overlayer, a coverage dependent study, showing different structural motifs of TD[9]H, was performed. This structural evolution was investigated using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). In combination, these methods reveal a chiral lattice, and the role of the different molecule-molecule and molecule-substrate interactions will be discussed.

O 50.3 Tue 18:00 P2

Determining the Epitaxial Relations of Lead Phthalocyanine on Graphitic Surfaces — •Marco Gruenewald, Roman Forker, Matthias Spoddeck, and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The epitaxial relations between lead phthalocyanine (PbPc) layers and single-crystal graphite (SCG) as well as few-layer graphene/SiC(0001) are determined. Compared to previous reports, we obtain a clearly improved precision by combining the following concepts: [i] the use of distortion-corrected, calibrated low-energy electron diffraction (LEED), [ii] the complementary use of large-scale scanning tunneling microscopy (STM) with high resolution, [iii] the evaluation of multiple scattering features in LEED and Moiré spots in Fourier-transformed STM images, [iv] the simulation of those reciprocal-space patterns with an objective numerical fitting to the experimentally discernible spots, and [v] the analysis of the STM Moiré patterns in real space. Our independently determined LEED and STM results mutually confirm each other due to the remarkably similar structural parameters obtained. For all systems investigated we find noncommensurate, point-on-line coincident registries, and the epitaxial relations of PbPc layers on SCG and on graphene/SiC(0001) are found to be nearly identical despite the different compositions of those substrates. https://doi.org/10.1021/acs.cgd.4c01055

O 50.4 Tue 18:00 P2

Solvent-Free Fabrication of Supported Lipid Bilayers Incorporating Carbon Quantum Dots and Gramicidin A for Biosensing Applications — •Daniel A. Saavedra[1], Benjamín Ruz[1], Nicolás Moraga[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], Susana D. Rojas[2], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Univ. de Valparaíso, Chile

This study employed two phospholipids for the formation of supported lipid bilayers (SLBs): DPPG, with a net negative charge for enhanced adsorption to surfaces and biomolecules, and DPPC, which is neutral. SLBs were fabricated using a solvent-free, dry, ultra-high vacuum (UHV) approach [1], designed for protein insertion and nanoscale biosensor development for Forster energy transfer (FRET) detection mechanism.

Gramicidin A, a stable ion-channel protein, was incorporated into SLBs via physical vapor deposition monitored by high-resolution ellipsometry, followed by thermal treatment to enhance stability. Carbon quantum dots (CQDs), synthesized through hydrothermal carbonization of chitosan, were added via spin-coating. CQDs were selected for their photostability, low toxicity, and tunable fluorescence [2].

Acknowledgements: ANID Ph.D. Fellowships (DAS, NM, NGV), PUENTE-UC 2024-25. References: [1] Cisternas, M.A. et al., IJMS, 21, 6819 (2020). DOI: 10.3390/ijms21186819 [2] Wu, Q., et al., Nano Research, 16, 1835-1845 (2023). DOI: 10.1007/s12274-022-5189-2

O 50.5 Tue 18:00 P2

Long range ordering of molecular layers on Ag(110) — •Ravi Priya, Weishan Wu, and Peter Jakob — Department of Physics, Philipps University of Marburg, Germany

Single domain molecular layers have been explored on the non-hexagonal Ag(110) substrate in terms of their long-range ordering using SPA-LEED and vibrational signature using high-resolution FT-IRAS. The absence of rotational domains for fcc(110) metal substrates allows for growing layers with uniform azimuthal orientation of deposited molecules. We have investigated various molecules and configurations that may form single domain molecular layers (including mirror domains). Specifically, monolayers of PTCDA, NTCDA, and regio-selectively substituted pentacene species (pentacene (PEN), pentacene-quinone (P2O), pentacene-tetrone (P4O), quinacridone (QA)) were deposited on Ag(110) and examined in terms of their structure using SPA-LEED, and their vibrational signature using IR - spectroscopy. Among them, PTCDA, NTCDA, PEN, and QA have been found to form parallel-oriented, single domain structures. For QA two novel heterochiral phases are found after annealing, in addition to the single-domain homochiral phase present T < 500K. For P2O and P4O, steric hindrance and hydrogen bonding lead to the formation of 1D islands and 2D islands, respectively, at sub-monolayer coverages. Another finding refers to the increased molecule - metal interaction on Ag(110) vs. Ag(111) that leads to an extra energy (down)shift of the LUMO, thereby having a significant impact on interfacial dynamic charge transfer (IDCT) of vibrational modes.

O 50.6 Tue 18:00 P2

Structural and vibrational properties of mixed (CuPc + P4O) molecular layers on Ag(111) — •Yeondu Kim, Ravi Priya, and Peter Jakob — Department of Physics, Philipps University Marburg, Germany

Structural properties of mixed layers comprising CuPc and P4O on Ag(111) and their thermal evolution have been investigated by means of Fourier-transform

infrared absorption (FT-IRAS) and electron diffraction (SPA-LEED). For this material combination several long-range ordered phases at different relative ratios are found. Their formation and thermal stability have been analyzed in the temperature range 80 - 500 K, limited by thermal desorption and/or dissociation of the CuPc and P4O compounds at high temperature. Lateral interactions between CuPc and P4O within the mixed layers lead to characteristic frequency shifts of out-of-plane modes. In parallel, the intensities of in-plane vibrational modes of CuPc and P4O are strongly attenuated when adsorbed at nearby locations, indicating a major change in the associated interfacial dynamical charge transfer (IDCT). Specifically, IDCT that is quite prominent for the pure CuPc/Ag(111) and P4O/Ag(111) monolayers, is substantially attenuated for the mixed layers. This is ascribed to a through-metal charge transfer from CuPc to P4O that is associated with an upshift of the CuPc former LUMO and the correlated downshift of the P4O former LUMO. These correlated shifts lead to substantially lower density of states at the fermi level for both molecular species and thereby a weakening of IDCT induced bands.

O 50.7 Tue 18:00 P2

Structure and thermal Stability of (C60+P2O) and (C60+P4O) Heterolayers on Ag(111) — •Mohammed Suhail Ansari, Ravi Priya, Keda Jin, and Peter Jakob — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the interactions between C_{60} fullerene and two organic semiconductors, 6,13-pentacenequinone (P2O) and 5,7,12,14-pentacenetetrone (P4O), on Ag(111) substrates using IRAS, SPA-LEED, and TDS. The aim is to elucidate the structural properties and transformation processes of C_{60} and P2O/P4O under varying preparation conditions and thermal processing. Our findings reveal three different vertical arrangement scenarios of the heterostructures based on the deposition sequence and thermal treatments: (a) Formation of a well-defined bilayer on a pre-deposited monolayer corresponding to the deposition sequence, (b) a complete interlayer exchange of molecules, and (c) a partial interlayer exchange leading to mixed layers. Scenario (a) is observed with a P2O bilayer deposited on a well-defined C_{60} monolayer. Interestingly, P2O adsorbs in an inclined orientation on the C_{60}/Ag(111) monolayer. Scenario (b) is observed with deposition of a monolayer of P2O followed by a bilayer of C_{60} at room temperature that results in P2O migration to the second layer, emphasizing the weaker interaction of P2O with the substrate Scenario (c) is found for the combination of C_{60} and P4O and it involves migration of P4O to the second layer if it was deposited in the first layer, and vice-versa. We will discuss in detail the evolution of the grown heterolayers in terms of molecular orientations, interlayer exchange, and intermixing.

O 50.8 Tue 18:00 P2

Molecular self-assembly of BDA on $CsPbBr_3$(100) — •Hannah Loh, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

$CsPbBr_3$ is a promising alternative to organic-inorganic perovskites in solar cells and light emitting diodes [1]. In these devices, organic layers are often used as charge transport layers and hence interface properties are of particular interest. By choosing particular anchoring groups of organic molecules (here the carboxylic COOH-group) the interaction with the perovskite material may be tuned.

In this contribution we investigate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial $CsPbBr_3$ on Au(100) [2] by STM. For submonolayer coverage of BDA on $CsPbBr_3$ we find that upon deposition at 305 K molecules grow epitaxially in compact islands. The islands consist of chains with a V-structure inside the chains similar to the way BDA self-assembles on Cu(111) [3].

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Schmitt T. et al., J. Phys. Chem. C, **120(2)**, 1043-1048, (2016)

O 50.9 Tue 18:00 P2

Structure and charge carrier dynamics of an organic donor/acceptor heterostructure: a LEEM/PEEM study — •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — IEPT, TU Clausthal, Germany

We combine low-energy electron microscopy (LEEM) and two-photon photoemission electron microscopy (2P-PEEM) to study the relation between structure and charge carrier dynamics in well-ordered organic donor/acceptor (D/A) heterostructures of para-sexiphenyl (*p*-6P) and copper-hexadecaphthalocyanine (F_{16}CuPc). While *p*-6P monolayers deposited on SiO_2 exhibit structural order only on a nanometer scale, *p*-6P islands in the second layer comprise micrometer sized single-crystalline domains. Using microspot low-energy electron diffraction (μLEED) and dark-field LEEM, on many islands we observe two mirror domains which we attribute to different tilt angles of the *p*-6P molecules in the second layer. Using μLEED we confirm epitaxial growth of monolayer F_{16}CuPc on SiO_2/*p*-6P which results in a structurally well-defined organic D/A interface. Especially on *p*-6P bilayer regions, large single-crystalline F_{16}CuPc domains are observed. With 2P-PEEM we observe increased photoemission from SiO_2/F_{16}CuPc after optical pumping at 810 nm. In contrast, for SiO_2/*p*-6P/F_{16}CuPc the photoemission signal decreases. Also, the reflectivity for low-energy electrons changes upon optical pumping. We relate these long-lived pump-induced effects to intermolecular charge transfer which is more pronounced for bilayer-*p*-6P/F_{16}CuPc than for monolayer-*p*-6P/F_{16}CuPc.

O 51: Poster Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:00–20:00 Location: P2

O 51.1 Tue 18:00 P2

Visualizing quantum states in fluorene-based organometallic quantum corrals — •Longfeng Huang[1], Wenchao Zhao[1], Ignacio Piquero-Zulaica[1], Johannes Barth[1], and Biao Yang[1,2] — [1]Physics Department E20, Technical University of Munich, 85748 Garching, Germany — [2]Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, 215123 Suzhou, China

Constructing well-defined and controllable quantum states holds promise for applications in quantum technology. As an exemplary quantum architecture, quantum corrals (QCs) which are considered as artificial atoms attract enormous attention.1, 2 Common strategies for manufacturing QCs have mainly involved atomic and molecular manipulations, molecular assembly, and on-surface synthesis.3-5 However, fabricating robust QCs simultaneously with a high yield and specific size still remains elusive. In this work, we realize stable QCs with a well-defined size via organometallic bonding between fluorine-based molecules and intrinsic Ag adatoms on Ag(111). In particular, we observe spatial quantum resonance states inside the QCs, which arise from the scattered two-dimensional electron gas. Additionally, stadium-shaped and triangular QCs exhibit intriguingly specific orbital-like quantum states in differential conductance maps. In addition, we tune the QCs by replacing the F to H atoms and tip manipulation. Our study provides new means to fabricate controllable exotic quantum states with atomically precise QCs, aiding in a rational design strategy towards materials with tailored electronic properties.

O 51.2 Tue 18:00 P2

Termination-dependent ARPES maps from novel magnetic Kagome metals GdV_6Sn_6 and $GdMn_6Sn_6$ — •Robin P. Forster[1], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]JCNS Forschungszentrum-Jülich

The magnetic Kagome metals GdV_6Sn_6 and $GdMn_6Sn_6$ combine in a single material phenomena such as flat Kagome bands [1,2], local moments of the 4f electrons of Gd, and itinerant Mn or V 3d electrons [3], providing a platform to study their complex magentic and electronic interactions. We have performed termination-dependent micro-ARPES measurements with 20 μm real-space resolution at 20 K of paramagnetic GdV_6Sn_6 [4] and ferrimagnetic $GdMn_6Sn_6$ [5]. Surface and bulk states could be distinguished in the series of scans made over a range of photon energies. We have chosen $h\nu$ of 80 and 130 eV for GdV_6Sn_6 and 80, 112, 140, and 200 eV for $GdMn_6Sn_6$ for detailed ARPES scans. In addition, XPS measurements were conducted, which provide an insight into the measured terminations. Preliminary circular-dirchroic ARPES maps exhibit multiple sign inversions that stem from a combination of initial state orbital angular momenta and photoemission final state scattering [6]. [1] PRL 127, 266401 (2021) [2] PRB 104, 15122 (2021) [3] JPSJ 90, 124704 (2021) [4] JMMM 202, 519 (1999) [5] PRB 104, 235139 (2021) [6] *arXiv:2410.19652 (2024).

O 51.3 Tue 18:00 P2

Structural fingerprints in the reflectance anisotropy of P-rich and In-rich AlInP(001) — •Isaac Azahel Ruiz Alvarado[1], Mohammad Amin Zare Pour[2], Thomas Hannappel[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The surface optical anisotropy of AlInP(001) surfaces is investigated through experimental and theoretical approaches. Comparison is made between spectra calculated for energetically favored AlInP(001) surface structures with data measured on epitaxially grown $Al_{0.52}In_{0.48}P$(001) epilayers lattice-matched to GaAs samples. The anisotropies for photon energies below 3 eV provide clear fingerprints for the structure of the outermost surface atomics layers. The negative anisotropies for P-rich AlInP(001) surfaces are related to transitions involving

surface states located at the top P-dimers. In contrast, In-rich AlInP(001) surfaces show anisotropies related to surface states localized on the In atoms of the In dimers of the second row. The spectral features at higher energies provide insight into the near surface bulk ordering of AlInP. In particular, optical anisotropies at the AlInP critical point energies are found to be related to the CuPt ordering in the material.

O 51.4 Tue 18:00 P2

Next-Gen ARPES: AI-controlled beam polarization through Graphene — •Ridha Eddhib[1], Balasubramanian Thiagarajan[2], and Jan Minar[1] — [1]New Technologies-Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic — [2]MAX IV Laboratory, Lund University, Lund, 22100, Sweden

Angle-Resolved Photoemission Spectroscopy (ARPES) stands as a cornerstone technique in condensed matter physics, offering deep insights into electronic structures and quantum states. However, the precision of ARPES measurements critically depends on the exact calibration of the photon beam polarization, a challenge that often confronts experimentalists. This study introduces an innovative application of artificial intelligence (AI) to revolutionize ARPES experiments by enabling precise calibration and tuning of photon beam polarization through graphene ARPES cross section, aiming for the ideal of 100% circular polarization. At the heart of our methodology is a neural network model, meticulously trained on datasets generated by the sophisticated one-step model of the SPRKKR [1] (Spin-Polarized Relativistic Korringa-Kohn-Rostoker) code, renowned for its accurate ARPES simulation capabilities. This study leverages the ase2sprkkr package for streamlined interfacing with SPRKKR, enriching our AI model training data with high-fidelity simulations. By implementing this AI-driven methodology, researchers can dynamically adjust their ARPES setups, ensuring that each measurement is conducted under optimal polarization conditions. [1] Ebert, H., Koedderitzsch, D., & Minar, J. (2011). 74(9), 096501.

O 51.5 Tue 18:00 P2

The CD-ARPES study of intercalated transition metal dichalcogenide V1/3NbS2 — •Jyoti Kaswan[1], Laurent Nicolaï[1], Raphaël Salazar[1], Aki Ismo Olavi Pulkkinen[1], Sunil W Dsouza[1], Zdeněk Sofer[2], and Jan Minár[1] — [1]University of West Bohemia, Plzeň, Czech Republic — [2]University of chemistry and technology Prague, Czech Republic

Intercalated transition metal dichalcogenides (TMDCs) have recently garnered significant attention from the condensed matter community due to the demonstration of exotic phenomena that depend on the intercalated transition metal [1]. We investigate the electronic structure of V-intercalated TMDC, V1/3NbS2, using Circular Dichroic Angle-Resolved Photoemission Spectroscopy (CD-ARPES) in combination with the one-step model of photoemission as implemented in the SPR-KKR package [2].The intensity asymmetry in CD contains a well-known dichroism component related to the measurement geometry, as well as a component associated with magnetic ordering, complicating the extraction of spin information from CD-ARPES data. To address this challenge, our group has developed a model of dichroism based on the one-step model of photoemission (SPR-KKR code). By incorporating the measurement geometry, the ab initio calculations enable the separation of geometric and spin contributions to the CD signal [3,4]. [1] B. Edwards et al, Nature Materials 22, 459*465 (2023). [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011) [3] O. Fedchenko et al., Sci. Adv. 10, eadj4883 (2024) [4] S. Beaulieu et al, Phys. Rev. Lett. 125, 216404 (2020)

O 52: New Methods: Experiment

Time: Tuesday 18:00–20:00 Location: P2

O 52.1 Tue 18:00 P2

Exploring novel scanning force microscopy schemes by stabilising unstable states — •Lukas Böttcher[1], Hannes Wallner[2], Niklas Kruse[2], Wolfram Just[2], Ingo Barke[1], Jens Starke[2], and Sylvia Speller[1] — [1]Universität Rostock, Institute of Physics — [2]Universität Rostock, Institute of Mathematics

Dynamic scanning Force Microscopy (SFM) is a versatile and popular method for investigation of surface properties on the nanoscale. When probing the surface with an oscillating cantilever bistabilities may occur [1, 2], which are a result of nonlinearities arising due to interaction between tip and sample. By implementing a control scheme, we track the unstable state arising between the two stable states [3]. These unstable states may enable ultra-sensitive imaging conditions and give access to virtually interaction free mapping of material parameters.

[1] Gleyzes, P., Kuo, P.K., Boccara, A.: Bistable behavior of a vibrating tip near a solid surface. Appl. Phys. Lett. 58, 2989 (1991) [2] Misra, S., Dankowicz, H., Paul, M.: Event-driven feedback tracking and control483 of tapping-mode atomic force microscopy. Royal Society of London Proceedings484 Series A 464, 2113*2133 (2008) [3] Böttcher et.al, Exposing hidden orbits in scanning force microscopy, in preparation

O 52.2 Tue 18:00 P2

Surface photovoltage spectroscopy for investigation of SiC surface quality — •Viktoriia Nikonova[1], Nadine Schüler[1], Steffen Fengler[1], Maaz Soomro[1], Knut Gottfried[2], Imme Ellebrecht[2], and Kay Dornich[1] — [1]Freiberg Instruments GmbH, Delfter Strasse 6, 09599, Freiberg, Germany — [2]ErzM-Technologies UG, Technologie-Campus 1, 09126, Chemnitz, Germany

The surface photovoltage (SPV) technique belongs to the advanced methods for studying charge separation and transfer processes in photoactive materials.

The measurements of the SPV signal amplitude and time constant maps for SiC wafers have been done using a compact HR-SPS tool with fixed energy excitation sources. It has a high flexibility, which for example enables the integration of up to four lasers in the measurement head, either for injection level dependent SPV measurements or extracting depth information by using different wavelengths. Presented method based on fixed capacitor approach, that is much faster and more sensitive than on Kelvin probe. Also it works for highly doped substrate for which microwave based methods are difficult.

The experiments show the difference in maps between surface quality of wafers: polished wafers, fine and coarse grinded surfaces. Thus, the presented technique can be used to make quantitatively based decisions on the goodness of surface treatment methods without damaging the samples and to improve production based on SiC and others wide bandgap materials.

O 52.3 Tue 18:00 P2

ESEM Automation - Advanced Acquisition & Dual Magnification — •Maurits Vuijk[1], Annika Kubsch[1], Johannes Zeininger[2], Karsten Reuter[1], Thomas Lunkenbein[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]TU Wien

In Environmental Scanning Electron Microscopy (ESEM) experiments, the acquisition parameters are generally kept constant throughout the collection of the data set. This requires human supervision and limits data collection to one data set at a time. We use a custom automation interface to minimize supervision and allow for the collection of multiple simultaneous data sets containing complementary information.

Slow oscillatory dynamics are observed on a Co surface under hydrogen and oxygen dosing conditions using traditional ESEM. With our automation interface, we can implement more advanced acquisition programs into the microscope that take advantage of different time scales of the surface dynamics. By using automation to change the settings of the acquisition after each frame, we are able to capture multiple interlaced views of the same process. In this case, we alternated between two different magnification values, allowing us to capture a low magnification overview of the propagation of the surface dynamics and a high magnification view of the ongoing local structural changes to a selected surface feature. Many acquisition parameters such as gun voltage, stage position or focus can be automatically adjusted in an intelligent fashion, allowing for more complex acquisition strategies to unravel complex dynamic processes.

O 52.4 Tue 18:00 P2

Simultaneous Grazing Incidence Small Angle X-Ray Scattering (GISAXS) and Absorption Spectroscopy (XAS) of Liquid Surfaces — •Carlo Schneider, Lukas Voss, Frederic Braun, and Dirk Lützenkirchen-Hecht — Bergische Universität Wuppertal

A method combining Grazing Incidence Small Angle X-ray Scattering (GISAXS) and X-ray Absorption Spectroscopy (XAS) has been developed to investigate liquid surfaces. The approach employs a specialized reaction cell and detection systems, including a PILATUS 100k detector for scattering data and a PIPS detector for absorption spectra, paired with a Quick EXAFS (QEXAFS) monochromator. Solutions of nickel chloride, cobalt nitrate, and zinc acetate were analyzed to evaluate the feasibility of integrating time-resolved GISAXS with XAS. Results demonstrate the capability of the method to provide structural and compositional information on nanometer and angstrom scales simultaneously. Challenges, such as interference patterns potentially caused by instrumental effects, were identified and suggest areas for further refinement. The developed technique offers potential for applications in materials science and chemistry, enabling insights into liquid systems.

O 52.5 Tue 18:00 P2

Surface-Sensitive Analysis of Liquid Interfaces: Grazing Incidence X-Ray Absorption Spectroscopy with a Double-Mirror Setup — •Lukas Voss, Dirk Lützenkirchen-Hecht, Frederic Braun, and Carlo Schneider — Bergische Universität Wuppertal, NRW

Grazing incidence X-ray absorption spectroscopy (GIXAS) is a powerful technique for surface-sensitive investigations. While the study of solid materials can be easily performed by adjusting the sample orientation to vary the X-ray incidence angle, the examination of liquids requires a specialized experimental setup. To address this challenge, a double-mirror system was integrated into an existing reflectometer, enabling GIXAS measurements on liquid samples. This setup was utilized to study the melting behavior of gallium and the formation of sol-gel-derived germanium oxide nanoparticles.

O 53: Poster Electronic Structure Theory

Time: Tuesday 18:00–20:00 Location: P2

O 53.1 Tue 18:00 P2

Enhancing Efficiency of Bethe-Salpeter equation calculations including spin-orbit coupling — •Seokhyun Hong, Cecilia Vona, Sven Lubeck, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

Calculating optical excitations in materials with significant spin-orbit coupling (SOC) effects is challenging due to the computational costs. We propose a new method to compute optical spectra including excitonic effects within an all-electron framework. This method extends recently introduced second variation with local orbital (SVLO) method[1] towards the Bethe-Salpeter equation (BSE) framework. The SVLO method is based on the conventional second variation (SV) approach for density-funtional theory calculations. In SV, SOC is treated as a perturbation through a two-step procedure. By solving the scalar relativistic (SR) Hamiltonian, we first obtain eigenvalues and states without SOC. A subset of these SR Kohn-Sham states is used as basis functions for evaluating the SOC terms. For many materials, this approach can require all available states for convergence and thus may not capture SOC effects accurately without resorting to huge matrix sizes. In the SVLO method, local orbitals (LOs) are included in the SV step as additional basis functions. It could be shown that this enhances the computational efficiency tremendously[1]. Through this work, we have implemented an analogous scheme in the BSE framework. We demonstrate, how we overcome current limitations and achieve highly precise results for materials with strong SOC, such as lead iodide, perovskites, MoS2,etc.

O 53.2 Tue 18:00 P2

First-Principles Calculations of X-ray Absorption Spectra: Supercell Core-Hole Method versus Bethe-Salpeter Equation — •Ziyu Wang[1], Lu Qiao[1], Ronaldo Rodrigues Pelá[2], and Claudia Draxl[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany — [2]Supercomputing Department, Zuse Institute Berlin (ZIB), Berlin, Takustraße 7, 14195 Berlin, Germany

Accurate simulations of X-ray absorption spectra (XAS) are essential for understanding core-level excitations and electronic structure. In this study, we compare two approaches for calculating XAS: the supercell core-hole (SCH) method based on density-functional theory and the Bethe-Salpeter equation (BSE) of many-body perturbation theory. In the SCH method, core excitations are simulated by removing a core electron from the system, thus treating electron-hole interaction on the DFT level. In contrast, excitonic effects are considered explicitly in the two-body Hamiltonian underlying the BSE. We apply the SCH method with various exchange-correlation (xc) functionals of DFT to calculate XAS in diverse materials (metals, semiconductors, and insulators) and absorption edges. By comparing them with XAS obtained from BSE, we evaluate in which cases the SCH method is appropriate to be applied.

O 54: Poster New Methods: Theory

Time: Tuesday 18:00–20:00 Location: P2

O 54.1 Tue 18:00 P2

Increasing the Transferability of Machine Learning Potentials by Learning Atomic Properties — •Johann Richard Springborn[1,2], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In the last decade, Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces (PESs) of complex systems. While they significantly speed up the evaluation of the energy and forces in comparison to *ab-initio* methods, they require high-quality reference data for training. Depending on the systems to be studied, generating this training data can become the computational bottleneck and it is of high interest to reduce the number of structures to be computed as well as their complexity. We propose to achieve this goal by training MLPs on atomic properties instead of global quantities such as the system's total energy. This approach aims to increase the transferability of the resulting MLPs to more complicated systems while still utilizing easily accessible reference data.

O 55: Poster Topology and Symmetry-protected Materials

Time: Tuesday 18:00–20:00 Location: P2

O 55.1 Tue 18:00 P2

Native Bi_2Se_3 bulk and surface defects calculated from first principles — •Juntao Kong[1], Timur Biktagirov[2], Uwe Gerstmann[3], and Wolf Gero Schmidt[4] — [1]Warburger Str. 100,33098 Paderborn,Germany — [2]Warburger Str. 100,33098 Paderborn,Germany — [3]Warburger Str. 100,33098 Paderborn,Germany — [4]Warburger Str. 100,33098 Paderborn,Germany

Bi_2Se_3 attracts great attention presently because it is a strong topological insulator with its surface state consisting of a single Dirac cone at Γ which is protected by timereversal symmetry. Defects in the bulk, such as selenium vacancies, may introduce charge carriers that interfere with these surface states and reduce the ability to isolate surface conduction, which is critical for applications in quantum computing and spintronic devices. Surface defects, on the other hand, may act as active sites for adsorbing gas molecules, enabling changes in electronic properties that can be used for gas sensing. Here, we present a first principles study of native point defects in Bi_2Se_3. In particular, the formation energies of vacancies, antisites and interstitials [1,2] are investigated in dependence on Fermi level position and preparation conditions.

O 55.2 Tue 18:00 P2

Exploring magnetism, topology, and magnetoresistance in rare-earth based compound GdAuSn: Ab initio study — •Sumit Mondal[1], Japsreet Singh[2], and Kanachana Venkatakrishnan[2] — [1]Central University of Haryana — [2]Indian Institute of Technology, Hyderabad

Among rare-earth intermetallics, Gd-based compounds have garnered particular interest due to their diverse magnetic ground states and interesting non-trivial topological properties. In the present work, we investigate the magnetic, electronic, and dynamical properties of the equiatomic ternary compound GdAuSn using first-principles calculations. We explore its crystal structure and analyse various magnetic configurations to determine the ground state. Our results indicate that the C-type antiferromagnetic configuration has the lowest energy. By correlating the spin configurations with the underlying Heisenberg spin model, we determine the exchange interactions and calculate the critical tempera- ture using the mean-field approximation. Additionally, we examine the electronic band structure and find evidences of nodal surface and Dirac points, indicative of non-trivial topology. Furthermore, we analyse the longitudinal and transverse magnetoresistance behaviour of GdAuSn under varying magnetic fields, observ-

ing intriguing trends that suggest a correlation between magnetic field strength and magnetoresistance. Finally, we assess the phonon dispersion of our compound and find the topological phononic states with nodal surfaces. Our findings shed light on the magnetism, topology, and transport properties in rare-earth-based intermetallic compound.

O 55.3 Tue 18:00 P2

Graphene intercalation of the large gap quantum spin Hall insulator bismuthene — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Bing Liu[1,2], Jonas Erhardt[1,2], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

Bismuthene, a honeycomb monolayer of bismuth atoms synthesized on a SiC(0001) substrate, is a topological insulator with a breakthrough bulk band gap of 800 meV due to giant spin-orbit coupling. The magnitude of this gap exposes bismuthene as a promising candidate for room temperature spintronic applications based on the quantum spin Hall effect. However, oxidation of bismuthene in air confines most experiments on this system to UHV conditions. Here we demonstrate the intercalation of bismuthene between SiC and a single sheet of graphene. This protective layer effectively prevents bismuthene from oxidation, while it fully conserves its structural and topological properties as we readily demonstrate by scanning tunneling microscopy and photoemission spectroscopy. This paves the way for ex-situ experiments and ultimately brings bismuthene closer to the fabrication of spintronic devices.

O 56: Overview Talk Pavel Jelinek

Time: Wednesday 9:30–10:15 Location: H24

Topical Talk O 56.1 Wed 9:30 H24

trends and perspectives in on-surfece UHV synthesis — •Pavel Jelínek — Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, Prague 6, Czechia

On-surface synthesis in ultra-high vacuum conditions has demonstrated the capability to synthesize molecular structures that are not available through traditional methods in solutions [1]. For example, the synthesis of radical PAH molecules on metal surfaces and their subsequent characterization with the help of UHV SPM contributed significantly to the progress in pi-magnetism [2]. In this talk, we will discuss the current status and perspectives of the field. We will also review what makes the on-surface synthesis on metallic surfaces unique concerning synthesis in solution. This includes the 2D constraint imposed by the proximity of the surface as well as the essential catalytic role of single atoms diffusing on metal surfaces [3], so-called adatoms, at elevated temperatures has been pointed out [4].

[1] S. Clair and D. G. de Otyeza Chem. Rev. 119, 4717 (2019); L. Grill et al, Nature Nano 2, 687 (2007). [2] D.G. de Otyeza and T. Frederiksen JPCM 34, 443001 (2022). [3] H. Brune, Surf. Sci. Rep. 31, 125 (1998). [4] J.I. Mendieta-Moreno et al, Angew. Chem. Int. Ed. 61 e202208010 (2022).

O 57: Ultrafast Electron Dynamics I

Time: Wednesday 10:30–13:00 Location: H2

O 57.1 Wed 10:30 H2

Imaging the subcycle dynamics of topological surface currents in two-dimensional momentum space — •Tim Bergmeier[1], Suguru Ito[1], Jens Güdde[1], and Ulrich Höfer[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fachbereich Physik, Universität Regensburg, Germany

Angle-resolved photoemission spectroscopy (ARPES), combined with THz-electric fields and subcycle temporal resolution, offers unique capabilites to explore light-matter interaction on timescales faster than the oscillation of a light-wave. With this approach, it is possible to directly observe the dynamics of lateral Dirac currents along the surface of topological insulators, as well as the ultrafast buildup and dephasing of Floquet-Bloch states. However, so far the momentum resolution of such experiments was restricted to only 1-dimensional cuts within the surface momentum space.

Here, we present first results on the subcycle dynamics of surface currents resolving the full Dirac cone of Bi_2Te_3. In our recently established setup in Marburg, a 200 kHz laser system allows for MV/cm field strengths by parametric amplification of frequency-tunable THz-pulses in the range of 20-40 THz, together with optimal focussing at large angles of incidence inside of the UHV chamber by astigmatism compensation. Combined with ultrashort 400nm two-photon probe pulses (<15 fs) and a Scienta DA30 photoelectron analyzer, we are able to measure the whole 2D-momentum space with subcycle resolution.

O 57.2 Wed 10:45 H2

Measuring the non-equilibrium electronic structure of phonon-driven 2D materials — •Niklas Hofmann and Isabella Gierz — University of Regensburg

Quasi-periodic driving of solids with tailored light fields has emerged as a promising pathway for non-equilibrium materials design. To bring this approach to the next level, tailored driving schemes targeting specific degrees of freedom need to be combined with ultrafast probes of the atomic and electronic structure. We combine pump pulses tunable all the way from the Terahertz to the visible spectral range with a time- and angle-resolved photoemission (trARPES) probe to gain access to the transient electronic structure of driven materials. We recently implemented a narrow-band, strong-field Terahertz source [1] that allows for the selective excitation of phonon modes in materials with strong spin-orbit coupling and extreme ultraviolet probe pulses with tunable pulse duration to trace band structure dynamics on sub-cycle as well as cycle-averaged time scales. In this talk we present proof-of-principle experiments on graphene and show the transient electronic structure of WS_2 driven at resonance to the E_{1u} phonon mode.

[1] Optics Letters 42, 129 (2017)

Invited Talk O 57.3 Wed 11:00 H2

Floquet engineering in black phosphorus — •Changhua Bao[1,2], Shaohua Zhou[2], Benshu Fan[2], Michael Schüler[3], Teng Xiao[2], Hui Zhou[4], Zhiyuan Sun[2], Peizhe Tang[5], Sheng Meng[4], Wenhui Duan[2], and Shuyun Zhou[2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Tsinghua University, Beijing, China — [3]Laboratory for Materials Simulations, Paul Scherrer Institute, Switzerland — [4]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [5]School of Materials Science and Engineering, Beihang University, Beijing, China

The time-periodic light field has emerged as a control knob for manipulating quantum states in solid-state materials, dubbed as Floquet engineering. In this talk, I will present our progress on the experimental realization of Floquet band engineering in a model semiconductor, black phosphorus. Driven by strong mid-infrared light fields, transient gap opening and band renormalization are directly resolved with exotic pseudospin selectivity. In addition to band-structure engineering, manipulation of symmetry properties through Floquet engineering is also explored, including ultrafast glide-mirror symmetry breaking and parity symmetry manipulation. This series of works provides a comprehensive understanding of Floquet engineering in semiconductors and important guidance for extending Floquet engineering into more materials.

Nat. Rev. Phys. 4, 33 (2022); Nature 614, 75 (2023); PRL 131, 116401 (2023); ACS Nano 18, 32038 (2024); Nat. Commun. in press

O 57.4 Wed 11:30 H2

Observation of Floquet states in graphene — •Marco Merboldt[1], Michael Schüler[2], David Schmitt[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Karun Gadge[3], Salvatore R. Manmana[3], Sabine Steil[1], G. S. Matthijs Jansen[1], Daniel Steil[1], Michael Sentef[4], Marcel Reutzel[1], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Department of Physics, University of Fribourg, Fribourg, Switzerland — [3]Georg-August-Universität Göttingen, Institut für Theoretische Physik, Germany — [4]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Recent advances in the field of condensed-matter physics have unlocked the potential to realize and control emergent material phases that do not exist in thermal equilibrium. One of the most promising concepts in this regard is Floquet engineering, the coherent dressing of matter via time-periodic perturbations. However, the broad applicability of Floquet engineering to quantum materials is in question, especially with respect to (semi-)metals and graphene in particular.

Here, we resolve this long-standing debate by using electronic structure measurements to provide direct spectroscopic evidence of Floquet effects in graphene [1]. We report light-matter-dressed Dirac bands by measuring the con-

tribution of Floquet sidebands, Volkov sidebands, and their quantum path interference to graphene's photoemission spectrum. Fully supported by experiment and theory, we demonstrate that Floquet engineering in graphene is possible.

[1] Merboldt *et al.*, arXiv:2404.12791 (2024)

O 57.5 Wed 11:45 H2

Theory of nonperturbative nonlinear transport in a Floquet-Weyl semimetal — •Juan Ignacio Aranzadi[1], Matthew Day[2,3], James McIver[2,3], and Michael Sentef[1,2] — [1]Institute for Theoretical Physics, University of Bremen/ Bremen Center for Computational Material Science, Bremen — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg — [3]Department of Physics, Columbia University, New York, NY, USA

Weyl semimetals exhibit unique topological properties characterized by pairs of Weyl nodes with opposite chirality. While their transport properties have been extensively studied [1], their behavior under strong optical driving fields remains poorly understood. In this regime, the material response is governed by photon-dressed Floquet-Bloch states. Here, we investigate the photocurrent production mechanisms in Td-MoTe2, a type-II Weyl semimetal, under strong circularly polarized fields. Recent transport measurements in this material revealed a linear scaling of photocurrents at strong fields (<0.4 MV/cm) for the circular photogalvanic effect and the light-induced Hall effect [2]. We explore the microscopic theory underlying the photocurrent production in this system and disentangle its various contributing mechanisms. [1] J. Hu, S. Xu, N. Ni, Z. Mao, Annual Review of Materials Research (2019) 49:1, 207-252 [2] M. Day et. al. Nonperturbative nonlinear transport in a topological light-matter hybrid (2024)

O 57.6 Wed 12:00 H2

Hybrid Frenkel-Wannier excitons facilitate ultrafast energy transfer at a 2D-organic interface — •Wiebke Bennecke[1], Ignacio Gonzalez Oliva[2], Jan Philipp Bange[1], Paul Werner[1], David Schmitt[1], Marco Merboldt[1], Anna M. Seiler[1], Daniel Steil[1], R. Thomas Weitz[1], Peter Puschnig[3], Claudia Draxl[2], G. S. Matthijs Jansen[1], Marcel Reutzel[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Institute of Physics, NAWI Graz, University of Graz, 8010 Graz, Austria

The combination of two-dimensional transition metal dichalcogenides (TMDs) and organic semiconductors (OSCs) is a highly promising material platform for the realization of future optoelectronic devices. While the excitonic properties of their individual components have been intensively studied, much less is known about excitons at the hybrid interface. Here, we use ultrafast momentum microscopy and many-body perturbation theory to investigate the exciton landscape at the PTCDA/WSe_2 interface [1]. In particular, we find an exciton state formed via Förster resonant energy transfer, which is of hybrid nature: Concomitant intra- and interlayer electron-hole transitions within the OSC layer and across the TMD/OSC interface, respectively, give rise to an exciton wavefunction with mixed Frenkel-Wannier character.

[1] Bennecke *et al.*, arXiv:2411.14993 (2024)

O 57.7 Wed 12:15 H2

Characterization of Excitons for bulk Black Phosphorus — •Juan Felipe Pulgarin Mosquera[1,2], Geoffroy Kremer[2,3], Claude Monney[2], and Michael Schueler[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Department of Physics, University of Fribourg, CH-1700 Fribourg, Switzerland — [3]Institut Jean Lamour, CNRS-Université de Lorraine

Excitons (coupled electron-hole pairs) in semiconductors can form collective states that exhibit spectacular nonlinear properties and possible applications in future optoelectronic devices. We present here some theoretical methods and a workflow for determining the excitonic wave functions and the corresponding excitonic binding energies for bulk Black Phosphorus. We solve the Bethe-Salpeter equations for coherent and incoherent excitations. The theoretical/numerical results are compared to the experimental ones of angle resolved photoemission spectroscopy (ARPES), by analyzing the spectra produced after including non-equilibrium electron-phonon dynamics; solving the time-dependent Boltzmann equation. These results allow us to understand the nature and characteristics of these two-particle bound states, together with some scattering effects, being challenging due to the stronger screened potential for 3D materials, resulting in short time excitations.

O 57.8 Wed 12:30 H2

Momentum-resolved valleytronic dynamics in TMDC monolayers — •Sarah Zajusch[1], Lasse Münster[2], Marcel Theilen[1], Marleen Axt[1], Yaroslav Gerasimenko[2], Jens Güdde[1], Robert Wallauer[1], and Ulrich Höfer[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Fachbereich Physik, Universität Regensburg

The lack of inversion symmetry allows to access the valley degree of freedom in TMDC materials. With circular polarized light, time-resolved momentum microscopy enables us to trace the formation of a rich variety of bright and dark excitons typical for these materials on an ultrafast timescale and throughout the whole Brillouin zone.

We performed measurements on both $MoSe_2$ and WS_2. In WS_2, we observe a valley depolarization at room temperature within 100 fs, whereas in $MoSe_2$, this happens on a slower timescale, with a slight polarization that is still visible long after 100 fs. There are mainly two proposed leading mechanisms for this relaxation process, exciton-phonon scattering and electron-hole exchange interaction, which are differently pronounced in W- and Mo-based TMDCs due to the differences in their excitonic energy landscapes. As the ultrafast formation of dark KK'- and KΣ-excitons in WS_2 shows, mainly exciton-phonon scattering contributes to the valley relaxation here. This process is strongly temperature-dependent.

O 57.9 Wed 12:45 H2

Formation and thermalization of non-equilibrium excitonic occupations — •Paul Werner[1], Jan P. Bange[1], Wiebke Bennecke[1], Giuseppe Meneghini[2], David Schmitt[1], Marco Merboldt[1], Anna Seiler[1], AbdulAziz AlMutairi[3], Samuel Brem[2], Junde Liu[1], Daniel Steil[1], Stephan Hofmann[3], R. Thomas Weitz[1], Ermin Malic[2], Stefan Mathias[1], and Marcel Reutzel[1] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany — [3]Department of Engineering, University of Cambridge, United Kingdom

Semiconducting transition metal dichalcogenides (TMDs) host a rich landscape of Coulomb-correlated electron-hole pairs, which makes them ideal candidates for future optoelectronic applications. After an initial optical excitation of bright excitons, it is known that subsequent scattering into optically dark excitons takes place [1]. However, these processes must involve non-thermal exciton distributions that thermalize to a quasi-equilibrium [2]. In this work we use time-resolved momentum microscopy to directly access these non-thermal exciton distributions in optically excited homobilayer MoS_2. We identify the exciton landscape and relaxation pathways, and we find clear signatures of the non-equilibrium exciton distributions that are involved in the thermalization process. We compare our data with a full microscopic model calculation that confirms our experimental findings.

[1] Bange *et al.*, 2D Materials **10** 035039 (2023)
[2] Rosati *et al.*, ACS Photonics **7**, 2756–2764 (2020)

O 58: Solid-Liquid Interfaces: Reactions and Electrochemistry II

Time: Wednesday 10:30–13:00 Location: H4

O 58.1 Wed 10:30 H4

Step Bunching Instability and its Effects in Electrocatalysis on Platinum Surfaces — •Francesc Valls Mascaró[1], Marc T. M. Koper[2], and Marcel J. Rost[3] — [1]Departement of Physical Chemistry, University of Innsbruck — [2]Leiden Institute of Chemistry, Leiden University — [3]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University

The atomic-scale surface structure plays a major role in the electrochemical behaviour of a catalyst. The electrocatalytic activity towards many relevant reactions, such as the oxygen reduction reaction on platinum, exhibits a linear dependency with the number of steps until this linear scaling breaks down at high step densities. In this work we show, using Pt(111)-vicinal surfaces and in situ electrochemical scanning tunnelling microscopy, that this anomalous behaviour at high step densities has a structural origin and is attributed to the bunching of closely spaced steps. While Pt(554) presents parallel single steps and terrace widths that correspond to its nominal, expected value, most steps on Pt(553) are bunched. Our findings challenge the common assumption in electrochemistry that all stepped surfaces are composed of homogeneously spaced steps of monoatomic height and can successfully explain the anomalous trends documented in the literature linking step density to both activity and potential of zero total charge [1].

[1] F. Valls Mascaró, M. T. M. Koper, and M. J. Rost, Nat. Catal. 7, 1165 (2024)

O 58.2 Wed 10:45 H4

ALD coatings on 1D and 3D structures for electrochemical applications — •Siow Woon Ng — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Atomic layer deposition (ALD) utilizes self-limiting surface reactions to construct ultrathin films layer by layer. Among many deposition techniques, ALD

uniquely offers conformal deposition and excellent coating thickness control. Hence, the technique is particularly attractive for depositing structures with complex geometries, such as spheres, foams, 1D nanostructures, and 3D structures. This presentation discusses the preparation of 1D nanostructure and 3D-printed structures, followed by ALD inorganic and semiconductor coatings on these scaffolds. The influence of surface properties on the ALD coatings, and how the coatings enhance the electrical, mechanical, optical, and chemical properties or introduce new functionalities to the host structures will be presented. In particular, we will demonstrate that thin coatings in nanometer thicknesses are optimized for sensing and photo- and electrocatalytic applications.

O 58.3 Wed 11:00 H4

echemdb - a Database for Electrochemical and -catalytic Data of Metal Single-Crystal Electrodes — •Johannes Hermann[1], Julian Rüth[2], Nicolas G. Hörmann[3], Nicolas Bergmann[3], Karsten Reuter[3], Timo Jacob[1], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, Ulm, DE — [2]Julian Rüth GmbH, DE — [3]Fritz-Haber-Institut der MPG, Berlin, DE

Over the last decades and still today, electrochemical and catalytic studies on metal single-crystal electrodes form the basis of our fundamental understanding of atomic-scale processes on such electrodes and more complex catalyst materials, such as supported nanoparticles, found in applications. So far, experimental data and information on the data are mostly only available as traces and plain text in published works, which limits the FAIR (findable, accessible, interoperable, and reusable) use of the data in further experimental and theoretical works. To mitigate this issue, we present an open-source community approach to store such data and metadata in a structured way in a dedicated database, using the frictionless framework combined with a simple metadata standard. We illustrate the challenges associated with setting up such a system for the underlying data types, highlight tools that allow recovering data from published works and storing new data from experimental and theoretical works similarly. We demonstrate that these tools are equally applicable to other research areas. Finally, we provide some examples of using such a database in daily routines (finding and comparing experimental and theoretical data) and system-specific studies (reusability).

O 58.4 Wed 11:15 H4

The direct comparison of Pt and Cu particles on a TiO_2 photocatalyst in the hydrogen evolution reaction — •Lucia Mengel[1], Pieter van den Berg[2], Martin Tschurl[1], Neill Goosen[2], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Department of Process Engineering, Stellenbosch University, Banghoek Rd, Stellenbosch Central, Stellenbosch, 7599, South Africa

Anatase TiO_2 loaded with a metal co-catalyst is a well-known photocatalyst for hydrogen evolution. Fundamental studies on this system often employ photoreforming of alcohols as model reaction, utilizing noble metals such as platinum as a co-catalyst. The hole-mediated photooxidation reaction of the alcohol yields hydrogen next to valuable organic compounds such as aldehydes. Recent efforts aim at a replacement of platinum as co-catalyst by the more abundant and less expensive copper. In our work, we focus on the evolution of hydrogen on copper-loaded anatase by performing ethanol photoreforming in the liquid phase in oxygen- and water-free conditions. We study the hydrogen evolution reaction under excitation with UV-light and compare the photoactivity of the system to a common platinum-loaded catalyst and discuss possible scenarios for the interpretation of the reaction behavior.

O 58.5 Wed 11:30 H4

Microkinetic Modeling of the Hydrogen Evolution Reaction in Alkaline Conditions — •Dipam Patel and Georg Kastlunger — Technical University of Denmark

The Hydrogen Evolution Reaction (HER) in alkaline media is distinguished from the acidic case by the source of H. Significant theoretical work has investigated and diagnosed activity in acidic conditions, but this understanding does not necessarily correspond to alkaline. The implications of the stronger O-H bond in H2O compared to that in H3O+ are not yet fully understood. Using constant-potential electrochemical barriers, we developed a microkinetic model of alkaline HER activity on a selection of close-packed metallic surfaces. By accounting for the different potential responses of catalysts, we are able to reproduce the relative rates and tafel slopes seen in experiment. By relating the calculated activities to electrochemical descriptors, we show that the application of solely hydrogen binding descriptors, as in acidic HER, does not fully explain HER activity in alkaline.

O 58.6 Wed 11:45 H4

Predicting Charge Effects at Electrified Solid/Liquid Interfaces — •Nicolas Bergmann[1], Nicéphore Bonnet[2], Nicola Marzari[2], Karsten Reuter[1], and Nicolas G. Hörmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Laboratory of Theory and Simulation of Materials, EPFL, Lausanne

Computational modeling of electrified solid-liquid interfaces must account for capacitive contributions at potentials beyond the point of zero charge (PZC) [1]. These contributions can approximately be obtained from first-principles calculations at constant charge, employing a second-order Taylor expansion that involves the surface's free energy, the work function, and the interfacial capacitance at the PZC [2]. Machine learning (ML) surrogate models have already successfully been employed to predict the PZC energies at significantly reduced computational costs. Here, we extend this by presenting a ML model for work functions and apply this to two standard electrode modeling setups. By including the derivatives of the atomic forces with charge, we stabilize our model and predict the atomic effective charge. As an outlook, we show how this methodology could be utilized to run molecular dynamics simulations at charged conditions and electrochemical barrier calculations.

[1] N. Bergmann, N.G. Hörmann, and K. Reuter, J. Chem. Theory Comput. **19**, 8815 (2023).
[2] N.G. Hörmann and K. Reuter, J. Chem. Theory Comput. **17**, 1782 (2021).

O 58.7 Wed 12:00 H4

Dynamics at metal-water interfaces for catalytic hydrogenation — Tien Le[1], Shoutian Sun[1], and •Bin Wang[1,2] — [1]University of Oklahoma, Norman, Oklahoma, US — [2]Max Planck Institute for Sustainable Materials GmbH, Düsseldorf, Germany

The presence of water has been shown to enhance hydrogenation of polar chemical functional groups, such as C=O and N=O bonds, through proton shuttling. To demonstrate such rather sophisticated reaction pathways, explicit solvent models with dynamic change of local solvent structures should be considered. Beyond what we reported previously for water-promoted C=O hydrogenation in furfural, in this presentation, we will highlight how the dynamics of the local water structures within the first solvation shell may affect the hydrogenation kinetics. Specifically, we find that the activation barriers correlate well with some collective variables that determine the local configuration and relative positions of surface hydrogen and water. We further show that such dynamics of the metal-water interfaces can be manipulated by different approaches to tune the reaction kinetics. Our findings thus provide fundamental insights of this dynamic transformation at the solid-liquid interface and its impact on catalytic activity and selectivity.

O 58.8 Wed 12:15 H4

Rough Choice: Comparing 1- and 2D Representations of Electrocatalyst Morphology in Multiscale Models — •Hemanth S. Pillai, Hendrik H. Heenen, Karsten Reuter, and Vanessa J. Bukas — Fritz Haber Institute der MPG, Berlin

While electrocatalyst morphology is often used to tune product selectivity in electrochemical systems, the precise mechanism underpinning this relationship still remains elusive. Recently, we highlighted the role of morphology impacting product selectivity through a "Desorption–Re-adsorption–Reaction" mechanism [*Nat. Catal.* 7, 847*854 (2024)]. In particular, the catalyst morphology steers the competition between two elementary steps: either the desorption and diffusion of an intermediary byproduct or its re-adsorption and further reaction. Within such a model, morphology is captured in an effective manner via a surface roughness descriptor, however some systems may require a more explicit representation of the catalyst morphology. To assess this we employ a transport coupled kinetic model and systematically improve the representation of the catalyst from an effective one-dimensional descriptor to an explicit two-dimensional catalyst morphology. We find that deviations between the two descriptions are governed by morphological and transport parameters, i.e. diffusion length, particle size, shape, and interparticle distance. To conclude, we demonstrate that detailed morphological descriptions are only necessary within a narrow parameter window, thus providing guidance for selecting appropriate representations.

O 58.9 Wed 12:30 H4

Atomistic Simulation of Platinum-Water Interface: Deep Potential Molecular Dynamics (DP-MD) — •Muhammad Saleh[1], Alexander Lozovoi[2], Riccardo Martina[1], Matthew Darby[2], Clotilde Cucinotta[2], and Marialore Sulpizi[1] — [1]Theoretical Physics of electrified liquid-solid interface, Ruhr-University Bochum, Germany — [2]Department of Chemistry, Imperial College London, UK

The interaction between platinum surfaces and water holds significant importance due to its extensive applications in catalysis and electrochemical reactions. However, investigating these interactions at the atomistic level presents considerable experimental challenges. Moreover, accurately modeling such systems demands a substantial number of atoms (exceeding 1000), which can impede computational efficiency, particularly when using high-quality methods. In this study, we utilize the capabilities of machine learning potentials, specifically Deep Potential Molecular Dynamics (DP-MD), to overcome these challenges and achieve comprehensive simulation trajectories. This approach allows for an in-depth analysis, providing valuable insights into the surface properties.

O 58.10 Wed 12:45 H4

Preparation and Electrochemical Characterization of Metal Bicrystal Electrodes — •Nadine Wölfel, Albert K. Engstfeld, and Timo Jacob — Institute of Electrochemistry, Ulm, DE

The activity of a metal-based electrocatalyst strongly depends on its structural properties, where grain boundaries (GB) can play a significant role. One approach to study the impact of GBs is by varying the grain size of a material, which changes the GB density. In our study we aim at gaining fundamental insights into the atomic scale electrochemical and -catalytic processes at a GB, separating two surfaces with specific crystallographic orientation. We demonstrate how such electrodes can be prepared from Pt wires using the controlled atmosphere flame fusion method [1]. Here, poly-oriented single crystals are formed from two wires, crystallizing as a poly-oriented bicrystal from a common melt. By carefully polishing the poly-oriented crystal along the surface orientation of interest, a planar bicrystal surface with a single GB can be created. The structural properties of the prepared electrodes are determined by Laue X-ray diffraction, scanning electron microscopy (SEM), and electron backscatter diffraction (EBSD) spectroscopy. Electrochemical measurements, such as cyclic voltammetry (CV) are presented, which, based on the features in the CV, provide insights into the available facets and defects. The local electrocatalytic activity of the GB can be elucidated by scanning electrochemical microscopy (SECM) measurements.

[1] FM Schuett et al., Angewandte Chemie, 132 (2020) 13348-13354

O 59: Spins on Surfaces at the Atomic Scale I

Time: Wednesday 10:30–13:00 Location: H6

O 59.1 Wed 10:30 H6

Quantum spin engineering in bottom-up assembled molecular nanostructures — •Taner Esat[1,2], Dmitriy Borodin[3,4], Jeongmin Oh[1,2], Andreas Heinrich[3,4], Stefan Tautz[1,2,5], Yujeong Bae[3,4], and Ruslan Temirov[1,2,6] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance, Germany — [3]Center for Quantum Nanoscience, Institute for Basic Science, South Korea — [4]Ewha Womans University, South Korea — [5]RWTH Aachen University, Germany — [6]University of Cologne, Germany

Scanning tunneling microscopy (STM) is a powerful technique for fabricating and studying artificial nanostructures with purpose-engineered quantum states. Using the manipulation capabilities of the STM, we place aromatic molecules in an upright geometry on a pedestal of two transition metal atoms on the surface [1] and on the STM tip. These nanostructures carry electron spins that are well decoupled from the metallic substrate [2]. Based on this, we fabricate a single-molecule quantum sensor at the apex of the STM tip and address it by electron spin resonance. We use this sensor to measure the magnetic and electric dipole fields emanating from a single atom with sub-angstrom spatial resolution [3]. Finally, we show that varying the transition metal atoms in the pedestal alters the spin state of the molecular nanostructures, leading to exceptionally long spin lifetimes of up to several minutes. [1] Esat et al., Nature 558, 573 (2018) [2] Esat et al., Phys. Rev. Research 5, 033200 (2023) [3] Esat et al., Nat. Nanotechnol. 19, 1466 (2024)

O 59.2 Wed 10:45 H6

Tuning the Kondo temperature of Porphyrin molecules via adsorption configurations. — •Xiangzhi Meng[1], Jenny Möller[2], Rodrigo Menchón[3], Alexander Weismann[1], Daniel Sánchez-Portal[3], Aran Garcia-Lekue[3], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany — [3]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain

Magnetic molecules may serve as building blocks for spintronic devices at the ultimate limit of miniaturization. This sort of application requires an understanding of their spin properties. An important example is the Kondo effect that originates from the exchange interaction between a localized magnetic moment and the conduction electrons of the host metal. The interaction strength is reflected by a characteristic temperature, the Kondo temperature TK. In this work, we will show the Kondo effect of cobalt(II)-5,15-bis(4'-bromophenyl)-10,20-bis(4'-iodophenyl)porphyrin (CoTPPBr2I2) molecules on an Au(111) surface with a low-temperature STM. In comparison with the molecules reported before, the Kondo temperature of CoTPPBr2I2 can be tuned over a much broader range (8 K to 250 K) by switching their configurations. Additionally, we show that surface reconstruction plays a crucial role in modulating the molecular Kondo effect.

O 59.3 Wed 11:00 H6

Fock-Darwin states in tunable artificial atoms with high spin-orbit coupling — •Julian H. Strik, Hermann Osterhage, Kira Junghans, Niels P.E. van Mullekom, Emil Sierda, Anna M.H. Krieg, Danis Badrtdinov, Daniel Wegner, Mikhail I. Katsnelson, Malte Rösner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Quantum simulators are a pathway to study novel physical phenomena which are difficult to predict or observe in synthesized materials. To date, there is still a lack of viable platforms for quantum simulation to study confined electrons in strong magnetic fields, namely in the limit that the magnetic length is on the order of the Bohr radius. For typical crystals, this corresponds to field strengths that are unattainable in a laboratory.

In this talk I will discuss the magnetic response of atomic-scale quantum dots based on individual Cs atoms on the semiconducting surface of InSb [1]. Using low-temperature scanning tunnelling microscopy and spectroscopy, we pattern quantum dots of various sizes and geometries, by sculpting the potential of the underlying 2DEG. We then study the LDOS of these various structures to an external magnetic field. We relate this to the Fock-Darwin model of atomic states [2]. We review the experimental results in this context and discuss the role of structure size, symmetry and spin-orbit coupling.

[1] E. Sierda, et al, Science 380, 1048 (2023).
[2] L. P. Kouwenhoven et al., Rep. Prog. Phys. 64, 6 (2001).

O 59.4 Wed 11:15 H6

Nickelocene-functionalized tips as a molecular spin sensor — •Diego Soler-Polo[1], Ana Barragán[2], Andrés Pinar Solé[1], Manish Kumar[1], Oleksandr Stetsovych[1], Ben Lowe[1], Elena Pérez-Elvira[2], Koen Lauwaet[2], Pavel Jelínek[2], and José Ignacio Urgel[2] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]IMDEA Nanoscience, Cantoblanco, Madrid, Spain

Polyradicals nanographenes with low-lying spin excitations have almost degenerate states with different spins. Even Many-Body methods such as CASSCF and NEVPT2 might not provide enough accuracy to determine the spin of the real ground state. Here, we demonstrate that scanning probe microscopy with a nickelocene-functionalized tip can distinguish between nearly degenerate spin states of single molecular π-magnets. The nickelocene molecule has a spin 1 and a small magnetic anisotropy of 4 meV that interacts with the molecular spins of the sample. The spectroscopic patterns as we the tip is approached can be related to the number of radicals and their couplings. Such patterns are well reproduced by simple spin models and the corresponding simulated inelastic current. First, the molecular radicals are fitted to a spin hamiltonian, which is then coupled to the S=1 modelling the nickelocene. A cotunneling formalism adapted to spin hamiltonians provides the dIdV maps comparable with the experimental measurements, thus revealing the spin of the sampled system.

O 59.5 Wed 11:30 H6

Vibrational excitations in magnetic triangular nanographenes — Nils Krane[1], •Elia Turco[1], Annika Bernhardt[2], Michal Juríček[2], Roman Fasel[1,3], and Pascal Ruffieux[1] — [1]Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland — [2]University of Zurich, Zurich, Switzerland — [3]University of Bern, Bern, Switzerland

Inelastic electron tunneling spectroscopy has become a powerful tool for the investigation of excited states in single molecules and other quantum dot systems. These excited states can be of various origins, notably from higher energy spin states but also from vibrational modes. Especially in the case of carbon-based molecules, featuring π-magnetism with strong exchange coupling, both excitation mechanisms can be found within one system. Here, we present a simple method to distinguish between these two mechanisms by spatial map-ping of the excited states without any need for high magnetic fields. As a model system, we investigate the spin $S = 1/2$ phenalenyl radical on Au(111) and observe the featuring of two excited states via inelastic tun-neling spectroscopy. Comparison with DFT calculations proofs the vibrational origin of the observed inelastic features and allows us to assign them to distinct vibrational modes.

O 59.6 Wed 11:45 H6

Realization of separation of time scales in a heterogeneous atomic Boltzmann machine — •Kira Junghans, Hermann Osterhage, Werner M. J. van Weerdenburg, Niek M. M. Aarts, Anna M. H. Krieg, Tren Jacobs, Niels P. E. van Mullekom, Ruben Christianen, Eduardo J. Domínguez Vázquez, Hilbert J. Kappen, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The Boltzmann machine (BM) describes an energy-based neural network formed by coupled, fluctuating Ising spins [1]. A material realization of the Boltzmann machine was constructed using the complex stochastic dynamics of coupled Co atoms on the surface of black phosphorus (BP) [1]. Neurons and synapses were realized by a separation of time scales exploiting the anisotropic electronic structure of BP [1]. Using the anisotropy of the substrate is a limita-

tion in scaling this concept.
Here, we study the coupled dynamics of different types of atoms on BP, which exhibit orbital memory [2,3]. We study the influence of the coupling on stochastic dynamics in heteroatomic dimer and trimer configurations with scanning tunneling microscopy (STM). Further, we discuss how the multi-well energy landscape can be influenced by an applied AC signal.
[1] B. Kiraly et al., Nat. Nanotechn. 16, 414 (2021).
[2] B. Kiraly et al., Nat. Comm. 9, 3904 (2018).
[3] B. Kiraly et al., Phys. Rev. Research 4, 033047 (2022).

O 59.7 Wed 12:00 H6

Spin-surface interactions of S=1/2 molecular magnets on superconductors — •Susanne Baumann[1], Lukas Arnhold[1], Nicolaj Betz[1,2], Matteo Briganti[3], Andrea Sorrentino[4], Giulia Serrano[4], Federico Totti[3], Roberta Sessoli[3], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology, Stuttgart, Germany — [3]Department of Chemistry 'Ugo Schiff', University of Florence, Italy — [4]Department of Industrial Engineering, University of Florence, Italy

The interaction between magnetic molecules and superconducting surfaces critically depends on the electronic properties of the surface and the molecules' binding configuration, which determines the wave function overlap between molecule and surface. Using scanning tunneling microscopy (STM), we study the organometallic molecule ((η8-cyclooctatetraene)(η5-cyclopentadienyl)titanium) (CpTicot) on two different superconducting surfaces. On lead (Pb) nanoislands on Si(111), CpTicot exhibits multiple binding orientations with varying surface coupling strengths, that can be strong enough to generate Yu-Shiba-Rusinov bound states within the superconducting gap. Conversely, on vanadium (V(100)), the molecules adsorb in a single orientation with minimal coupling to the superconductor. Their spin states remain largely decoupled from the substrate, preserving their S=1/2 properties. These findings offer valuable insights into chemical design principles for molecular qubits where individual adressability and decoupling from superconducting substrates is desired.

O 59.8 Wed 12:15 H6

Edge states in bottom-up designed spin chains on a superconducting Rashba surface alloy — •Harim Jang, Khai That Ton, Lucas Schneider, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, Germany

The experimental quest for topological superconductors and emergent Majorana modes (MMs) at their edges have attracted significant interest recently in both directions of fundamental understanding of topology-driven quantum states and their potential applications in quantum computation leveraging the robustness by topological protection. A spin chain on a conventional superconductor in the presence of spin-orbit coupling is one of the promising platforms for realizing topologically non-trivial Yu-Shiba-Rusinov (YSR) bands, which can show signatures of MMs at the chain boundaries in the form of zero-energy states [1]. In this talk, we report on bottom-up designed Fe chains on the Rashba surface-alloy $BiAg_2$ grown on Ag(111)/Nb(110) and the detailed investigation of prominent states near the Fermi level at both chain ends, which are studied using scanning tunneling spectroscopy at sub-Kelvin temperatures. The atomically constructed Fe chains on the $BiAg_2$ alloy with proximity-induced superconductivity originating from the bulk Nb substrate show YSR bands with minigaps on the verge of our energy resolution inside the chain and edge states near the Fermi level at the chain's ends. The results are systematically compared to chains composed of other 3*d* transition metals, Mn and Co, on the same surface, revealing the absence of edge states for both cases. [1] S. Rachel and R. Wiesendanger, Phys. Rep. 1099, 1 (2025)

O 59.9 Wed 12:30 H6

Second harmonic driving of paramagnetic resonance of molecular spin through non-linear transport phenomena — •Stepan Kovarik[1], Richard Schlitz[1], Jose Reina-Gálvez[2,3], Aishwarya Vishwakarma[1], Dominic Ruckert[1], Nicolas Lorente[4,5], Christoph Wolf[2,3], Pietro Gambardella[1], and Sebastian Stepanow[1] — [1]ETH Zurich, Switzerland — [2]QNS, Seoul, Korea — [3]Ewha Woman University, Seoul, Korea — [4]CFM, Donostia-San Sebastian, Spain — [5]DIPC, Donostia-San Sebastian, Spain

The second harmonic excitation of electron paramagnetic resonance (EPR) originates from nonlinear processes. In this talk, I will demonstrate the presence of second and higher harmonic driving of a single spin in a pentacene molecule on 2ML MgO on Ag(001) when applying a radio-frequency electric field in an STM. Comparing our results to a theory considering EPR driven by a periodic modulation of the tunneling barrier [1] yields qualitative agreement, indicating the presence of higher harmonic driving. The key observation is that the barrier modulation can introduce nonlinearities to the electronic transport, leading to the excitation of magnetic resonance at the driving frequency [2] and at its multiples. Our work enhances the capabilities of EPR measurements in STM by introducing the frequency upconversion mechanism, showcasing the key role of electronic transport in driving the EPR. The presented findings apply also to other quantum transport systems, where the electrons are transported through discrete energy levels. References: [1]J. Reina-Gálvez et al., Phys. Rev. B 107, 235404 (2023)., [2]S. Kovarik et al., Science 384, 1368-1373 (2024).

O 59.10 Wed 12:45 H6

A quantum simulator to study electronic structure of matter in the Hofstadter limit — •Hermann Osterhage, Julian H. Strik, Kira Junghans, Niels P. E. van Mullekom, Anna M. H. Krieg, Emil Sierda, Danis Badrtdinov, Daniel Wegner, Mikhail I. Katsnelson, Malte Rösner, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The Hofstadter limit describes electronic structure in strong magnetic fields, where the magnetic length is on the order of the periodicity of the crystal. In this limit, the electronic structure shows self-similarity, namely fractal behavior. Experimentally, it is challenging to reach this limit for conventional crystals due to the high required field strengths. Therefore, one solution is to investigate structures with effectively larger periodicities. [1]. However, finding platforms that allow to study this limit with control over orbital and lattice symmetries is a current challenge.

Here, I will present a quantum simulator based on patterning Cs atoms on the surface of InSb(110) by scanning tunneling microscopy [2]. Cs atoms can be patterned into nanostructures that exhibit multi-orbital wavefunctions reminiscent of an artificial atom, and can be coupled to each other. We detail how the electronic spectrum evolves in magnetic field, and discuss the role of finite size effects and temperature, as well as link this to the expected spectra in the Hofstadter limit.
[1] R. Krishna Kumar et al., Science 357, 181 (2017).
[2] E. Sierda, et al, Science 380, 1048 (2023).

O 60: Plasmonics and Nanooptics: Fabrication, Characterization and Applications I

Time: Wednesday 10:30–12:45 Location: H8

O 60.1 Wed 10:30 H8

Infrared beam-shaping via geometric phase metasurfaces with the plasmonic phase-change material In_3SbTe_2 — •Lukas Conrads, Florian Bontke, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Conventional optical elements are bulky and limited to specific functionalities, contradicting the increasing demand of miniaturization and multifunctionalities. Optical metasurfaces enable tailoring light-matter interaction at will, especially important for the infrared spectral range which lacks commercially available beam-shaping elements. While the fabrication of those metasurfaces usually requires cumbersome lithography techniques, direct laser writing promises a simple and convenient alternative. Here, we exploit the non-volatile laser-induced insulator-to-metal transition of the plasmonic phase-change material In_3SbTe_2 (IST) [1] for optical programming of large-area metasurfaces for infrared beam-shaping. We tailor the geometric phase of metasurfaces with rotated crystalline IST rod antennas to achieve beam steering, lensing, and beams carrying orbital angular momenta. Finally, we investigate multi-functional and cascaded metasurfaces exploiting enlarged holography, and design a single metasurface creating two different holograms along the optical axis. Our approach facilitates fabrication of large-area metasurfaces within hours, enabling rapid-prototyping of customized infrared meta-optics for sensing, imaging and quantum information.[2] [1] Heßler et al. *Nat. Com.* **12**, 924 (2021) [2] Conrads et al. *arXiv:2408.05044* (2024)

O 60.2 Wed 10:45 H8

Investigation of lithiated carbon as active plasmonic material system — •Valentin Maile, Mario Hentschel, and Harald Giessen — 4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Active plasmonic structures are integral to recent advancements in optical technologies due to their ability to confine and manipulate light on the nanoscale, enabling the miniaturization of optical devices. A pivotal aspect of future devices is the switchability and tunability of their optical resonances. However, only very few material systems can intrinsically switch the ability of the individual resonator to support plasmonic resonances via a metal-to-insulator transition.

Here, we introduce a novel concept based on lithium-intercalated carbon, a material system widely studied in battery research. The electrically driven, re-

versible lithium intercalation in the carbon lattice leads to an increase in charge carrier density and a corresponding shift in the optical material properties, visibly changing its color from black to golden. This unique optical modulation demonstrates its potential for integrating dynamic plasmonic functionalities.

In this work, lithiated forms of carbon and their change in optical reflectance are investigated as a switchable material system for plasmonics. Furthermore, we explored multiple fabrication techniques for nanostructuring the material, demonstrating that the nanostructures can be electrically switched while maintaining their structural integrity. This approach promises to expand the toolkit of active plasmonic structures for metasurfaces and nano-optics.

O 60.3 Wed 11:00 H8

Hybrid resonant metasurfaces combining dielectric nanocup metasurfaces and plasmonic networks — Jelena Wohlwend, Anna Hilti, Claudiadele Polinari, Ralph Spolenak, and •Henning Galinski — Laboratory for Nanometallurgy Department of Materials ETH Zurich, 8093 Zurich, Zurich Switzerland

State-of-the-art dielectric metasurfaces commonly consist of geometric primitives, such as cylinders or nanofins, and their integration into hybrid systems is fundamentally limited as confinement of light occurs only in their interior. In this talk, we report on a simple fabrication scheme that unlocks a new degree of freedom in the optical design space, as it enables the design of complex metasurfaces that break the out-of-plane symmetry [1]. We showcase the versatility of this approach on the specific example of nanocup metasurfaces made of amorphous silicon. We outline the extraordinary modal properties of these resonant sub-wavelength structures including confinement of light in air, lattice resonances and optical non-reciprocity. Creating complex hybrid metasurfaces, which combine such ordered silicon nanocups and disordered plasmonic networks [2, 3], we demonstrate that the generation of configurable structural colors can be tailored by the local near-field coupling between the ordered and disordered optical elements.

References: [1] Adv. Optical Mater. 2024, 12, 2401501. [2] Adv. Optical Mater. 2023, 11, 2300568. [3] Nano Letters 2022, 22 (2), 853-859

O 60.4 Wed 11:15 H8

Optical programming of Hyperbolic Phonon Polariton Resonators with the plasmonic phase-change material In_3SbTe_2 — •Aaron Moos, Lina Jäckering, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Germany

Tailoring light at the nano scale is mandatory for creating new nanophotonic devices and is achievable with polaritons. Hexagonal Boron Nitride (hBN), a 2d van der Waals material, hosts Hyperbolic Phonon Polaritons (HPPs) featuring high volume-confinement and low losses [1]. Restricting HPPs to resonators enables ultra-confined resonances, but their fabrication requires cumbersome etching processes [2]. Instead, resonators can be fabricated via optical programming of a phase-change material like In_3SbTe_2 (IST) with a metallic and a dielectric state in the infrared enabling rapid fabrication and reconfigurability. IST resonators combined with surface polaritons on bulk SiC were exploited before [3]. Here, we show optical programming of circular IST resonators below 2d hBN and investigate the HPP mode structures with scattering-type scanning near-field optical microscopy (s-SNOM). Influences of hBN thickness and resonator-size on resonances are studied. Furthermore, we show focussing of free propagating HPPs launched by a crystalline IST structure with tuneable focal length by reconfiguring. Our results enable rapid prototyping of confined polariton resonators for infrared nanophotonics. [1] Dai et al., *Science* **343**, 1125-1129 (2014), [2] Sheinfux et al., *Nat. Mat.* **23**, 499-505 (2024), [3] Conrads et al., *Nat. Com.* **15**, 3472 (2024)

O 60.5 Wed 11:30 H8

Optical Response of High-refractive Index Nanodisk Arrays with Hyperuniform Disorder — •Davy Tesch, Koundinya Upadhyayula, Bodo Fuhrmann, Alexander Sprafke, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, 06120 Halle, Germany

Light-scattering metasurfaces with tailored disorder, in particular hyperuniform disorder (HUD), have recently attracted interest in the photonics community. HUD promises several properties that were previously associated only with either periodic or random structures. The combination of the strong diffraction of periodic structures and the broadband spectral response of disordered structures holds promise for tailored light scattering.

In this work, we use a scalable fabrication process to experimentally fabricate HUD nanodisk arrays using hydrogenated amorphous silicon (a-Si:H) optimised for low absorption as the nanodisk material. Optical measurements of such fabricated samples show a strong dependence of the scattering response on the form factor of the individual scatterers and their HUD arrangement, given by the structure factor. By tuning these quantities, we were able to tailor the scattering response. One of the most striking results is the ability of the fabricated samples to suppress scattering at small angles (below 45°) due to the HUD arrangement and to enhance scattering at large angles (up to 80°) due to the dominance of electric dipoles in single a-Si:H scatterers.

We have also studied a more complex system: nanodimers consisting of two stacked nanodisks, separated by a spacer layer.

O 60.6 Wed 11:45 H8

Edge-state imaging of high-precision plasmonic SSH chains — Benedikt Schurr[1], Luisa Brenneis[2], Philipp Kessler[2], Jin Qin[1], Victor Lisinetskii[2], •Matthias Hensen[2], Ronny Thomale[3], Tobias Brixner[2], and Bert Hecht[1] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Topological nanophotonics offers the possibility to precisely control nanoscale light–matter interaction via states that are topologically protected from disorder and impurities. A prominent example are Su–Schrieffer–Heeger (SSH) chains, in which the staggered nearest-neighbor coupling strength leads to topologically protected and localized edge states. Here, we present plasmonic SSH chains of nanoslot dipole antennas fabricated by helium ion-beam milling in a single-crystal Au micro-platelet. The chains are characterized by individual antenna distances down to 12 nm, strong coupling amplitudes, and negligible next-nearest-neighbor coupling. Furthermore, the near-field distribution of plasmonic eigenmodes is consistent with the amplitude distribution of the eigenfunctions of a quantum mechanical SSH model. We prove the existence of topological edge states experimentally by imaging corresponding mode patterns with aberration-corrected photoemission electron microscopy (PEEM) under wide-field excitation.

O 60.7 Wed 12:00 H8

Analytical study of Mie void resonances — Timothy J. Davis[1,2], •Julian Schwab[1], Harald Giessen[1], and Mario Hentschel[1] — [1]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany — [2]School of Physics, University of Melbourne; Parkville Victoria 3010, Australia

The preferential light scattering at particular wavelengths by mall particles is a well know phenomenon since the introduction of an analytical theory by Gustav Mie in 1908. Over the decades, this theory has helped in understanding, designing, and optimizing a multitude of plasmonic and dielectric nanophotonic systems. Just recently it was shown that Mie scattering can also be observed from voids in high-index dielectric media, such as silicon or gallium arsenide. This phenomenon is particularly counterintuitive as the void sizes are on the order of the resonant wavelength, rendering full-wave simulations and thus a deeper understanding challenging. Here, we present a new analytical model to study and understand the resonance properties of Mie voids. In particular, we derive analytical expressions of the electric field distribution based on solutions of Maxwell's equations for cylindrical holes in the substrate. These solutions are used in a simple three-layer model of the void that gives predictions of the void resonances, the observed spectra, as well as the microscopic appearance. Our model will aid in the future design of Mie-void based systems and applications, such as nanophotonic sensors, metasurfaces, and nanoscale detection.

O 60.8 Wed 12:15 H8

In-situ Plasmonic Sensing of Surfactant Structures — •Esmée Berger[1], Narjes Khosravian[1], Ferry Nugroho[2], Joakim Löfgren[3], Christoph Langhammer[1], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Physics, Universitas Indonesia, Depok, Indonesia — [3]Department of Applied Physics, Aalto University, Espoo, Finland

Surfactants play an important role in many areas of chemistry and have immense technological relevance. Their functionality is dictated by their frequently complex phase diagrams, which are very difficult to probe, especially *in situ*. Here, by combining experiment and multi-scale modeling, we demonstrate that the structure and dynamics of surfactant layers can be very efficiently probed using plasmonic sensing. Considering a prototypical surfactant-surface system (CTAB on silica), we show that the plasmonic response not only reveals changes in the structure of the surfactant layer as the CTAB concentration varies but also provides access to the kinetics of the phase transition. The approach demonstrated in the present work is minimally intrusive, efficient, and widely applicable. It thus constitutes a very powerful tool for exploring surfactant-surface structures, representing a large step forward in understanding these systems of enormous scientific and technological importance.

O 60.9 Wed 12:30 H8

Optical Sieve for Nanoplastic Detection — •Dominik Ludescher[1], Lukas Wesemann[2], Julian Schwab[1], Julian Karst[1], Shaban B. Sulejman[2], Monika Ubl[1], Ann Roberts[2], Harald Giessen[1], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]ARC Center of Excellence for Transformative Meta-Optical Systems (TMOS), The University of Melbourne, Australia

Micro- and nanoplastics contaminate marine ecosystems and endanger aquatic life, even in remote locations. These minute synthetic fragments, persisting for

hundreds of years, infiltrate the food chain, posing potential health risks due to toxic chemicals. Besides improving the quality of plastic disposal and reducing plastic production, determining the existence of micro- and nanoplastics in aqueous environments like water or blood is essential for biological studies. We present an optical sieve for nanoplastic detection based on the recently discovered Mie void resonances. Our devices are able to detect, size, and count nanoplastic particles by observing apparent color changes of the emitted light in the presence of a sphere in the void. The proposed method profits from its simplicity and only requires a conventional microscope setup with CMOS RGB imaging sensor.

O 61: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

O 61.1 Wed 10:30 H11

The Bell-Shaped Component in Diffraction from 2D Materials — •Birk Finke[1], Christian Brand[1], Karim Omambac[1,2], Pascal Dreher[1], Hannah Kohler[1], Frank-J. Meyer zu Heringdorf[1,3,4], and Michael Horn-von Hoegen[1,3] — [1]Universität Duisburg-Essen — [2]Polytechnique Montréal Canada — [3]Center for Nanointegration Duisburg-Essen — [4]Interdisciplinary Center for Analytics on the Nanoscale

In 2D materials, the formation of moiré superlattices with graphene or hBN on crystalline surfaces alters electronic, vibrational, and chemical properties. Here we analysed an unusual broad diffraction background observed in low energy electron diffraction from 2D material systems, which is called the bell-shaped component (BSC). Employing SPA-LEED, LEEM, and μ-LEED we propose the origin to be the inelastic scattering of the low energy electrons at the vertically polarized ZA-phonons of the weakly bound graphene and hBN layers on Ir(111) and SiC(0001). For these systems the ZA-phonon branch exhibits a parabolic dispersion with a finite phonon frequency of a few meV at the Γ point. This results in a high phonon density at low energy, but high momentum causing the strong intensity of the BSC in diffraction. In the framework of kinematic scattering theory, we performed simulations of the inelastic diffuse scattering which quantitively confirm our proposal.

O 61.2 Wed 10:45 H11

Combining DFT and ML to Explore the Electronic Properties of Nanoporous Graphene — •Bernhard Kretz and Ivor Lončarić — Institut Ruder Bošković, Zagreb, Croatia

Nano-porous graphene (NPG) holds great potential in electronics due to its tunable electronic properties. However, establishing a comprehensive understanding of how structural parameters influence these properties remains a challenge. This work employs density functional theory (DFT) calculations combined with machine learning (ML) to systematically investigate both static and dynamic electronic properties across a set of 460 NPG structures derived from four distinct templates.

Our DFT results reveal correlations between structural features and band gaps within subsets of our NPG structures. Notably, we identify certain NPG configurations exhibiting band gap behavior analogous to armchair graphene nanoribbons. To predict the dynamic response of our NPG structures, we train two distinct ML networks: one for predicting forces and total energies, and another one for predicting band gaps. Using the former allows us to perform temperature-dependent molecular dynamics simulations for all 460 NPG structures, while the latter enables us to predict band gap evolution under varying operating temperatures, a crucial factor for semiconductor device performance. Our findings identify several NPG structures exhibiting band gaps suitable for semiconductor applications while demonstrating sufficient thermal stability to function effectively at typical operating temperatures.

Invited Talk O 61.3 Wed 11:00 H11

Polaritons in two-dimensional materials and hybrids probed by electron beams — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel

Polaritonic quasiparticles in two-dimensional (2D) materials have garnered significant attention in recent years, emerging as a promising platform for studying novel photon- and phonon-mediated correlations between various material excitations. In this work, we employ electron beams to investigate exciton and plasmon polaritons in diverse 2D materials, including transition-metal dichalcogenides, perovskites, hexagonal boron nitride, borophene, and hybrid systems. By comparing cathodoluminescence and photoluminescence spectroscopy, we uncover differences in the selection rules governing the excitation of quasiparticles by coherent light versus electron beams. Furthermore, leveraging a recently developed method that utilizes electron-driven photon sources inside an electron microscope for Ramsey-type spectroscopy, we examine the coherence of cathodoluminescence emitted by exciton polaritons (Nature Physics 19, 869 (2023)) and defects in hexagonal boron nitride (arXiv:2404.09879). These results provide new insights into the temporal coherence of the radiation from 2D materials excited by coherent and incoherent excitations.

O 61.4 Wed 11:30 H11

Electron-phonon interaction in polar two-dimensional materials — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We recently developed a generally applicable ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation, which are usually neglected [1].

Incorporating effects from macroscopic electric fields into our implementation allows us to extend our calculations to the class of polar materials. In this presentation we discuss our results for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

O 61.5 Wed 11:45 H11

Structural modulations of unidirectional charge density waves in rare earth tellurides — •Eunseo Kim[1], Sanghun Lee[1], Junho Bang[1], Hyungryul Yang[1], Jongho Park[2], Changyoung Kim[2], Dirk Wulferding[2], Doohee Cho[1], Makoto Hashimito[3], Donghui Lu[3], and Sunghun Kim[4] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea — [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Department of Physics, Ajou University, Suwon 16499, Korea

Charge density waves (CDWs) in rare earth tellurides (RTe_3) provide a unique platform for exploring the interplay between lattice deformations and electronic order. Using scanning tunneling microscopy and spectroscopy (STM/S), we investigate unique surface features in two different materials, $GdTe_3$ and $DyTe_3$, that influence the CDW behavior. In $GdTe_3$, twin domain boundaries provide a static platform for observing the spatial "melting" of unidirectional CDWs and the emergence of bidirectional CDWs. Our spatial lock-in analysis demonstrates the attenuation of CDW order parameters and the proliferation of topological defects at these boundaries, correlating with enhanced local density of states near the Fermi level. In $DyTe_3$, nanowrinkles act as topological interfaces, hosting phase-winding CDWs and confining one-dimensional metallic states. These findings emphasize the role of local structural distortions in shaping CDW phenomena, offering insights into manipulating quantum states via lattice engineering.

O 61.6 Wed 12:00 H11

Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field — •Jan-Philip Joost and Michael Bonitz — Kiel University, Institute for Theoretical Physics and Astrophysics, 24098 Kiel, Germany

When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [1]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [2]. Further, we demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects greatly benefit from surface screening, while in free-standing systems the targeted charge excitation is restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

[1] J.-P. Joost et al., Nano Lett. **19**, 9045 (2019)

[2] J.-P. Joost et al., Phys. Rev. B **105**, 165155 (2022)

O 61.7 Wed 12:15 H11

Two-dimensional breathing Kagome lattice of antimony atoms on a SiC substrate — •Bing Liu[1], Kyungchan Lee[1], Jonas Erhardt[1], Manish Verma[1], Stefan Enyner[1], Cedric Schmitt[1], Philipp Kessler[1], Lukas Gehrig[1], Chris Jozwiak[2], Aaron Bostwick[2], Martin Kamp[1], Eli Rotenberg[2], Jörg Schäfer[1], Simon Moser[1], Giorgio Sangiovanni[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The Kagome lattice, characterized by flat electronic bands, which represents a class of candidate materials for charge order, time-reversal symmetry-breaking and exotic superconductivity. In this work, we report the successful synthesis of a breathing Kagome lattice of Sb on SiC surface. Band mapping reveals a significant gap opening at the K point near the Fermi level, driven by different hopping parameters within the breathing Kagome lattice. Scanning tunneling microscopy measurements of this phase confirm a well-ordered 2x2 lattice reconstruction, consistent with the breathing Kagome unit cell. Furthermore, DFT calculations elucidate the role of the Sb p-orbitals. Specifically, near the Fermi level the physics is dominated by px and py orbitals, which are sensitive to hopping and possibly electron correlation, giving rise to an energy gap, and by their splitting reflect the breathing Kagome lattice situation. Our findings demonstrate a pathway for constructing two-dimensional Kagome lattices on semiconductor surfaces, and are encouraging further research into their spin and electronic properties.

O 61.8 Wed 12:30 H11

Ultrafast lattice dynamics of monolayer ReS_2 — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Within the transition metal dichalcogenide (TMDC) material family, TMDCs containing rhenium stand out due to their low crystal symmetry. Instead of the common hexagonal structure, ReS_2 exhibits in-plane 1D chains of rhenium ions due to a Peierls-like distortion. This highly anisotropic crystal structure results in a range of material properties, such as anisotropic effective carrier masses, polarization dependent optical absorption, and extremely weak interlayer coupling.

We present femtosecond electron diffraction (FED) measurements of monolayer ReS_2. FED is a direct probe of photoexcited lattice dynamics, providing quantitative information on coherent and incoherent atomic vibrations on femtosecond timescales. In ReS_2 monolayers we observe a strong and complex lattice response to photoexcitation. In particular, we observe a rapid (<1 ps) collective response, indicative of a concerted change in ionic positions within the unit cell. We measure the fluence dependence of this response and investigate the effect of the pronounced polarization dependence of the optical excitation, which results from the material's in-plane anisotropy.

O 62: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation III

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Wednesday 10:30–13:00 Location: H24

O 62.1 Wed 10:30 H24

Selective On-Surface Synthesis of Isokekulene Facilitated by Strong Molecule-Substrate Interaction — Qitang Fan[1], Alexander Reichmann[2], Zilin Ruan[1], Faming Kang[1], Tim Naumann[1], Simon Werner[1], Olaf Kleykamp[1], Jose Martinez[3], Felix Lüpke[3], François C. Bocquet[3], Christian Kumpf[3], Serguei Soubatch[3], Jörg Sundermeyer[1], Peter Puschnig[2], F. Stefan Tautz[3], J. Michael Gottfried[1], and •Sabine Wenzel[1,3] — [1]Fachbereich Chemie, Philipps-Universität Marburg — [2]Institute of Physics, University of Graz — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich

The role of different facets of metal nanoparticles in steering reaction pathways is crucial for the design of heterogeneous catalysts with superior selectivity. Transition-metal-catalyzed C-H bond activation is widely used for the synthesis of different chemicals. Here, we report orthogonal selectivity in intramolecular cyclodehydrogenation of a nonplanar cyclic precursor steered by different facets of a copper single crystal. On Cu(110), the previously unknown cycloarene isokekulene is formed with a high selectivity of 92 %, while reaction on Cu(111) is known to result in kekulene (> 99 %). Combining scanning tunneling microscopy with CO-functionalized tips and density functional theory, we identify two adsorption geometries of the precursor which react to the respective products. The isokekulene molecule appears in two nonplanar adsorption configurations and shows a strong molecule-substrate interaction including charge transfer, which accounts for the more favorable energetics of isokekulene on Cu(110).

O 62.2 Wed 10:45 H24

On-surface synthesis and characterization of long azaacenes — •Zilin Ruan[1], Liping Ye[2], Jakob Schramm[3], Tim Naumann[1], Faming Kang[1], Ralf Tonner-Zech[3], Michael Mastalerz[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, 35037 Marburg, Germany — [2]2Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, 69120 Heidelberg, Germany — [3]Wilhelm Ostwald Institute of Physical and Theoretical Chemistry, Universität Leipzig, 04103 Leipzig, Germany

Introducing electronegative nitrogen into the backbone of acenes yields azaacenes, enabling fine-tuning of the energy alignment of frontier orbitals while enhancing resistance to oxidation, photodegradation, and dimerization. Here, we demonstrate the on-surface synthesis of tetraazanonacene and hexaazatridecacene, the latter being the longest azaacene known to date and here reported for the first time via atom-manipulation-induced dissociation of a triethenobridged precursor on a Au(111) surface in UHV. The geometric and electronic structures of the generated azaacenes were investigated by combined scanning tunneling microscopy/spectroscopy and non-contact atomic force microscopy. For tetraazanonacene, we observed an increase of the frontier orbital gap compared to pristine nonacene, attributed to a more pronounced downshift of occupied states. Meanwhile, hexaazanonacene exhibited an open-shell singlet ground state with a singlet-triplet gap of 110 meV, slightly smaller than that observed for long acenes.

O 62.3 Wed 11:00 H24

On-surface synthesis and characterization of polyynic carbon chains — •Wenze Gao[1,2], Wei Zheng[1], Luye Sun[1], Faming Kang[1], Zheng Zhou[1], and Wei Xu[1] — [1]Interdisciplinary Materials Research Center, School of Materials Science and Engineering, Tongji University, Shanghai, China — [2]Empa-Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

Carbyne, an elusive sp-hybridized linear carbon allotrope, has fascinated chemists and physicists for decades. Due to its high chemical reactivity and extreme instability, carbyne was much less explored in contrast to the sp2-hybridized carbon allotropes such as graphene. Herein, we report the on-surface synthesis of polyynic carbon chains by demetallization of organometallic polyynes on the Au(111) surface; the longest one observed consists of 60 alkyne units (120 carbon atoms). The polyynic structure of carbon chains with alternating triple and single bonds was unambiguously revealed by bond-resolved atomic force microscopy. Moreover, an atomically precise polyyne, C14, was successfully produced via tip-induced dehalogenation and ring-opening of the decachloroanthracene molecule (C14Cl10) on a bilayer NaCl/Au(111) surface at 4.7 K, and a band gap of 5.8 eV was measured by scanning tunnelling spectroscopy, in a good agreement with the theoretical HOMO-LUMO gap (5.48 eV).

O 62.4 Wed 11:15 H24

The odd-number cyclo[13]carbon and its dimer, cyclo[26]carbon — •Florian Albrecht[1], Igor Rončević[2], Yueze Gao[2], Fabian Paschke[1], Alberto Baiardi[3], Ivano Tavernelli[3], Shantanu Mishra[1], Harry L. Anderson[2] und Leo Gross[1] — [1]IBM Research Europe - Zurich — [2]Department of Chemistry, Oxford Univeristy — [3]IBM Quantum, IBM Research Europe - Zurich

Using CO-functionalized tips, we generate the odd-numbered cyclocarbon molecule cyclo[13]carbon (C13) on an ulatra-thin insulating film by applying voltage pulses to a stable precursor molecule. The geometric and electronic properties of C13 were characterized experimentally as well as theoretically, determining the electronic ground state to be an open-shell triplet. In addition to the C13 monomer, we also generated its dimer, cyclo[26]carbon, from two precursor molecules [1].

[1] Albrecht et al., Science 384, 677 (2024)

Invited Talk O 62.5 Wed 11:30 H24

On-Surface Synthesis with Hydrogen Atoms — •Szymon Godlewski — Jagiellonian University, Krakow, Poland

In recent years the on-surface manipulation and chemical reactions created a playground for atomically precise synthesis and development of new atomic and molecular nanostructures. However, the abilities to produce desired systems are limited, among others, by relying on the catalytic role of the substrate in initiating selected reactions. Therefore striving for the generation of desired systems forces the search of new reaction pathways and catalytic transformations.

In this talk I will demonstrate our approach based on the application of hydrogen atoms in the on-surface experiments. First, I will discuss the synthesis of the acene series based on the application of *extra* hydrogen atoms. The application of atomic hydrogen in on-surface transformations will be exemplified by organometallic hybrids and graphene nanoribbons.

While the surface assisted synthesis approach has proven its effectiveness in the precise formation of new organic compounds on metallic surfaces one of the most challenging limitations arises from the dependence on the catalytic activity of the substrate. This makes the direct transfer to the non-metallic surfaces extremely challenging. In this talk I will present our pathway for the synthesis of new molecular compounds on non-metallic surfaces with prospects for circumventing the need to exploit the catalytic role of metallic substrates.

This work was supported by the National Science Center, Poland (2019/35/B/ST5/02666)

O 62.6 Wed 12:00 H24

On-Surface Synthesis of Hydrogen-Substituted γ-Graphdiyne with High Efficiency — •Faming Kang[1,3], Wei Zheng[1], Luye Sun[1], Wenze Gao[1], Lina Shang[1], Lifeng Chi[2], and Wei Xu[1] — [1]Interdisciplinary Materials Research Center, School of Materials Science and Engineering, Tongji University, 201804 Shanghai, China — [2]Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials and Devices, Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, 215123 Suzhou, China — [3]Department of Chemistry, University of Marburg, 35032 Marburg, Germany

Graphyne-family structures, a group of hybrid carbon allotropes with sp- and sp2-hybridized carbon atoms, are expected to have unique features, including a natural direct bandgap, unlike graphene. Here, we developed and synthesized precursors with one and three tribromoethenyl groups. In mild conditions, metal-free dimer and network (HsGDY) products were synthesized in big scale and good quality. The geometric structure of synthesized dimer and network products was accurately characterized by scanning tunneling microscopy and non-contact atomic force microscopy. The electronic structures of produced hydrogen-substituted graphdiyne were studied using DFT calculations. Our research may motivate theoretical and experimental efforts to create more sensitive two-dimensional carbon nanostructures with sp-hybridized carbon atoms.

O 62.7 Wed 12:15 H24

Tip-induced nitrene generation — •Leonard-Alexander Lieske[1], Aaron Oechsle[1], Ilias Gazizullin[2], Matthias Krinninger[3], Igor Rončević[4], Florian Albrecht[1], Leonhard Grill[2], Friedrich Esch[3], and Leo Gross[1] — [1]IBM Research Europe - Zurich, Rueschlikon, Switzerland — [2]Physical Chemistry Department, University of Graz, Graz, Austria — [3]Chair of Physical Chemistry and Catalysis Research Center, Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [4]Department of Chemistry, University of Manchester, Manchester, United Kingdom

We have successfully generated mono-, di- and trinitreno-*s*-heptazine by tip-induced chemistry from the precursor 2,5,8-triazido-*s*-heptazine[1,2] on bilayer NaCl and on bare Au(111). The precursor's azide groups are cleaved off sequentially in a controlled manner, demonstrating the generation of single molecules with one, two and three nitrene moieties, which are highly reactive.[3] We characterized the mono-, di- and trinitrene species by high-resolution atomic force microscopy with CO functionalized tips[4] and by scanning tunneling microscopy. Broken-symmetry density functional theory and multi-reference complete active space calculations of inter- and intra-nitrene exchange couplings J and J^* suggest a high-spin (S = 3) ground state for trinitreno-*s*-heptazine. [1] D. Miller et al., *J. Am. Chem. Soc.*, 126, 5372 (2004). [2] M. Krinninger et al., *Chem. Mater.*, 35, 6762 (2023). [3] M. Janssen et al., *Science*, 385, 318 (2024). [4] L. Gross et al., *Science*, 325, 1110 (2009).

O 62.8 Wed 12:30 H24

On-Surface Synthesis and Reactivity of Biphenylene Network on Au(788) — •Ye Liu, Yingling Zhang, Zilin Ruan, Tim Naumann, Faming Kang, Ulrich Koert, and J. Michael Gottfried — Department of Chemistry, University of Marburg, 35032 Marburg, Germany

The recently synthesized biphenylene network (BPN), a new sp2-hybridized carbon allotrope comprising four-, six-, and eight-membered rings, significantly differs from graphene in its electronic and chemical properties. Theoretical studies predict that BPN features a multiradical ground state, with its open-shell character predominantly localized at the four-membered rings. However, experimental confirmation of these predictions has been hindered by the limited quality of the material currently available. To address this challenge, we employed Au(788), a surface characterized by narrow terraces, and designed an extended molecular precursor to promote the formation of the desired structure. For comparison, we also investigated interpolymer dehydrofluorination (HF-zipping) reactions of the precursor on Au(111). Scanning probe microscopy (SPM) analysis revealed that pure BPN fused chains formed on Au(788) exhibit superior structural quality compared to those synthesized on Au(111). These findings provide a solid experimental foundation for probing the theoretically predicted properties of BPN, opening avenues for the further exploration of its distinctive electronic and chemical behavior.

O 62.9 Wed 12:45 H24

Incorporating Nonhexagonal Polygons into Carbon-Based Nanostructures via On-Surface Synthesis — •Dong Han[1], Jakob Schramm[2], Zilin Ruan[1], Tim Naumann[1], Konstantin Y. Amsharov[3], Ralf Tonner-Zech[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Marburg, Germany — [2]Faculty of Chemistry and Mineralogy, Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Universität Leipzig, Leipzig, Germany — [3]Institute of Chemistry, Organic Chemistry, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The incorporation of nonhexagonal rings offers a powerful strategy for designing novel carbon-based nanostructures with unique physicochemical properties. Herein, we report the on-surface synthesis of: (1) Quasi-planar, furan-containing cycloparaphenylenes (CPPs): Synthesized via Ullmann coupling and cyclodehydrogenation on Au(111), these CPPs show a decreasing energy gap with increasing size. Orbital confinement at edges and pores is observed, which is associated with the slower wave function decay above the CPP plane. (2) Carbon nanoribbons (CNRs) embedded with nonbenzenoid rings: Zigzag nanoribbons bearing 5-6-7 membered rings and linear nanoribbons containing 4-5-6-8 carbon polygons are formed through the lateral fusion of polymer chains on Au(111). Low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) reveals their geometric and electronic properties, and X-ray photoelectron spectroscopy (XPS) unravels the reaction process.

O 63: Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules II

Time: Wednesday 10:30–12:30 Location: H25

O 63.1 Wed 10:30 H25

Unravelling the Photocatalysis of Alcohol on Rutile(110) — •Philip Petzoldt, Lucia Mengel, Anna Lemperle, Moritz Eder, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Heterogeneous photocatalysis is a promising tool for the environmentally benign production of chemical fuels such as hydrogen. However, the structural complexity of state-of-the-art materials makes mechanistic investigations and, in consequence, the targeted design of new catalysts extremely challenging. We employ surface science methods to explore fundamental mechanisms in photocatalysis. In this contribution, we focus on the photocatalytic hydrogen evolution from alcohols over rutile(110) loaded with Pt cluster co-catalysts. Our experimental evidence reveals a new reaction mechanism, which substantially differs from the generally assumed model of independent redox reactions. By changing active sites for both the alcohol oxidation and the hydrogen evolution reaction, we further show that the overall photoactivity strongly depends on the equilibrium of a reaction network of several elementary photo- and thermal reaction steps. Our results provide new mechanistic insights into the photocatalytic hydrogen evolution from Pt loaded titania and illustrate the importance of a comprehensive understanding of the photocatalysts (surface) chemistry.

O 63.2 Wed 10:45 H25

Characterization of rhodium single atoms as dicarbonyls on TiO_2(110) — •Moritz Eder, Faith Lewis, Panukorn Sombut, Johanna Hütner, David Rath, Jan Balajka, Jiri Pavelec, and Gareth Parkinson — Institute of Applied Physics, TU Wien, Austria

Single-atom catalysts (SACs) have garnered significant attention in recent years due to their potential to minimize noble metal usage by isolating active atoms on metal (oxide) surfaces. However, stabilizing these single atoms remains a major challenge. Ligands, such as carbon monoxide, can stabilize single atoms by transforming them into surface-bound metal complexes, closely resembling the well-defined species in homogeneous catalysis. In this contribution, we present a comprehensive characterization of a ligand-stabilized single atom: a rhodium gem-dicarbonyl ($Rh(CO)_2$) bound to rutile TiO_2(110). Using XPS, TPD, scanning probe, and a newly developed IRRAS apparatus, we provide a detailed analysis of these sites. Our findings are contextualized through comparisons with theoretical models and insights from powder catalyst studies in the literature. This work demonstrates that multi-technique approaches are essential for the accurate characterization of single-atom catalysts, offering a deeper understanding of their structure and stability.

O 63.3 Wed 11:00 H25

Desorption of water from microcline (001) — Tobias Dickbreder[1,2], Florian Schneider[1], Lea Klausfering[1], Kim Noelle Dreier[1], Franziska Sabath[1,3], Adam S. Foster[4], Ralf Bechstein[1], and •Angelika Kühnle[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]University of Vienna, 1090 Vienna, Austria — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [4]Aalto University, Finland and Kanazawa University, Kanazawa 920-1192, Japan

Feldspar minerals are highly abundant in the Earth's crust. They play a significant role in a plethora of geochemical processes, including, e.g., weathering and ice nucleation. For many of these processes, the interaction of water with the feldspar surface is decisive. However, little is known about binding and desorption of the first water layer on feldspar. Here, we present temperature-programmed desorption (TPD) experiments of water desorbing from the thermodynamically most stable cleavage plane of potassium-rich feldspar, microcline (001). From the interplay of these experimental data with density-functional theory (DFT) results we shed light onto the binding of the first water layer. Our work confirms previous theory results from literature and provides molecular-scale insights into the binding of water onto microcline (001).

O 63.4 Wed 11:15 H25

Cleaved feldspar surfaces under dry and humid conditions: an AFM study — •Luca Lezuo[1], Sandra Boigner[1], Rainer Abart[2], Michael Schmid[1], Ulrike Diebold[1], and Giada Franceschi[1] — [1]Inst. of Applied Physics, TU Wien, 1040 Wien, Austria — [2]Dep. of Lithospheric Research, Universität Wien, 1090 Wien, Austria

The Earth's surface is largely shaped by the interaction between water and the minerals of its crust. Feldspars, the most common aluminosilicates, are made of a framework of corner-sharing silica and alumina tetrahedra, enclosing cations such as potassium (K^+), sodium (Na^+), and calcium (Ca^{2+}). The chemical reactions at the feldspar-water interface contribute to geological processes such as erosion and weathering [1], clay formation [2], and ice nucleation [3], with implications for geology, agriculture, atmospheric chemistry, and climate science.

We exposed cleaved surfaces of different feldspars to air and Ar with defined humidity and examined the evolution of their mesoscale morphology with atomic force microscopy (AFM). Overlayers with distinct patterns develop over time. They remain stable after rinsing the surface with ultrapure water, suggesting a permanent alteration of the surface morphology. We attribute the distinct patterns to local chemistry differences and different cation leaching rates [1].

[1] Brantley and White, Chem. Weath. Rates of Sil. Min. (2018)
[2] Bleam., Clay Min. and Chem., 87-146 (2017)
[3] Atkinson, et al., Nature 498, 355-358 (2013)

O 63.5 Wed 11:30 H25

Tracking the redox cycle of CeO_2 by Infrared spectroscopy via a titration of the defect states by O_2 adsorption. — •Lachlan Caulfield, Eric Sauter, Hicham Idriss, and Christof Wöll — Karlsruhe Institute of Technology

CeO_2 is probably the most stable reducible metal oxide known. It is the main component of automobile three-way catalysts and is the chief prototype for the thermochemical water splitting to H_2 and O_2 reaction as well as for CO_2 thermal reduction to CO. This is largely due to the relative stability of the $Ce4f_1$ electron formed upon the removal of surface oxygen atoms during the reduction process. While these are commonly studied by photoelectron spectroscopy (XPS Ce3d or UPS Ce4f), less attention in general has been given to the Ce^{3+} (2F5/2 to 2F7/2) spin orbit transition of this process that appears in infrared spectroscopy at ca. 2150 cm^{-1}. In this work we have monitored the formation of these transition on reduced polycrystalline CeO_2 exposed to molecular O_2 as a function of temperature using the DRIFT technique. Results have shown that there is a linear relationship between the disappearance of the observed electronic transition at ca. 2130-2160 cm^{-1} and the IR signal of the superoxo (O^{2-}). species upon exposure of the reduced surface to different partial pressures of O_2. Moreover, it was found that the oxidation process is irreversible: the spin-orbit transition signal does not recover upon the removal of adsorbed oxygen species. Work in progress to track the catalytic activity of these adsorbed O_2 species and spin-orbit transition by probe molecules suitable for the redox cycle.

O 63.6 Wed 11:45 H25

Nucleation of TMDAH on CoO nanoislands on Au(111) — •Jonas Hauner, Nikolai Sidorenko, Hanna Bühlmeyer, and Jörg Libuda — Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany

Atomic layer deposition (ALD) has recently received considerable attention as a promising method to precisely grow thin films of a wide variety of materials. This work focuses on the ALD of HfS_2 on oxide substrates. In specific, we report on the nucleation behavior of the ALD precursor tetrakis(dimethylamido)hafnium(IV) (TMDAH) on cobaltoxide nanoislands on Au(111). The samples were prepared by deposition of Co in oxygen atmosphere and subsequent deposition of TMDAH. We investigated the adsorption of TMDAH by scanning tunneling microscopy (STM) and infrared absorption reflection spectroscopy (IRAS). At 300 K, TMDAH nucleates at OH groups at the CoO surface by means of a Brønsted acid-base reaction. At 400 K, the mechanism changes and involves a Lewis acid-base reaction due to the lack of OH groups on the substrate. Presaturation of the substrate with H_2O further modifies the reaction mechanism of nucleation.

O 63.7 Wed 12:00 H25

Maghemite (γ-Fe_2O_3): From Bulk Phases to (001) Oriented Surfaces — •Muhammad Munawar[1,2] and Rossitza Pentcheva[1] — [1]Department of Physics and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]International Max Planck Research School on Sustainable Metallurgy, Max-Planck-Straße 1, 40237, Düsseldorf, Germany

Maghemite (γ-Fe_2O_3) finds applications across a wide range of fields, including spintronics, magnetic recording, and nano-medicine, to name a few. It can be derived from the magnetite (Fe_3O_4) structure by introducing Fe vacancies in the B layers containing octahedral Fe ions and oxygen. A stoichiometric phase is achieved by tripling the cubic cell along the c-axis, resulting in a charge-transfer insulator with band gap of 1.90 eV. Phonon dispersion indicates that the cubic structure is stable without imaginary frequency modes. *Ab initio* molecular dynamics (AIMD) simulations confirm the stability at 300 K. Additionally, we explore the stability of the (001) surface within the framework of *ab initio* thermodynamics. The A and B layer terminations are favored at oxygen-poor and oxygen-rich conditions, whereas at intermediate oxygen chemical potentials, a 0.5A layer termination is stabilized. While the A termination exhibits only a minor band gap change, a significant decrease occurs for the B-layer termination due to reduction of magnetic moments and Fe-O bonds up to 0.21 Å. These surfaces serve as a starting point to explore the mechanism of hydrogen adsorption and reduction of the material in view of green steel production.

O 63.8 Wed 12:15 H25

New insights into CO adsorption on TiO_2(110): Enhanced IRAS characterisation — •Nail Barama, Moritz Eder, Igor Sokolović, Michele Reticcioli, David Rath, Michael Schmid, Ulrike Diebold, Jiri Pavelec, and Gareth Parkinson — Institute of Applied Physics, TU Wien, 1050 Vienna, Austria

TiO_2(110) serves as a model system for investigating surface reactivity and catalytic behavior, with CO adsorption commonly employed as a probe molecule. While previous IR spectroscopy studies identified two distinct adsorption sites for low coverages, regular Ti sites, and Ti sites near oxygen vacancies[1,2], recent work based on DFT and microscopy suggests the existence of additional adsorption configurations influenced by the polaronic nature of the substrate[3]. In this contribution, we present experimental results obtained using our custom-built reactivity and infrared reflection absorption spectroscopy (IRAS) setup[4]. This design, optimized for detecting small concentrations of adsorbates on metal oxide surfaces, delivers high-resolution spectra with a high signal-to-noise ratio, allowing us to observe new features. Our data reveal multiple CO adsorption configurations on TiO_2(110), which agrees with STM observations from a recent study[3]. References: [1] Xu, M. et al. Angew. Chem. Int. Ed. 51, 4731-4734 (2012). [2] Petrik, N. G. & Kimmel, G. A. J. Phys. Chem. Lett. 3, 3425-3430 (2012). [3] Reticcioli, M. et al. Phys. Rev. Lett. 122, 016805 (2019). [4] Rath, D. et al. Rev. Sci. Instrum. 95, 065106 (2024).

O 64: Focus Session Atomic Scale Investigation of Magnetic 2D Materials

The rapid expansion of the family of magnetic two-dimensional (2D) materials led to the observation of various types of magnetic order in the 2D limit, such as (anti-)ferromagnetism, noncolinear structures, and magnetic moiré effects. On the fundamental level, there are various open questions regarding the mechanisms that underlie these ground states, as well as the understanding of the role of the interface and dimensionality.

Epitaxial growth of 2D magnetic materials on inert substrates under ultrahigh vacuum conditions and respective in situ investigation allows direct and unambiguous comparison between experimental findings and theoretical calculations. Experimentally, (spin-polarized) scanning tunneling microscopy methods are ideal to explore the electronic structure and magnetic properties of emerging 2D magnetic phases with ultimate real-space and energy resolution at low temperatures. These results are often corroborated by averaging techniques such as X-ray magnetic circular dichroism or magneto-optic Kerr effect. Theoretically, the use of model Hamiltonians requires atomically well-defined systems to precisely predict the electronic and magnetic properties. Combining these complementary approaches helps to elucidate the role of the substrate, defects, and the coupling between quasiparticles in stacked heterostructures.

This focus session aims at highlighting recent progress in the growth and characterization of magnetic states in epitaxial 2D materials and 2D heterostructures on metal substrates, bringing together experts from the fields of scanning probe techniques and first-principles calculations. The overall goal of the session is to gain fundamental insights into the driving mechanisms of 2D magnetic phases.

Organized by Jeison Fischer, University of Cologne, Germany and Wouter Jolie, University of Cologne, Germany.

Time: Wednesday 15:00–18:00 Location: H2

Invited Talk O 64.1 Wed 15:00 H2

Topological spin structures in two-dimensional van der Waals magnets and heterostructures — •Stefan Heinze — Institute of Astrophysics and Theoretical Physics, University of Kiel, Germany

Two-dimensional (2D) van der Waals (vdW) magnets offer exciting opportunities for topological magnetism due to high-quality interfaces, the possibility of single-atomic layer systems, and easy control of magnetism via external stimuli [1]. Here, we explore nano- and atomic-scale topological spin structures in 2D vdW magnets and heterostructures based on first-principles calculations and atomistic spin simulations. A focus is given to heterostructures based on the 2D vdW magnet Fe_3GeTe_2 which is experimentally accessible and exhibits favorable properties such as a high transition temperature. An essential pre-requisite to apply topological spin states such as skyrmions in future applications is a sufficient stability which we quantify by calculating their lifetime using transition-state theory [2,3]. All-electrical skyrmion detection is proposed via the tunneling anisotropic and non-collinear magnetoresistance considering both a scanning tunneling microscopy geometry and a planar tunnel device structure [4]. Finally, the all-magnetic vdW heterostructure $Fe_3GeTe_2/Cr_2Ge_2Te_6$ is studied and the stability of bimerons in $Cr_2Ge_2Te_6$ is discussed [5].

[1] Q. H. Wang *et al.*, ACS Nano **16**, 6960 (2022).
[2] D. Li *et al.*, Nano Lett. **22**, 7706 (2022).
[3] D. Li *et al.*, Phys. Rev. B **109**, L220404 (2024).
[4] D. Li *et al.*, Nano Lett. **24**, 2496 (2024).
[5] D. Li *et al.*, arxiv: 2408.15974 (2024).

Invited Talk O 64.2 Wed 15:30 H2

Ferromagnetic Order in 2D Layers of Transition Metal Dichlorides — Andrea Aguirre[1], Andres Pinar[2], Diego Soler[2], Carmen Gonzalez-Orellana[1], Jon Ortuzar[3], Oleksandr Stesovych[2], Celia Rogero[1], Jose Ignacio Pascual[3], Pavel Jelinek[2], Maxim Ilyn[1], and •Martina Corso[1] — [1]Centro de Fisica de Materiales, San Sebastian, Spain — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]CIC NanoGUNE, San Sebastian, Spain

Transition metals dihalides are an ideal class of van der Waals materials that enable the study of magnetic phases as function of the transition metal and halide composition as predicted by theory. Here, we characterize the magnetic and electronic properties of 2D magnets based on metallic dichlorides. The materials form flat epitaxial layers on Au(111) with semiconducting character. By X-Ray Magnetic Circular Dichroism (XMCD) measurements we find that single layers of FeCl2 and NiCl2 are soft ferromagnets on Au(111) and their magnetization can be switched from out-of-plane to in-plane by substituting the metal ion from Fe to Ni. Using low temperature scanning tunnelling microscopy with tips functionalized with a nickelocene molecule as magnetic sensor, we confirm the magnetic order of the materials at the atomic scale even at zero applied magnetic field. We thus established a correlation between the mesoscopic magnetic properties probed by XMCD and the atomic spins. Our results suggest that these 2D semiconducting magnets could be implemented in van der Waals heterostructures for applications in spintronics and opto-spintronics.

Invited Talk O 64.3 Wed 16:00 H2

Tailoring spin lattice in van der Waals monolayer crystals — •Ying-Shuang Fu — Huazhong University of Science and Technology, Wuhan, Chinaina

Spin lattices in monolayer van der Waals (vdW) crystals provide a paradigm for exploring both fundamental spin physics at the 2D limit and miniaturized spintronic applications. Here, we present our recent research in the construction of spin lattices with molecular beam epitaxy and addressing their spin states with both spin-averaged and spin-polarized scanning tunneling microscopy. We explored artificial Kondo lattices in monolayer vdW crystals aiming to emulate protocol heavy fermion systems. We realized quasi-1D Kondo lattice in monolayer stripe-phase 1T-NbSe2 and superconducting 2D Kondo lattice in monolayer VSe2 grown on NbSe2. We also investigated intrinsic magnetic order in monolayer vdW crystals using spin-polarized scanning tunneling microscopy. We identified an antiferromagnetic order in monolayer CrTe2, unraveling the indispensable role of interlayer coupling in determining the magnetic order. Based on that finding, we further fabricated Janus CrTeSe monolayer, and regulates the magnetic anisotropy energy via the symmetry breaking introduced from the Janus structure. Our study resolves intrinsic magnetism with atomic-scale resolution down to monolayer limit, opening up an avenue for studying the unusual spin excitations.

Invited Talk O 64.4 Wed 16:30 H2

Spin excitations in 2D heterostructures from realistic fermionic models — •António Costa — Center of Physics of the University of Minho, Braga, Portugal — International Iberian Nanotechnology Laboratory

Spin excitations dominate the magnetic response of ferromagnetic two-dimensional crystals. The interplay between low dimensionality, reduced symmetry and spin-orbit coupling endows spin excitations in those materials with intriguing properties, such as non-trivial topology and non-reciprocity. Moreover, spin-orbit coupling connects spin and charge degrees of freedom, opening up paths to electrical control and detection of magnetic states. I will present a microscopic description of the spin response of nanostructured materials based on Hamiltonians for itinerant fermions, derived from DFT calculations. This approach incorporates spin-orbit coupling, does not rely on postulated spin models, and can be applied to insulating or conducting 2D heterostructures, with any kind of magnetic order. I will discuss the properties of magnons in insulating and metallic van der Waals ferromagnets, as well as in 2D molecular crystals. I will also discuss the proximity effect in a heterostructure formed by a 2D ferromagnet and graphene.

O 64.5 Wed 17:00 H2

Monolayer Multiferroic - Superconductor van der Waals Heterostructures — •Büşra Gamze Arslan, Mohammad Amini, Ziying Wang, Robert Drost, and Peter Liljeroth — Department of Applied Physics, Aalto University, P.O. Box 15100, 00076 Aalto, Espoo, Finland

Topological superconductivity, a quantum phase hosting robust edge modes like Majorana zero modes (MZMs), holds promise for fault-tolerant quantum computation due to its stability against disturbances. Stacked van der Waals materials offer a promising platform to engineer topological superconductors, as they arise from the interactions between superconductors and magnetic materials. With its helical magnetic order and intrinsic spin-orbit coupling, multiferroic NiI_2 is an excellent component for heterostructures realising topological superconductivity.

Here we present our study on monolayer NiI_2 grown on superconducting bulk $NbSe_2$. This system is characterized using scanning tunneling microscopy (STM) and spectroscopy (STS). The effect of doping due to the growth of NiI_2 on different substrates is investigated. Our observations revealed that NiI_2 does not show ferroelectricity, likely due to the charge transfer from the $NbSe_2$ substrate. In addition, we have investigated the edges of the NiI_2 islands, where we found clear signatures of edge modes in the $NiI_2/NbSe_2$ system. Whether these arise from topological effects remains to be seen in future studies. Our results show that combining 2D materials can create custom materials with relevant properties.

O 64.6 Wed 17:15 H2

Engineering the electronic and magnetic properties of MPS_3 (M=Fe, Ni, Co, Mn) materials through alkali metal doping — Jonah Nitschke[1], •Preeti Bhumla[2], Till Willershausen[1], Patrick Merisescu[3], Lasse Sternemann[1], Valentin Mischke[1], Michele Capra[1], Mira Arndt[1], David Janas[1], Giovanni Zamborlini[4], Silvana Botti[2], and Mirko Cinchetti[1] — [1]TU Dortmund — [2]Research Center Future Energy Materials and Systems, ICAMS, Ruhr University Bochum — [3]University of Bath — [4]Universität Graz

Transition metal phosphorus trichalcogenides, MPX_3 (where M represents a transition metal and X represents a chalcogen), have emerged as promising candidates for exploring two-dimensional (2D) magnetism. In this study, we focus particularly on MPS_3 (M = Fe, Ni, Co, Mn) materials, both above and below the Néel temperature TN. We investigate the electronic and magnetic properties of these materials using micrometer-scale angle-resolved photoelectron spectroscopy (ARPES) and density functional theory (DFT+U) calculations. We observe an increase in the band gaps and shifts in the M d and S p states below TN in the antiferromagnetic (AFM) phase. The density of states reveals the orbital character of the observed bands, and the strong hybridization between the M d and S p orbitals suggests that the superexchange mechanism, in which the S atom mediates the magnetic interaction between neighboring M ions, is relevant for these materials. Further, we examine the effect of alkali metal doping on the magnetic properties of these transition metal phosphorus trichalcogenides.

O 64.7 Wed 17:30 H2

Conflicting magnetic anisotropy in 2D metal-organic networks — •Diego Radillo[1,2], Céline Hensky[1,2], Quy Hien Le[1,2], Manfred Parschau[3], Egzona Isufi Neziri[3], Christian Wäckerlin[1,2], and Pierluigi Gargiani[4] — [1]EPFL, Switzerland — [2]PSI, Switzerland — [3]Empa, Switzerland — [4]ALBA, Spain

This talk presents insights into the properties of 2D metal-organic coordination networks embedded with atoms of conflicting magnetic anisotropies. In particular, we look into the coordination networks of tetracyanoethylene with Ni atoms (NiTCNE), Fe atoms (FeTCNE) and a mixture of both (NiFeTCNE), on a gold(111) surface. NiTCNE is known to be a ferromagnet with an out-of-plane easy axis of magne- tization. Whereas, for the conflicting in-plane ferromagnet, we propose FeTCNE as a suitable candidate. In our mixed-network experiments, where the magnetic exchange energy enforces that the preferences of the two metal ions cannot be perfectly satisfied, we observe that the magnetization along the out-of-plane and in-plane axes at the Ni and Fe centers mutually influence each other in a rather rational way. This interaction suggests the potential for fine-tuning the magnetization axis and highlights the importance of investigating spin alignment at the per-atom scale. Scanning probe microscopy (SPM) and non-contact atomic force microscopy (AFM) are employed to inspect the morphology of the networks, while X-ray absorption spectroscopy (XAS) and X-ray mag- netic circular dichroism (XMCD) were utilized to analyze the magnetic properties.

O 64.8 Wed 17:45 H2

Non-van der Waals 2D Materials: Magnetic State Control — •Tom Barnowsky[1,2] and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Non-van der Waals (non-vdW) 2D materials – exfoliated from non-layered bulk structures [1] – offer unique opportunities for exploring magnetic properties and their surface-assisted manipulation.

In recent data-driven studies [2,3], we predict several dozen exfoliable candidates. Many of these materials exhibit intrinsic magnetism, notably due to magnetic surface cations, which lead to strong surface spin polarization. Furthermore, the exposed "dangling" bonds at their surfaces – created by bond breaking during exfoliation from the bulk – enable passivation that can significantly modify their electronic and magnetic properties [4]. This passivation-based tuning can, for example, switch the magnetic state of these materials, *i.e.*, alter their local spin symmetry. Most notably, non-vdW 2D $CdTiO_3$ – a diamagnetic compound in its pristine form – becomes ferromagnetic upon hydrogenation. Using data mining and autonomous density functional theory, we demonstrate the potential of these materials as a powerful platform for magnetic state control, opening new possibilities for spintronics.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Adv. Electron. Mater. **9**, 2201112 (2023).
[4] T. Barnowsky *et al.*, Nano Lett. **24**, 3874 (2024).

O 65: Solid-Liquid Interfaces: Reactions and Electrochemistry III

Time: Wednesday 15:00–17:45 Location: H6

O 65.1 Wed 15:00 H6

Potential Pulsed CO2 Reduction Reaction on Polycrystalline Copper Electrodes Studied with Operando Plasmonic Interface Analysis — •Hagen Übele, Katharina Krischer, and Moritz Josef Feil — Chemische Physik fern des Gleichgewichts Technische Universität München, München, Deutschland

This contribution highlights the use of polished polycrystalline Cu electrodes for the CO2 reduction reaction. By applying time-periodic potential pulses, long-term stability and enhanced selectivity towards hydrocarbon products like methane, ethylene, and ethanol are achieved. These methods rival the performance of nano-structured oxide-derived catalysts or Cu single crystal electrodes while improving electrode longevity.

Operando monitoring is conducted using a plasmonic interface analysis technique with a time resolution of 100 ms. This enables real-time tracking of the Cu oxidation state and the nano-morphology of the electrode surface during potential pulses. The study demonstrates that optimized pulsing protocols can significantly extend the stability of Cu electrodes without the need for premanufactured nanostructures.

O 65.2 Wed 15:15 H6

Au(111) in the Ionic Liquid [MPPip][TFSI]: Corrosion, Reconstruction and Other Surface Restructuring Phenomena — •Maren-Kathrin Heubach[1] and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany. — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany. — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany.

In fundamental electrochemistry, Au single-crystals are a good benchmarking standard because of the ease of their preparation and high chemical stability.[1-4] Nevertheless, the morphological stability of Au under measurement conditions is rather limited. In this study, we utilize *in situ* scanning tunnelling microscopy (STM) to investigate the stability of a Au(111) electrode in the ionic liq-

uid *N*-methyl-*N*-propylpiperidinium bis(trifluoromethane)sulfonimide ([MPPip][TFSI]). We will provide an overview of the observed surface structures and the corresponding potential ranges in which they remain stable.

[1] J. M. Hermann, *et al.* Electrochim Acta 2020, 347, 136287. [2] M.-K. Heubach, *et al.* ChemElectroChem 2022, 9, e202200722. [3] X. Hu, *et al.* Sci. Bull. (Beijing) 2015, 60, 877-883. [4] L. A. Kibler, *et al.* in Encyclopedia of Solid-Liquid Interfaces, Elsevier, 2024, pp. 426-449.

O 65.3 Wed 15:30 H6

The relationship between composition, structure and activity of well-defined Pt-Ru alloys during electroreduction of acetone — •Robert Hübsch[1], Pankaj Kumar Samal[2], Frederike Jäschke[1], Tomáš Skála[2], Nataliya Tsud[2], Josef Mysliveček[2], Olaf Brummel[1], Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

The isopropanol/acetone couple can be used as an electrochemically active liquid organic hydrogen carrier (EC-LOHC). PtRu-based alloys are the state-of-the-art catalysts for the electrooxidation of isopropanol. We have investigated the reverse reaction, i.e. electrochemical reduction of acetone, on well-defined PtxRu1-x alloys by means of cyclic voltammetry (CV), synchrotron radiation photoelectron spectroscopy (SRPES) coupled with an ex-situ emersion electrochemical cell, electrochemical infrared reflection absorption spectroscopy (EC-IRRAS), and differential electrochemical mass spectrometry (DEMS). In a systematic study, we established structure-activity relationships for well-ordered PtxRu1-x alloys and surfaces subjected to dealloying in pure and acetone-containing electrolyte. We found that the active state of the catalyst corresponds to the presence of ultra-small Pt aggregates supported on partially oxidized Ru(0001). While Pt(110) forms propane as reduction product, the dealloyed catalysts form the target product isopropanol and suppress propane formation.

O 65.4 Wed 15:45 H6

Electrochemical XPS for probing the electrified solid-liquid interface of tungsten carbide — Christoph Griesser, Toni Moser, Sergio Diaz-Coello, and •Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria

A profound understanding of the solid/liquid interface is central in electrochemistry and electrocatalysis, as the interfacial properties determine the electroreactivity of the system. This study reveals the in-situ surface chemistry evolution of tungsten carbide (WC) powders during electrochemical polarization. WC is known for its platinum-like properties and its high activity towards the hydrogen evolution reaction (HER), but prone to passivation upon air or electrolyte exposure. It is found that the unpreventable surface passivation layer on WC dissolves into the electrolyte under HER conditions, which explains the typically measured high HER electrocatalytic activity of this compound material. The electrochemical (EC-)XPS data provide profound chemical understanding of the electrode/electrolyte interface during operation. This enables fundamental contribution to bottom-up electrocatalyst development, and thus to the advancement of energy conversion and storage technologies.

We thank the FWF for financial support within the Cluster of Excellence MECS.

O 65.5 Wed 16:00 H6

Degradation of TiO_2/Pt catalyst interfaces during operation — •Sergej Levashov[1], Tim Rieth[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]TUM School of Natural Sciences — [2]Walter Schottky Institut

Photoelectrochemical (PEC) water splitting is a promising approach for generating green fuels. However, photosystems often degrade in the harsh chemical environment required for PEC water splitting. To overcome this limitation, understanding the starting point of the degradation and the exact degradation mechanism at the nanoscale is required. In this work, we study TiO_2 thin films grown by atomic layer deposition (ALD) combined with Pt catalyst layers, deposited by sputtering and two different ALD processes, by in-situ/operando atomic force microscopy and elucidate their changes in topography and mechanical properties under operation conditions. The main difference between the Pt is the growth mechanics: while sputtering yields a continuous film, the ALD growth results in Pt islands. On the macroscale, the ALD grown Pt catalysts show similar onset potentials and saturation current densities as the sputtered ones. At the nanoscale, we observe that the ALD Pt films are more stable than sputtered Pt under operation conditions. Complementary, we performed X-ray photoelectron spectroscopy (XPS) before and after PEC operation to reveal chemical changes. Overall, ALD grown Pt catalysts improve the system performance compared to sputtered Pt. These measurements provide important insights into the underlying reaction mechanism and the role of surface restructuring and delamination of catalyst interfaces.

O 65.6 Wed 16:15 H6

TiO2 passivation of GaInP(100) surfaces — •David Ostheimer[1], Julius Kühne[2,3], Sahar Shekarabi[1], Agnieszka Paszuk[1], Mohammad Amin Zare Pour[1], Ian D. Sharp[2,3], Wolfram Jägermann[4], and Thomas Hannappel[1] — [1]TU Ilmenau, Inst. of Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]TU Munich, Walter Schottky Institute, Garching, Germany — [3]TU Munich, Physics Department, TUM School of Nat. Sciences, Garching, Germany — [4]TU Darmstadt, Surface Science Lab, Darmstadt, Germany

GaInP is widely used in III-V-based photoelectrochemical devices as a top photoabsorber or charge-selective contact, achieving high solar-to-fuel conversion efficiencies. To enhance stability under HER conditions, a thin TiO2 protection layer can be applied. This study investigates the electronic structure of the TiO2/GaInP(100) interface. TiO2 was deposited via atomic layer deposition (ALD) on p-type GaInP(100) grown on GaAs(100) substrates. Two surfaces were prepared: a phosphorus-rich (P-rich) (2x1)-like surface transferred contamination-free under ultra-high vacuum (UHV) and a naturally oxidized surface. X-ray and UV photoelectron spectroscopy revealed a slightly thinner interfacial oxide in the UHV-transferred sample. Initial ALD cycles formed an oxide nearly stoichiometric to the native oxide, but both samples exhibited strong Fermi level pinning, resulting in similar band alignments. These findings highlight the influence of initial oxides on interface control in III-V semiconductors.

O 65.7 Wed 16:30 H6

Influence of pH and Electrolyte Flow on the Oxidation of Ni anodes at High Overpotentials — •Justus Leist[1], Timo Jacob[1,2,3], and Albert K. Engstfeld[1] — [1]Institute of Electrochemistry, Ulm, Germany — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

The electrocalalytic splitting of aqueous electrolytes is typically impeded by the sluggish kinetics of the oxygen evolution reaction (OER). Ni-based catalysts are considered as cost-effective alternatives to the currently used rare metal oxides, such as Ir or Ru. While the fundamental properties of Ni have been studied intensively usually at or around the onset potential for the OER, here we study the OER activity at high overpotentials, which are more closely related to application.

The OER characteristics are studied by means of cyclic voltammetry and polarization curves using Ni electrodes in alkaline solutions. Depending on the experimental conditions, electrolyte pH and flow, the current voltage traces show several features at high overpotentials, which can be attributed to the pH-dependent change in OER kinetics. Based on additional in-situ Raman spectroscopy and electrochemical quartz crystal microbalance measurements we discuss possible structures formed and the degradation of the Ni electrodes under these conditions.

O 65.8 Wed 16:45 H6

DFT Study of Aldehyde Oxidation and Hydrogen Evolution on Flat and Stepped Gold Surfaces — •Samuel Mattoso[1], Stefan Wipperman[1,2], Mira Todorova[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf — [2]Philipps-Universität Marburg, Renthof 5, Marburg, 35032, Germany

Significant investments are being made in the development of greener industrial processes, with heterogeneous electrocatalysis playing a major role. Gold is known as a catalyst, which selectively oxidizes aldehydes to carboxylic acid. It may also catalyze the hydrogen evolution reaction (HER). These chemical reactions take place at the solid-liquid interface, where the role of step sites, pH, adsorption of intermediates, solvation and applied bias are largely unknown but may be relevant to understand in order to improve performance. We employ DFT simulations to provide mechanistic insights into this system, by probing the interaction of Au(111) and Au(331) surfaces with H, OH and acetaldehyde. The adsorption energies and work function changes as a function of H and OH coverage for different observed patterns will be reported for the two surfaces. In addition, we find that surface imperfections such as step edges are essential for the HER and aldehyde oxidation to proceed, as they dissociatively bind the aldehyde, leading to adsorbed H.

O 65.9 Wed 17:00 H6

On the pH-dependence of the H_{upd} peak in cyclic voltammograms of Pt-group nanoparticles — •Hedda Oschinski[1,2], Simeon Beinlich[1,2], Karsten Reuter[1,2], and Nicolas Hörmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Universität München, München

Understanding the electrochemical behavior of hydrogen adsorption at Pt-group metal surfaces, particularly in the context of non-well-defined nanoparticle surfaces, is crucial for advancing electrocatalytic applications such as the hydrogen evolution reaction (HER). To this end, we provide insights into the non-Nernstian pH shifts observed for underpotential deposited H_{upd}-like cyclic voltammetry (CV) peaks on Pt, Ir, Pd, and Rh nanoparticles. Utilizing density-functional theory, we explore the potential-dependent stability of H and OH adsorbates at undercoordinated surface sites, emphasizing the role of non-ideal electrosorption valencies in these shifts. This identifies direct H-OH replace-

ment as predominant mechanism behind the CV peaks and reveals a primary influence of partial charge transfer. The theoretical predictions show good agreement with experimental observations across various Pt-group metals, even over various surface coordinations, and provide insights into cation-specific effects at Pt across the entire pH scale. This work not only clarifies the origin of the H_{upd}-like peak shift within the water stability region, but also suggests the interfacial capacitance as a main descriptor for cation effects in the HER, paving the way for more detailed analyses of cation type, concentration, and interfacial solvent structure.

O 65.10 Wed 17:15 H6

From model to realistic copper sulfide electrocatalyst — •Roser Fernandez Climent, Jesus Redondo, and Martin Setvín — Charles University, Prague, Czech Republic

Copper sulfide is a widely studied material in electrocatalysis. In this study, we synthesized copper sulfide thin films electrochemically under inert conditions, enabling precise control of material properties and minimizing contamination risks. The films were transferred in-vacuum for surface characterization using X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning transmission electron microscopy (STEM).

O 65.11 Wed 17:30 H6

Stability of Pd-Rh core-shell electrocatalysts supported on Co3O4(111) in alkaline environment — Alexander Simanenko[1], Jan Škvára[2], Pankaj Kumar Samal[2], Evanie Franz[1], Robert Hübsch[1], Tomáš Skála[2], Nataliya Tsud[2], Sascha Mehl[3], Viktor Johánek[2], Josef Mysliveček[2], Olaf Brummel[1], •Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Charles University, Prague, Czech Republic — [3]Elettra-Sincrotrone Trieste SCpA, Basovizza-Trieste, Italy

The electronic metal-support interaction (EMSI) is considered as an efficient strategy to stabilize the noble metal nanoparticles against sintering, but its consequences under the electrochemical conditions remain elusive. We investigated the effect of the EMSI on the stability of bimetallic Pd@Rh and Rh@Pd core@shell nanoparticles supported on well-ordered Co3O4(111) films in alkaline electrochemical environment by means of synchrotron radiation photoelectron spectroscopy (SRPES) coupled with ex-situ emersion electrochemical cell. We found that the EMSI promotes strong oxidation of Rh metal. The extent of Rh oxidation strongly depends on the specific metal/oxide interface configuration below the core@shell nanoparticles. Our study suggests that decoupling the Rh metal and the Co3O4(111) substrate by constructing the Pd/Co3O4(111) interface below Pd@Rh core@shell nanoparticles reduces the effect of the EMSI and improves the stability of the electrocatalyst toward oxidation.

O 66: Vacuum Science Technology: Theory and Applications

Time: Wednesday 15:00–18:00 Location: H8

Invited Talk O 66.1 Wed 15:00 H8

Unveiling the crucial role of kinetic modeling of gas flows in vacuum and fusion technologies — •Christos Tantos and Thomas Giegerich — Institute for Technical Physics, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, 76344, Germany

Accurate and reliable modeling of non-equilibrium flows is not only of academic interest within the scientific community, including the field of vacuum gas dynamics, but is also crucial for the design and enhancement of engineering processes, such as those in vacuum and fusion technologies. In these applications, the flow is characterized by molecular mean free paths that are comparable to the reference characteristic length, making a particle-based description of the flow field essential. This requires the use of the Boltzmann equation and widely accepted numerical methods for solving it, such as the stochastic Direct Simulation Monte Carlo (DSMC) and the deterministic Discrete Velocity Method (DVM).

This talk discusses key aspects of rarefied gas dynamics in vacuum and fusion technologies, emphasizing the link between theory and practice. It is divided into two parts. The first covers recent advances in modeling multicomponent transport phenomena in vacuum technology using DSMC and DVM methods, with a focus on gas separation in multicomponent flows. The second part analyzes vacuum gas dynamics in fusion systems, presenting numerical simulations (2D and 3D) of pumping systems in fusion machines and highlighting their design impact.

Invited Talk O 66.2 Wed 15:30 H8

Advances in traceable vacuum and outgassing rate measurements — •Matthias Bernien[1], Annas Bin Ali[1], Thomas Bock[1], Tom Rubin[1], Janez Setina[2], Perrin Waldock[3], Kirk Madison[3], and Karl Jousten[1] — [1]PTB, Abbestr. 2-12, 10587 Berlin — [2]IMT, Lepi pot 11, 1000 Ljubljana, Slovenia — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, B.C. V6T 1Z1, Canada

For the pressure range from 10 mPa to 130 Pa, a fully automated static expansion system made of aluminum has been set up and validated. Its principle involves transferring a fixed amount of gas from a smaller volume to a larger one, creating a well-defined lower pressure, provided that the initial pressure and the volume ratio are accurately known. Relative standard measurement uncertainties between 0.08% and 0.012% are achieved. Primary standards utilizing cold atom traps offer a promising new approach for realizing the pascal in the UHV range by measuring the loss rate caused by collisions with gas molecules. To establish these standards, the University of British Columbia and PTB have carried out a comparison between a mobile standard based on cold atoms and a continuous expansion system for N_2, Ar and H_2. In the semiconductor industry, outgassing from components in vacuum must be well controlled. Contaminants are monitored using QMSs which lack stability. This is particularly problematic when maximum levels of contaminants must be agreed between manufacturers and suppliers. To improve the comparability of outgassing rate measurements, reference samples for dodecane and water have been developed suitable for in-situ calibration of QMSs.

O 66.3 Wed 16:00 H8

BeamPipes4ET: Innovative On-Site Production and Welding of the Einstein Telescope Vacuum Tubes — Charlotte Benning, •Robert Joppe, Oliver Pooth, and Achim Stahl — III. Physikalisches Institut B, RWTH Aachen

The Einstein Telescope will be the first gravitational wave detector of the third generation. It requires about 120 km of vacuum tubes with a diameter of 1 m to achieve the design sensitivity and reduce scattered light. BeamPipes4ET introduces an innovative production concept for vacuum pipes, incorporating a new welding technology and adapting existing flange and T-section production methods. This approach enhances reliability, significantly reduces labor, welding, and finishing efforts. By manufacturing pipes on-site from coils of sheet metal in a continuous process, transportation needs are minimized, and pipe connections are eliminated. Additionally, the project pioneers laser beam welding under mobile vacuum and transfers advanced pipe feature integration technologies to further streamline production.

This talk presents the current status and ongoing activities in the BeamPipes4ET project.

O 66.4 Wed 16:15 H8

Aluminum fiber optical vacuum feedthroughs for challenging environments — •Christoph Bartlitz, Kristian Kirsch, Marco John, Marcel Hannemann, Andreas Trützschler, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, In den Brückenäckern 3, 07751 Großlöbichau, Germany

Fiber optical components are used in a wide variety of places, both in scientific experiments and in production processes in vacuum systems. In principle, these components enable interference-free transmission of the finest measurement signals over long distances, robust sensor technology and maximum transmission speed. Hermetic optical fiber feedthroughs based on stainless steel, ceramics and quartz glass have become established for coupling light signals to vacuum- and process chambers.

We designed and tested a novel optical fiber feedthrough whose metallic components are made entirely of aluminum.

These technologies enable the application of optical fibers as in-vacuum diagnostic within challenging environments. Thereby, the diagnostic is driven by fiber Bragg gratings (FBGs) in the optical fiber itself. The application of FBGs as an in-vacuum temperature sensor is demonstrated, where an optical fiber containing a bunch of several FBGs becomes a compact, stable, robust, and flexible network of local sensors at different positions in vacuum with up to km-length signal path.

O 66.5 Wed 16:30 H8

Comparative Measurements of Ion Pump pumping speed according to ISO/DIS 3556 and DIN 28429 — •Marcel Herrmann, Kristian Kirsch, Marco John, Christoph Bartlitz, Andreas Trützschler, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH, In den Brückenäckern 3, 07751 Großlöbichau

Sputter Ion Pumps (SIP) offer an appealing strategy to efficiently maintain ultra-high and extremely-high vacuum conditions in a vacuum chamber. The pumping speed, i.e. the volume flow of gas extracted from the vacuum in a specific

period of time, can be determined according to various standards. However, recorded pumping speeds may vary severely, depending on the standard chosen and the detailed procedure applied. This talk compares experimentally obtained pumping speeds of several SIPs, acquired according to the most commonly applied standards, DIN 28429:2014 05 and ISO/DIS 3556 1.2(1992).

O 66.6 Wed 16:45 H8

Performance and future of the KATRIN experiment after 6 years of tritium operation — •Joachim Wolf — Karlsruher Institut für Technologie (for the KATRIN Collaboration)

The Karlsruhe Tritium Neutrino experiment (KATRIN) searches for the effective electron neutrino mass with electrons from the β-decay of tritium with an unprecedented sensitivity of <0.3 eV/c2. The β-electrons are guided magnetically through the 70-m long setup, moving from the gaseous tritium source through a differential pumping section (DPS) and a cryogenic pumping section (CPS) to the high-resolution spectrometer. In the spectrometer, the kinetic energies of the decay electrons are analysed in an electrostatic high-pass filter (MAC-E-filter). Background considerations require a very good vacuum in the order of 10-11 mbar in the large spectrometer vessel (volume 1240 m^3, surface: 1222 m^2). A combination of NEG pumps and turbo-molecular pumps reliably provides the necessary pumping speed since more than 10 years. In addition, a very clean surface and low outgassing rates are mandatory.

After several years of engineering runs, the experiment started full tritium operation in March 2019, searching for the effective mass of electron-antineutrinos. These measurements will finally end in December 2025, followed by hardware upgrades and a new physics program. This talk reports on the performance of the components, after almost 20 years of R&D and 6 years of tritium operation with special emphasis on vacuum-related issues, followed by a description of future plans for the KATRIN setup.

O 66.7 Wed 17:00 H8

Miniaturized Pirani vacuum sensor with active heat-loss compensation — •Julian Eiler[1], Stefan Weber[2], Peter Gerlesberger[2], Heinz Plöchinger[2], and Rupert Schreiner[1] — [1]Faculty of Applied Natural Sciences and Cultural Studies, OTH Regensburg, D-93053 Regensburg, Germany — [2]Thyracont Vacuum Instruments GmbH, D-94036 Passau, Germany

Pirani sensors measure the thermal conductivity of the residual gas in a vacuum by creating a thermal gradient between a heated sensor element and a heat sink. The heat flux from the sensor element to the heat sink over the residual gas is a measure of the vacuum and can be determined by the electrical power applied.

In addition to the heat flux over the gas, there are further energy losses from the heating structure due to radiation and parasitic heat fluxes via the suspensions of the sensor element. These losses reduce the sensitivity of the sensor.

For this reason, a Micro-Pirani sensor in the shape of a micro-hotplate was developed that actively compensates the heat flux via the suspensions. This was achieved by placing additional heating structures on the suspensions, which interrupt the heat flow from the sensor element via the suspensions during operation. This active compensation improves the sensitivity at low pressures, enabling vacuum measurements from atmospheric pressure down to 10e-6 mbar.

O 66.8 Wed 17:15 H8

Feasibility Study on Laser-Based Real-Time Monitoring of Hydrogen Atom Beams — •Tobias Geier, Alexander Marsteller, and Robin Grössle — Karlsruher Institute for Technology, IAP-TLK, for the KAMATE Collaboration

Through the observation of neutrino oscillations, it has been shown that there are three different neutrino mass eigenstates. Current measurements of the oscillation length of the flavor states yield a lower limit for the effective electron neutrino mass of ~ 0.05 eV (inverted ordering) or ~ 0.01 eV (normal ordering). The sensitivity of the KATRIN experiment is limited to ~ 0.3 eV. Therefore, future experiments which aspire to achieve inverted ordering or better need new technologies. For the next generation of experiments aiming at the direct determination of the neutrino mass using high-resolution beta spectroscopy on tritium, atomic tritium is to be used. The advantage over the currently used molecular tritium (T_2) lies in the avoidance of molecular excitations in the $^3HeT^+$ daughter molecule, which lead to a smearing of the beta spectrum, thus limiting the maximum achievable resolution. In order to employ atomic tritium for beta spectroscopy, it is essential to cool it to a few mK and trap it magnetically. A method for contactless real-time analysis of the beam is required to monitor and control the operation of the atomic source. This talk presents a method for characterizing the beam profile based on Rayleigh scattering of a laser beam. By measuring the intensity with a sensitive camera, the particle density can be mapped. In this contribution, the results of a first experimental feasibility study are presented.

O 66.9 Wed 17:30 H8

Challenging tasks in modern vacuum technology applications — •Kristian Kirsch, Andreas Trützschler, Christoph Bartlitz, Marcel Herrmann, Marco John, and Klaus Bergner — VACOM Vakuum Komponenten & Messtechnik GmbH In den Brückenäckern 3 07751 Großlöbichau / Germany

Cutting-edge technology from the field of particle accelerators, quantum technology applications and lithography is pushing the limits of vacuum technology. In general, off-the-self" products are not sufficient for that. In this context, product developers and scientists need to find a joint language to deal with this task. The focus of this talk is to explain needs and challenges of today's cutting edge technology applications related to vacuum requirements. Therefore, we address different state-of-the-art applications. One focus is the fundamental difficulty to fulfill demanding vacuum conditions in one compact system. On the other hand, we address the complex and demanding task of isolating quantum objects within a quantum application like quantum computing, quantum gravimetry, and quantum metrology. Based on this, benefits and drawbacks of different vacuum technology solutions to all of these requirements are shown within the transition from customized single components to standardized and industrial ready serial components.

O 66.10 Wed 17:45 H8

Different Approaches to Vacuum System Performance Improvement for the Einstein Telescope — •Charlotte Benning, Robert Joppe, Maike Kühler, Stefan Krischer, Oliver Pooth, and Achim Stahl — III. Physikalisches Insitut B, RWTH Aachen

The Einstein Telescope will be the next European gravitational wave detector. It requires about 120 km of vacuum tubes in tunnels with a diameter of 1 m for a laser beam to achieve the design sensitivity. The required pressure of less than 10^{-11} mbar introduces the need for innovations that help with performance improvement and cost reduction. The current baseline concept of the vacuum system includes passive sections of stainless steel welded inside the tunnels and connected to pumping stations. Achieving ultra-high vacuum (UHV) in these tubes requires high pumping capacities and long bake-out times of the tubes, which are associated with high energy and equipment costs.

This talk discusses two possible improvements over the baseline design: Integrating non-evaporable getter (NEG) surfaces into the inside of the tubes to reduce costs and aiming for a more homogeneous distribution of pumping power (distributed pumping). Furthermore, forming seamless flanges from the pipe material eliminating the need for welding is presented, which is especially relevant for the underground environment of the Einstein Telescope.

O 67: Ultrafast Electron Dynamics II

Time: Wednesday 15:00–17:45 Location: H11

O 67.1 Wed 15:00 H11

Polaron formation in NiO analysed by transient absorption spectroscopy — •Mahendra Kabbinahithlu[1], Björn Sothmann[1], Fred Hucht[1], Sergey Kovalenko[2], Tobias Lojewski[1], Nico Rothenbach[1], Katharina Ollefs[1], Heiko Wende[1], Uwe Bovensiepen[1], Julia Stähler[2], and Andrea Eschenlohr[1] — [1]Universität Duisburg-Essen, Fakultät für Physik und Center for Nanointegration (CENIDE), Lotharstraße 1, 47057 Duisburg, Germany — [2]Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Straße 2, 12489 Berlin, Germany

Polaron formation is the process by which free electrons in a material find a lower energy localized state by distorting their surrounding lattice. The polaron formation timescales and its fluence dependent dynamics in nickel oxide (NiO) from time-resolved optical absorption studies is discussed here.

NiO is pumped above the band gap with 3.98 eV energy photons, and is probed using a time-delayed supercontinuum. The time-resolved absorption spectrum shows negative ground state bleach and positive excited state absorption and in addition, a time-delayed and energy separated appearance of a positive feature at 3.35 eV that is discussed as the signature of polaron formation. With increasing fluence,the build-up time of this 3.35 eV signature decreases from 4 ps down to 1.1 ps, indicating the transition from isolated polarons to the formation of a polaron band. The spectrally distinct transition between low fluence and high fluence regimes is used to estimate the polaron size and the dynamics is modelled by coupled rate equations.

O 67.2 Wed 15:15 H11

Sharp Exciton Mott Transition in WS_2 and its Ultrafast Decay — •Subhadra Mohapatra[1], Lukas Gierster[1], Samuel Palato[1], Nicholas Michael Olsen[2], Xiaoyang Zhu[2], and Julia Stähler[1] — [1]Humboldt-Universität zu Berlin, Institut für Chemie — [2]Columbia University

The excitonic Mott transition (EMT) in transition metal dichalcogenides is reported to be either discontinuous [1] or continuous [2]. To resolve the ambiguity,

here we study the optical response of WS_2 across the Mott density. Using a complex lineshape analysis, we separate the optical response in the photo-excited part of the sample from the unexcited regimes. In agreement with a continuous EMT, a gradual increase in the bleach of the sample-averaged absorption is observed. However, the lineshape analysis unveils a sharp discontinuity in the transient dynamics of the A and B exciton resonances above a critical photoexcitation density. This is attributed to plasma formation followed by band gap renormalization. The plasma decays with a laser fluence-independent time constant of 0.65 ps which is attributed to phase separation into excitonic and plasma regions, in agreement with the literature [3,4]. This work not only provides the first detailed experimental investigation of the EMT close to the critical limit but also highlights the role of spatial inhomogeneous charge carrier distribution for the widely used transient optical spectroscopies of 2D materials. [1] Bataller et al. Nano Lett 19(2) (2019). [2] Chernikov et al. Nat Photonics 9(7) (2015). [3] Steinhoff et al. Nat Commun 8 (1) (2017). [4] Koch et al. Physica status solidi (b) 238(3) (2003).

O 67.3 Wed 15:30 H11

Ultrafast formation of electron polarons in rutile TiO_2(110) — •Xiang Zhang, Lukas Gierster, and Julia Stähler — Humboldt-Universität zu Berlin, Institut für Chemie

The electron dynamics at TiO_2 surfaces are widely studied, mainly focusing on the defect-induced electronic states [1,2]. Additionally, recent calculations suggest that upon across-bandgap excitation, electron polarons form within 25 fs by trapping of photoexcited electrons inside the deformed lattice [3]. Using time-resolved photoelectron spectroscopy, we observe the instrument response-limited (<30 fs) rise of a photoinduced electron population at 0.3 eV below E_F. To elucidate whether this feature originates from polaron formation, experiments are conducted with different laser fluences, photon en- ergies and under varying surface conditions. Based on this, competing mechanism as exciton formation, surface photovoltage effects and band gap renormalization can be excluded. Our results suggest that photoexcitation of the rutile TiO_2(110) surface creates small sub-surface polarons within only 30 fs.

[1] A. Argondizzo et al. J. Phys. Chem. C 120, 12959-12966(2016).
[2] Y. Zhang et al. J. Phys. Chem. Lett. 10, 5265-5270(2019).
[3] C. Gao et al. J. Phys. Chem. C 125, 27275-27282(2021).

O 67.4 Wed 15:45 H11

Time-resolved two-photon photoemission of antiferromagnetic $LaFeO_3$ — •Friederike Wührl, Antonia Rieche, Anne Oelschläger, Kathrin Dörr, and Wolf Widdra — MLU Halle-Wittenberg

Basic quantities as band gaps or the lifetime of electrons at the conduction band minimum are of strong interest for optoelectronic devives. In this context, strongly correlated oxides are rarely studied. One such example is NiO, which shows a remarkable short lifetime of < 10 fs at the conduction band minimum, relaxing in a many-body in-gap state, which couples to the antiferromagnetic spin system [1].

We present time-resolved two-photon photoemission (2PPE) data on above band gap excitation of electrons in $LaFeO_3$, a charge-transfer insulator with antiferromagnetic order, which exhibits weak ferromagnetism through spin canting. The band gap opens between hybridized O 2p – Fe $3d_\uparrow$ and minority Fe 3d $t_{2g\downarrow}$ states. Thin films of 9 nm $LaFeO_3$ were prepared on $SrRuO_3$/$DyScO_3$ substrates using pulsed laser deposition. Low-energy electron diffraction confirmed the formation of single crystalline layers with a c(2x2) superstructure, indicative for the long-range magnetic ordering. In one-colour and two-colour UV-UV pump-probe experiments ($h\nu$ = 3.4 eV and 4.2 eV) we find three unoccupied states at 0.3, 1.3, 2.1 eV above E_F, the middle one being resonantly pumped from Fe $e_{g,\uparrow}$ states and exhibiting a short lifetime of 22 fs. At the conduction band minimum we observe a biexponential decay with lifetimes of 40 fs and 1.1 ps.

[1] Gillmeister *et al.* Nat. Commun. **11**, 4095 (2020).

O 67.5 Wed 16:00 H11

Photo-induced charge-transfer renormalization in NiO — •T. Lojewski[1], D. Golez[2,3], K. Ollefs[1], L. Le Guyader[4], L. Kämmerer[1], N. Rothenbach[1], R. Y. Engel[5], P. S. Miedema[5], M. Beye[5,6], G. S. Chiuzbaian[7], R. Carley[4], R. Gort[4], B. E. Van Kuiken[4], G. Mercurio[4], J. Schlappa[4], A. Yaroslavtsev[4,8], A. Scherz[4], F. Döring[9], C. David[9], H. Wende[1], U. Bovensiepen[1,10], M. Eckstein[11], P. Werner[12], and A. Eschenlohr[1] — [1]Univ. Duisburg-Essen & CENIDE — [2]Jozef Stefan Inst. — [3]Univ. of Ljubljana — [4]European XFEL — [5]DESY — [6]Stockholm Univ. — [7]Sorbonne Univ. — [8]MAX IV Lab. — [9]PSI — [10]Univ. of Tokyo — [11]Univ. of Hamburg — [12]Univ. of Fribourg

For strongly correlated materials, like the charge transfer insulator NiO, the interplay between the interaction-based localization and the itinerant behaviour of electrons is essential in determining the electronic properties. In these materials, resonant photoexcitations result in convoluted dynamics involving dynamical screening induced band shifts, charge redistributions and *d-d* type excitations. By combining fs time-resolved X-ray absorption spectroscopy and dynamical mean-field theory, we disentangle the intertwined dynamics. We find long-lived redshifts of the Ni *L* and O *K* edges (> 10 ps), arising from a combination of Hartree shifts and renormalization of local interactions. We also identify a short-lived Ni L_3 pre-edge feature (< 1 ps) related to photo-induced *d-d* transitions [1]. Financial support by DFG through SFB 1242 is acknowledged. - [1] T. Lojewski et al., Phys. Rev. B, in press (ArXiv:2305.10145)

O 67.6 Wed 16:15 H11

Non-equilibrium carrier dynamics and band structure of graphene on 2D silicon — •Maria-Elisabeth Federl[1], Theresa Glaser[1], Niclas Tilgner[2], Thomas Seyller[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Technical University Chemnitz

Confinement heteroepitaxy, where novel 2D structures are stabilized at the interface between epitaxial graphene and SiC substrate, provides a pathway to engineer proximity-coupling between the massless carriers in graphene and the carriers in the underlying layer. If the latter is a Mott insulator, exotic electronic properties might emerge due to hybridization between itinerant and localized electrons. The Si-rich (3x3) structure on the surface of SiC(0001) was proposed to be Mott insulating with a bandgap of 1eV [1]. We used confinement heteroepitaxy to prepare a graphene monolayer on top of this putative 2D Mott insulator [2] and searched for indications of interlayer hybridization using time- and angle-resolved photoemission spectroscopy (trARPES). Our findings are consistent with the occurrence of ultrafast charge transfer between graphene and the Si-rich surface structure that we attribute to interlayer hybridization in agreement with predictions from density functional theory [2].

[1] Surf. Sci. 445, 109 (2000)
[2] Phys. Rev. B 94, 245421 (2016)

O 67.7 Wed 16:30 H11

Direct view on ultrafast charge transfer between C60 molecules and graphene — •Michael Herb, Maria-Elisabeth Federl, and Isabella Gierz — University of Regensburg

Interfacing 0D molecules with 2D materials holds great potential for various applications in materials science, electronics, and nanotechnology. For example, C60/graphene hybrids have been proposed to serve as supercapacitors or sensitive UV-visible photodetectors. We use time- and angle-resolved photoemission spectroscopy (trARPES) to investigate the interfacial non-equilibrium charge carrier dynamics of a sub-monolayer C60 film deposited on single-layer graphene. Upon excitation below the HOMO-LUMO gap of C60, we observe a shift of the graphene Dirac cone towards higher binding energies and a concurrent shift of the C60 molecular levels towards lower binding energies. These shifts indicate a photoinduced hole doping of graphene that persists for several picoseconds. Based on these findings we propose a possible microscopic pathway for ultrafast charge transfer across the C60-graphene interface.

O 67.8 Wed 16:45 H11

Light-induced hidden state studied by ultrafast angle-resolved photoemission spectroscopy — •Junde Liu[1], Pei Liu[3], Liu Yang[3], Sung-Hoon Lee[4], Mojun Pan[2], Famin Chen[2], Jierui Huang[2], Bei Jiang[2], Mingzhe Hu[2], Yuchong Zhang[2], Zhaoyang Xie[3], Gang Wang[3], Mengxue Guan[3], Wei Jiang[3], Huaixin Yang[2], Jianqi Li[2], Chenxia Yun[2], Zhiwei Wang[3], Sheng Meng[2], Yugui Yao[3], Tian Qian[2], and Xun Shi[3] — [1]University of Göttingen, I. Physikalisches Institut, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]Beijing Institute of Technology, Beijing, China — [4]Kyung Hee University, Yongin, Republic of Korea

The non-volatile and ultrafast optical manipulation of material properties offers profound insights into light-matter interactions and holds great potential for optoelectronic applications. However, the discovery of such transitions is often serendipitous, and their practical implementation remains limited, underscoring the need for systematic investigation. In this talk, I will focus on laser-induced nonvolatile phase transitions in transition metal dichalcogenides (TMDs), highlighting the critical role of interlayer order in the formation of hidden states. By employing ultrafast laser excitations (single-pulse writing, pulse-train erasing and pulse-pair control), systematic angle-resolved photoemission spectroscopy (ARPES) characterizations, and comparative density functional theory (DFT) calculations, I aim to unravel the mechanisms that form and stabilize these hidden states, paving the way for novel methods to optically control low-dimensional materials.

O 67.9 Wed 17:00 H11

A machine-learning approach to understanding ultrafast carrier dynamics in the 3D Brillouin zone of $PtBi_2$ — Paulina Majchrzak[1], Charlotte Sanders[2], Yu Zhang[2], Andrii Kuibarov[3], Oleksandr Suvorov[3], Tami Meyer[1], Gesa Siemann[1], Emma Springate[2], Iryna Kovalchuk[3,4], Saicharan Aswartham[3], Grigory Shipunov[3], Bernd Büchner[3], Sergey Borisenko[3], and •Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]IFW Dresden, Germany — [4]Kyiv Academic University, UA

We examine the electron dynamics of the type-I Weyl semimetal $PtBi_2$ by time- and angle-resolved photoemission spectroscopy. By varying the probe photon energy over a wide range, we are able to explore differences throughout the three-

dimensional Brillouin zone. For these experiments, the photoemission intensity is measured as a function of emission angle, electron kinetic energy, time delay and probe photon energy. In order to discover trends in this multi-dimensional data set, we apply k-means, an unsupervised machine learning technique. This reveals k_z-dependent differences in dynamics–in particular, we observe dynamics that are faster in the parts of the Brillouin zone that host most of the bulk Fermi surface than in parts close to the Weyl points.

O 67.10 Wed 17:15 H11

Tracing thermal and athermal electrons in laser-excited metals — •Markus Uehlein[1], Henry Snowden[2], Christopher Seibel[1], Tobias Held[1], Sebastian T Weber[1], Reinhard J Maurer[2,3], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Germany — [2]Department of Chemistry, University of Warwick, United Kingdom — [3]Department of Physics, University of Warwick, United Kingdom

Understanding the energy- and time-resolved electronic properties in metals at the initial athermal stage after femtosecond laser irradiation is of fundamental importance for many applications in surface science. In the time domain, where no electron temperature is defined, the non-equilibrium dynamics are usually described with microscopic methods, such as the Boltzmann equation. However, especially when investigating ballistic transport processes, a description with full Boltzmann collision integrals [1] is challenging due to the numerical effort.

We present a model that describes the athermal carriers efficiently. To that end, we consider thermal and athermal electrons separately. We use a temperature-based approach for the thermal electrons and the phonons, while we trace the distribution of the athermal electrons explicitly. Such a separation allows to conserve particles and energy even when a relaxation time approach is applied. We show the energy-resolved dynamics and find good agreement with time-resolved two-photon photoemission spectroscopy measurements [2].

[1] B. Y. Mueller and B. Rethfeld; Phys. Rev. B **87**, 035139 (2013)
[2] F. Kühne *et al.*; Phys. Rev. Res. **4**, 033239 (2022)

O 67.11 Wed 17:30 H11

Influence of carbon buffer layer on non-equilibrium carrier dynamics of epitaxial graphene on SiC(0001) — •Johannes Gradl[1], Leornard Weigl[1], Neeraj Mishra[2,3], Stiven Forti[2], Camilla Coletti[2,3], and Isabella Gierz[1] — [1]University of Regensburg, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy — [3]Istituto Italiano di Tecnologia, Genova, Italy

The carbon buffer layer resting at the interface between epitaxial graphene and SiC(0001) substrate is believed to be electronically dead with two non-dispersing bands located well below the Fermi level [1]. We use time- and angle-resolved photoemission spectroscopy (trARPES) to show that this picture breaks down away from thermal equilibrium and on ultrafast time scales. We find that photodoping of the graphene - buffer layer heterostructure increases the carrier concentration inside the Dirac cone. Supported by pump fluence and pump wavelength dependent measurements we attribute this transient charging to direct electronic transitions between the buffer layer and the graphene layer and subsequent relaxation of the non-equilibrium charge carrier distribution.

[1] Phys. Rev. B 77, 155303 (2008)

O 68: Focus Session Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation IV

This focus session aims to discuss recent advances in the on-surface synthesis, manipulation, characterization, and understanding of complex molecular architectures on surfaces. The interest in surface-confined molecular nanostructures emerges from their prospective applications in nanoscale (opto-) electronics, spintronics, solar cells, energy storage devices, and other fields. The bottom-up fabrication of surface-supported nanostructures can be based on molecular self-assembly utilizing non-covalent intermolecular interactions, covalent on-surface synthesis, or the direct manipulation of molecules. Molecular self-assembly usually leads to highly ordered nanostructures, controlled by non-covalent interactions, adsorbate-substrate interactions, as well as thermodynamic and kinetic factors. On-surface synthesis by covalent coupling of reactive precursors adsorbed on metallic, semiconducting, or even insulating surfaces has emerged as a powerful method that has opened new possibilities in exploring new routes towards the synthesis of complex low-dimensional nanostructures with unprecedented material properties, often via novel chemical reactions not available in conventional organic chemistry. Finally, the direct manipulation of molecules with the tip of a scanning probe microscope allows for unprecedented chemical transformations or structural modifications, as envisioned by the pioneers of nanotechnology. This focus session is intended to provide a platform for addressing current trends in these closely linked fields from various perspectives in experiment and theory.

Organized by Sabine Wenzel (University of Marburg) and Christian Wagner (Forschungszentrum Jülich)

Time: Wednesday 15:00–17:45 Location: H24

O 68.1 Wed 15:00 H24

On-surface Synthesis of Aza-Coronoids — •Tim Naumann[1], Zilin Ruan[1], Olaf Kleykamp[1], Alix Kaczmarek[2], Linus Pohl[2], Andreas Achazi[2], Eugen Sharikow[1], Doreen Mollenhauer[2,3,4], Jörg Sundermeyer[1], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Justus Liebig Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen, Germany — [3]Helmholtz-Institut für Polymere in Energieanwendungen, Lessingstr. 12-14, 07743 Jena, Germany — [4]Institut für Technische Chemie und Umweltchemie, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

The properties of nanographenes can be tailored by altering the topology, introducing defect sites like vacancies, or doping with heteroatoms. Coronoids represent a versatile sub-class of the nanographenes and can be regarded as benzenoids featuring a cavity. In-solution synthesis of extended coronoids has shown to be challenging due to their low solubility. To gain access to various aza-coronoids, we combined in-solution and on-surface techniques. By modification of the precursor's substituents, the edge termination of the coronoids is controlled. Besides planar armchair-edge and zigzag-edge terminated coronoids, a curved coronoid was synthesized. Nitrogen functionalization of the cavity allows for hosting a metal atom, giving rise to the formation of coronoid-metal complexes. The electronic and geometric properties of the nanostructures were investigated by low temperature scanning tunneling microscopy/spectroscopy (STM/STS) and non-contact atomic force microscopy (nc-AFM) and supported by DFT calculations.

O 68.2 Wed 15:15 H24

Sequential on-surface synthesis of planar and curved fused anthracenyl-porphyrins — •Miloš Baljozović[1], Joffrey Pijeat[2], Stéphane Campidelli[2], and Karl-Heinz Ernst[1,3,4] — [1]Empa, Dübendorf, Switzerland — [2]Université Paris-Saclay, CEA, Gif-sur-Yvette, France — [3]University of Zürich, Zürich, Switzerland — [4]The Czech Academy of Sciences, Prague, Czech Republic

On-surface synthesis has lately provided means for C-C bond formation that would otherwise hardly be accessible by conventional solution chemistry. Porphyrins are of particular interest in this regard, due to the ability to fine tune their physical and chemical properties via central metal incorporation or peripheral functionalization. Nevertheless, the formation of π-extended porphyrins bearing unsubstituted anthracenyl moieties was so far not achieved.

In this contribution we demonstrate temperature controlled (cyclo)dehydrogenation of bis- and tetra-anthracenyl Zn(II) porphyrins on a Au(111) substrate. Notably, on-surface dehydrogenation is not limited to the first dehydrogenation step involving fusion of anthracenyl units to the macrocycle. Sequential dehydrogenation with temperature elevation is leading to novel planar and curved porphyrin products beyond ones obtained by wet synthesis that could be identified in our combined STM, XPS and ToF-SIMS study.[1]

Support by Swiss National Science Foundation and University of Zürich Research Priority Program LightChEC is gratefully acknowledged.

[1] Baljozović, M. et al. J. Am. Chem. Soc. - just accepted.

O 68.3 Wed 15:30 H24

On-surface synthesis of porphyrin-capped carbon nanocones — Nemanja Kocic[1], Andreas Dörr[1], Moritz Villmow[1], Kevin Dhamo[2], Michael Ruppel[2], Norbert Jux[2], Bernd Meyer[2], and •Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We demonstrate the surface-assisted transformation of porphyrin-based precursor molecules into bowl-shaped nanographenes through cyclization reactions on an Au(111) surface. The structures are visualized by scanning probe techniques with submolecular resolution, directly revealing intramolecular bonding and compared to density-functional theory calculations. Distinct configurations that suggest bowl-to-dome inversion are identified on the surface. Additionally, we report the accompanying metallation of the macrocycle with Au substrate adatoms. This combination of porphyrin and nanographene with a periphery solely consisting of six-membered all-carbon rings might serve as a seed for growing porphyrin-doped graphene sheets.

O 68.4 Wed 15:45 H24

Relating Radical Delocalization, Charge Transfer and Magnetic Ground State in Open-Shell Molecules — Tao Wang[1], Sergio Salaverria[2], Fernando Aguilar-Galindo[3], Javier Besteiro-Saez[4], Luis M. Mateo[4], Paula Angulo-Portugal[5], Jonathan Rodriguez-Fernandez[6], Dolores Perez[4], Martina Corso[1,5], Diego Peña[4], and •Dimas G. de Oteyza[1,2] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Nanomaterials and Nanotechnology Research Center (CINN), El Entrego, Spain — [3]Universidad Autónoma de Madrid, Madrid, Spain — [4]CiQUS, Santiago de Compostela, Spain — [5]Centro de Fisica de Materiales, San Sebastián, Spain — [6]University of Oviedo, Oviedo, Spain

At the same time as our capabilities to synthesize open-shell carbon-based materials are rapidly growing with the development of on-surface synthesis under vacuum conditions, the interest in pi-magnetism is rising due to its excellent prospects for potential applications. As a result, increasing efforts are being focused on the detailed understanding of open-shell carbon nanostructures and all the parameters that determine their spin densities and magnetic ground states. Here we present a facile route to synthesize different open-shell acene derivatives with closely related structures. A systematic comparison allows us to draw conclusions on the role of the functional groups, their number and distribution, as well as on the role of the radical state delocalization in relation with the presence or absence of charge transfer at interfaces, which consequently impacts the molecules pi-magnetism.

O 68.5 Wed 16:00 H24

A route toward the on-surface synthesis of organic ferromagnetic quantum spin chains — •Fabian Paschke[1], Ricardo Ortiz[2], Shantanu Mishra[1], Manuel Vilas-Varela[3], Florian Albrecht[1], Diego Peña[3], Manuel Melle-Franco[2], and Leo Gross[1] — [1]IBM Research Europe - Zurich, 8803 Rueschlikon, Switzerland — [2]CICECO - Instituto de Materiais de Aveiro, 3810-193 Aveiro, Portugal — [3]CiQUS and Department of Organic Chemistry, 15782 Santiago de Compostela, Spain

Engineering a sublattice imbalance is an intuitive way to induce high-spin ground states in bipartite polycyclic conjugated hydrocarbons. Such high-spin molecules can be employed as building blocks of quantum spin chains, which are outstanding platforms to study many-body physics and fundamental models in quantum magnetism [1].

In contrast to antiferromagnetism, demonstration of ferromagnetic coupling between polycyclic conjugated hydrocarbons has been scarce. Here, we demonstrate the on-surface synthesis of short ferromagnetic spin chains based on dibenzotriangulene, a polycyclic conjugated hydrocarbon with a triplet ground state. We achieve a direct majority-minority sublattice coupling between adjacent units, which leads to a global sublattice imbalance in the chains and therefore a ferromagnetic ground state with a strong intermolecular ferromagnetic exchange. By means of scanning probe measurements and quantum chemistry calculations, we confirm quintet and septet ground states in dimers and trimers, respectively.

[1] S. Mishra et al., Nature 598, 287 (2021).

O 68.6 Wed 16:15 H24

Atomically Precise Control of Topological State Hybridization in Conjugated Polymers — Alejandro Jiménez-Martín[1,2], Zdenka Sosnová[2], Diego Soler[2], Benjamin Mallada[1], Héctor González-Herrero[1], Shayan Edalatmanesh[1,2], Pavel Jelínek[1,2], and •Bruno de la Torre[1,3] — [1]Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN), Palacký University, 78371 Olomouc, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences, 16200 Prague, Czech Republic — [3]Nanomaterials and Nanotechnology Research Center (CINN), CSIC-UNIOVI-PA, 33940 El Entrego, Spain

Realization of topological quantum states in carbon nanostructures has recently emerged as a promising platform for hosting highly coherent and controllable quantum dot spin qubits. However, their adjustable manipulation remains elusive. Here, we report the atomically accurate control of the hybridization level of topologically protected quantum edge states emerging from topological interfaces in bottom-up-fabricated π-conjugated polymers. Our investigation employed a combination of low-temperature scanning tunneling microscopy and spectroscopy, along with high-resolution atomic force microscopy, to effectively modify the hybridization level of neighboring edge states by the selective dehydrogenation reaction of molecular units in a pentacene-based polymer and demonstrate their reversible character.

O 68.7 Wed 16:30 H24

On-surface encapsulation of azafullerene radicals: towards 2D spin networks — •Marion A. van Midden Mavrič[1], Bastien Anézo[1,2], Gregor Kladnik[3,4], Luca Schio[4], Gregor Bavdek[4,5], Yuri Tanuma[1,6], Ruben Canton-Vitoria[7], Ioanna K. Sideri[7], Nikos Tagmatarchis[7], Jannis Volkmann[8,9], Herman A. Wegner[8,9], Andrea Goldoni[10], Chris Ewels[2], Alberto Morgante[4,11], Luca Floreano[4], Erik Zupanič[1], Dean Cvetko[1,3,4], and Denis Arčon[1,3] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]IMN, Nantes University, France — [3]FMF, University of Ljubljana, Slovenia — [4]CNR-IOM, Trieste, Italy — [5]PF, University of Ljubljana, Slovenia — [6]CAREM, Hokkaido University, Sapporo, Japan — [7]T.P.C.I., Athens, Greece — [8]Center for Materials research, Giessen, Germany — [9]Justus Liebig University, Giessen, Germany — [10]Elettra Sincrotrone Trieste S.C.p.A., Italy — [11]Phys. dept., University of Trieste, Italy

While organic radicals on surfaces are a promising platform for realizing and controlling qubits, they are usually highly reactive. Here we present on-surface encapsulation of azafullerene $C_{59}N^{\bullet}$ into [10]cycloparaphenylene ([10]CPP) nanohoops on Au(111) as an efficient strategy to form supramolecular complexes with long-term spin protection. By vacuum depositing $C_{59}N^{\bullet}$ on a pre-deposited template layer of [10]CPP, extended networks of spin 1/2 radicals in a hexagonal lattice are formed. We find compelling evidence for electronic coupling between both molecular species, show that [10]CPP protects $C_{59}N^{\bullet}$ against dimerization and inhibits coupling to the Au(111) substrate.

O 68.8 Wed 16:45 H24

Remote debromination on ultrathin insulating film — •Tzu-Chao Hung[1], Lucía Gómez-Rodrigo[2], Lennart Moritz[1], Manuel Vilas-Varela[2], Leo Gross[3], Diego Peña[2], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, Spain — [3]IBM Research Europe, Zurich, Switzerland

Open-shell carbon-based structures are widely studied in recent years not only owing to their potential applications in spintronics and as quantum devices, but they can also serve as a platform to investigate electron-correlation phenomena. One way to study open-shell molecules despite their large reactivity, is to create them from a suitable precursor in a scanning probe microscope (SPM) under ultra-high-vacuum and low-temperature conditions. Here, we demonstrate a particularly efficient debromination reaction resulting in an open-shell molecule by means of SPM manipulation on ultrathin NaCl film on Cu(111). The debromination even works remotely with the tip being up to ~10 nm away from the molecule for both voltage polarities. Based on our observation, possible reaction mechanisms will be discussed.

Invited Talk O 68.9 Wed 17:00 H24

On-Surface Synthesis of Porphyrins and BN-Substituted Carbon Scaffolds — •Willi Auwärter — Technical University of Munich, Garching, Germany

On-surface synthesis protocols provide elegant routes to individual molecular complexes, oligomers, and other carbon-based nanomaterials on metal supports [1]. The resulting structural, physical, and chemical properties can be controlled by heteroatom-substitution. The talk will report on our activities employing thermally induced reactions on coinage metal surfaces, affording heteroatom-doped porphyrins and BN-substituted carbon scaffolds. Specifically, a route to peripherally O-doped porphyrins is addressed [2]. Furthermore, we will discuss the use of functionalized borazine precursors yielding covalent carbon networks with $(BN)_3$ motifs. These include random sheet-like BNC structures [3], which can be transferred to Si waver dices, and covalent organic frameworks (COFs) on Ag(111) and Au(111). The comprehensive characterization by scanning probe microscopy, complemented by theoretical modelling, reveals that COFs with distinct $(BN)_3$ densities, pore sizes, and electronic structures can be achieved. The findings open pathways to new O- and BN-substituted carbon-based nanoarchitectures on surfaces. [1] Grill, L.; Hecht S. Nat. Chem. 12, 115 (2020). [2] Deyerling, J. et al. Angew. Chem. Int. Ed., e202412978 (2024). [3] Tömekce et al., Chem. Eur. J., e202402492 (2024).

O 68.10 Wed 17:30 H24

An electrically controlled molecular spin switch — •Kwan Ho Au-Yeung[1], Wantong Huang[1], Paul Greule[1], Máté Stark[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Roberto Robles[2], Nicolas Lorente[2,3], and Philip Willke[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain

Precise control of spin states and spin-spin interactions in atomic-scale molecular complexes is key to developing multi-spin systems on surfaces for instance for applications in quantum technologies. This has been realized in a variety of systems, for instance in spin-crossover molecules. In this study, we explore the spin coupling and tunability of molecular dimer complexes on an insulating magnesium oxide film: When brought close to a single Fe adatom, a FePc molecule interacts with the Fe forming an interacting spin system. The calculated adsorption geometries by density functional theory (DFT) shed light on the two adsorption configurations of the two bistable states. The two states of the Fe-FePc complex can be successfully and reversibly switched using STM voltage pulses. Subsequently, by using scanning tunneling spectroscopy, we show that this is accompanied by an alteration of the total spin state and spin coupling in the complex. We further illustrate how the complex can be used to shift the resonance frequency of a nearby FePc in single spin resonance experiments, which demonstrates that this complex can function as a magnetic spin switch.

O 69: Nanostructures at Surfaces II

Time: Wednesday 15:00–17:30 Location: H25

O 69.1 Wed 15:00 H25

Thermally-activated molecular rotors organised by porous networks on Au(111) — •Vishakya Jayalatharachchi[1], Roberto Robles[2], Milan Kivala[3], Nicolás Lorente[2,4], Meike Stöhr[1,5], and Sabine Maier[1] — [1]Department of Physics, Friedrich- Alexander-Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]Institute of Organic Chemistry, University of Heidelberg, Germany — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain — [5]University of Applied Sciences of the Grisons, Switzerland

Gaining insights into the precise control of molecular rotation on surfaces is crucial for making progress in nanoscale device innovation. In this study, we investigate the thermally triggered rotational motion of bromine-functionalized decacyclene (Br-DC) molecules, which are confined within a host-guest network of 4,4',4"-nitrilotribenzoic acid (H3NTB) on Au(111). With scanning tunneling microscopy (STM) experiments at variable temperatures, we could determine both the onset of molecular rotation (around 110 K) and the barrier for rotation. Importantly, the Br-DC molecules do not possess a predefined intrinsic rotation axis. Instead, the rotational motion is facilitated by the attractive interactions between the Br-DC guests and the H3NTB host network. Computational simulations support our findings and provide further insights into the energetics. Our strategy provides greater flexibility and versatility compared to traditional confinement approaches based on precise size matching of rotor and host networks.

O 69.2 Wed 15:15 H25

Examination and Modification of Self-organized Nanostructures in the Ternary System Au/Co/Ge(001): Chain Growth and the Observation of a Zero-Bias Anomaly — •Nico Kubetschek, Till-Jakob Stehling, Ulrike Kürpick, Marcel Schlesag, Johann Tonhäuser, and René Matzdorf — Institute of Physics, University of Kassel, Heinrich-Plett-Str. 40, Kassel D-34132, Germany

The twofold symmetric reconstruction of the Ge(001) surface provides a template for the self-organized formation of various transition metal nanostructures [1]. We employed scanning tunnelling microscopy (STM) and spectroscopy (STS) at 77 K and 5 K to examine the nucleation, chain growth, and subsequent modification of hexagonal cobalt nanostructures embedded in Ge(001) [2] through the introduction of gold-induced defects [3]. Moreover, the introduction of additional amounts of Au resulted in the formation of previously unobserved nanorods [4]. The electronic properties of these rods were examined by STS, which revealed a zero-bias anomaly (ZBA) in the tunneling spectra. The formation of nanorods with high aspect ratios was subjected to a systematic statistical investigation.

[1] J. Schäfer et al. 2009, New J. Phys. 11 125011, [2] H. J.W. Zandvliet et al. 2011, Surface Science 605,1129, [3] J. Tonhäuser et al. 2022 Phys. Rev. B 106, 115404, [4] M. Schlesag et al. 2024 Phys. Rev. B 110, 195412

O 69.3 Wed 15:30 H25

Electrical Modulation of a Plasmonic Single Particle Resonance — Luka Zurak[1], Christian Wolff[2], Jessica Meier[1], René Kullock[1], •Asger Mortensen[2], Bert Hecht[1], and Thorsten Feichtner[1] — [1]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, 97074 Würzburg, Germany — [2]POLIMA Center for Polariton-driven Light-Matter Interactions, University of Southern Denmark, DK-5230 Odense M, Denmark

Acitive modulation of plasmonic resonances is a promising route towards optical switches smaller way that than the diffraction limit. However, due to the difficulties to directly electrically connect a single resonator most experiments in this direction have been performed on large scales and/or in electrochemical environments – hampering interpretation and application.

Here, we demonstrate fast modulation of the plasmonic resonance of a single electrically connected gold nano-rod [1]. We employ a lock-in amplifier to measure the relative change of scattering signal $\Delta S/S_0$ in the spectral range from 500 to 900 nm, while driving our structure with up to 50 kHz in frequency and up to 40 V in voltage amplitude. Results are of the expected order of magnitude according to existing theories. We discuss some of the theories in detail, like classical surface currents or the introduction of Feibelman parameters to account for non-classical electron spill-out at metal surfaces.

[1] Zurak, L., et al. (2024). Modulation of surface response in a single plasmonic nanoresonator. Science Advances, 10(36), eadn5227.

O 69.4 Wed 15:45 H25

On-surface induced fitting and mobility of conformationally flexible molecules inside nanometer-sized quantum confinements — Aisha Ahsan[1,2], •Aaron Oechsle[2,1], Luiza Buimaga-Iarinca[3], Lutz H. Gade[4], and Thomas A. Jung[2,1] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen, Switzerland — [3]CETATEA, National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania — [4]Institute of Inorganic Chemistry, University of Heidelberg, 69120 Heidelberg, Germany

Host-guest architectures provide ideal systems to investigate site-specific physical and chemical effects. Condensation events in nanometer sized confinements are particularly interesting for the investigation of inter-molecular and molecule-surface interactions. They may be accompanied by conformational adjustments representing induced-fit packing patterns. Here, we report that the symmetry of small clusters of cycloalkane molecules, formed by condensation, their registry with the substrate, their structure as well as their adsorption height is characteristically modified by their packing in confinements. While cyclopentane and cycloheptane display cooperativity upon filling of the hosting pores, cyclooctane and to a lesser degree cyclohexane diffusively re-distribute to more favored adsorption sites. The site-specific modification of the interaction and behavior of adsorbates in confinements plays a crucial role in many applications of porous materials, e.g., as gas storage agents or catalysts and biocatalysts.

O 69.5 Wed 16:00 H25

Areas of lower local contact potential difference in the wetting layer in the system Pb/Si(111)-(7x7) — •Paul Philip Schmidt[1], Felix Hartmann[1], Ralf Metzler[1,2], Janet Anders[1,3], and Schmidt Hoffmann-Vogel[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

The description of the diffusion of Pb atoms on Si(111)-(7x7) is highly nontrivial. Previous studies show that although Pb grows in the Stranski-Krastanov mode, it exhibits explosive island growth and ultrafast mass transport [1,2]. The developing wetting layer plays a special role [3]. We have investigated this system using non-contact scanning force microscopy and Kelvin probe force microscopy. We have worked under ultrahigh vaccum conditions at variable temperatures between 120K and 300K. Our studies show inhomogeneities of the work function in the wetting layer. The areas with different work function seem to be related to the position of the islands and the step edges of the Si(111). We assume that the different work function values are caused by different Pb concentrations in the wetting layer, which are probably related to the preferred direction of growth of the islands, so that in certain areas Pb is extracted from the wetting layer with varying effectiveness. [1] M. Hupalo et. al. Phys. Rev. B, 23 (2007), [2] K. L. Man et al. Phys. Rev. Lett., 101 (2008), [3] M. T. Hershberger et al. Phys. Rev. Lett. 113 (2014)

O 69.6 Wed 16:15 H25

Pyridyl-functionalized tripod molecules on Au(111): Inter-play between hydrogen bonding and metal coordination — •Sajjan Mohammad[1], Neeta Bisht[2], Anjana Kannan[1], Anne Brandmeier[2], Christian Neiss[2], Andreas Görling[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Applied Sciences of the Grisons, Switzerland

Two-dimensional metal-organic coordination networks (MOCNs) offer rich opportunities for fabricating materials with potential applications in catalysis and molecular electronics. We investigated the self-assembly of pyridyl-functionalized triazine (T4PT) on Au(111) using low-temperature scanning tunneling microscopy (STM) complemented by density functional theory (DFT) calculations. T4PT forms a well-ordered, close-packed structure stabilized by hydrogen bonds upon adsorption at 300 K. Upon post-deposition annealing, the assemblies are additionally stabilized by metal-ligand bonding between the pyridyl ligands and native Au adatoms. Further post-deposition annealing to 473 K led to the breaking of the N-Au bonds, with the molecular assemblies transforming into a second close-packed hydrogen-bonded structure. Above 503 K, few covalently linked dimers formed, likely as a result of CH-bond activation. Our findings highlight the challenge of predicting and controlling 2D structure formation for porous MOCNs on metal surfaces due to competing interactions.

O 69.7 Wed 16:30 H25

Active manipulation of interface electronic structures by two-dimensional metal-organic coordination on metallic substrates — •Lu Lyu[1,2], Jonas Gödde[2], Martin Anstett[2], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, 86159 Augsburg, Germany — [2]Department of Physics, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Designing two-dimensional metal-organic coordination networks (2DMOCNs) on metallic substrates provides a unique approach for engineering interface electronic structures. To achieve this goal, we first investigate a protocol of pyridine-functionalized T4PT molecules with Co coordination (Co-T4PT) adsorbed on Au(111). In this system, the surface state electrons are bound to the Co metal centers, and charge transfer occurs between the Co and the substrate. By substituting the Co center with a Cu atom, the surface state electrons in the Cu-T4PT coordination exhibit weaker binding to the Cu centers and are partially confined within the pores surrounded by the molecular potentials. Additionally, replacing T4PT with cyano-functionalized DCA enhances the coordination between Co and DCA, resulting in altered charge transfer within the Co-DCA plane. Consequently, the orbital states of DCA undergo modifications in both energy and momentum space. Our study demonstrates that the manipulation of coordinated metals and functionalized molecules can actively tailor electronic structures at a 2DMOCN-metal interface.

O 69.8 Wed 16:45 H25

Unveiling hybrid electronic bands in 2D metal-organic frameworks: insights from density functional theory and photoemission spectroscopy — Dominik Brandstetter[1], Simone Mearini[2], Yan Yan Grisan Qiu[2], Daniel Baranowski[2], Andreas Windischbacher[1], Claus Michael Schneider[2,3], Vitaliy Feyer[2,3], and •Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-6, FZ-Jülich, Germany — [3]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Two-dimensional metal-organic frameworks are atomically thin materials that combine properties of organic molecules with the characteristics of crystalline inorganic solids. The strong bonding between the organic linkers and transition metal centers may result in new electronic states with hybrid organic/inorganic character, from which two-dimensional, dispersing electronic bands emerge. However, until recently no experimental proof for such hybrid bands could be given and the requirements for efficient hybrid band formation remained unknown. Here, we combine density functional theory calculations with experimental angle-resolved photoemission spectroscopy to reveal the nature of the interaction between the transition metal atoms and the organic linker. On the example of the Ni-TCNQ network supported on Ag(100) and by employing photoemission orbital tomography, we observe how the molecular orbitals hybridize with the Ni d-states of appropriate symmetry. Our findings are not only based on electronic structure theory, but are also confirmed by the experimental photoemission fingerprints of the involved molecular orbitals.

O 69.9 Wed 17:00 H25

Atomic size effects in 1D metal-coordination polymers on silver — •Pengfei Zhao[1], Hongxiang Xu[1,3], Joachim Reichert[1], Anthoula C. Papageorgiou[1,2], and Johannes V. Barth[1] — [1]Technical University of Munich, Germany — [2]National and Kapodistrian University of Athens, Greece — [3]Peking University, China

Supramolecular coordination on solid surfaces provides a versatile approach to synthesize one-dimensional metal coordination polymers (1D-CPs), where the atomic size of metals plays a crucial role in determining the final structures and properties. Here, we systematically investigate 1H,1'H-2,2'-bibenzo[d]imidazole (H_2bbim) on silver substrates under ultra-high vacuum. Using scanning probe microscopy, we find that the shape of 1D-CPs can be steered by metal-coordination templating with different metal atom sizes. Specifically, H_2bbim molecules and cobalt atoms on Ag(100) allow the formation of micrometer-sized 1D-CPs with porphyrinoids formed by covalently fused H_2bbim dimers, which is distinct from its counterpart of holmium-coordinated chains of monomers. This suggests that size-tuned metal templating is a good strategy for tailoring the formation of 1D-CPs, demonstrating its potential for next-generation electronic devices.

O 69.10 Wed 17:15 H25

An insight into the thermally activated organometallic-to-covalent transition in novel Graphdiyne Molecular Wires Frameworks — •Alice Cartoceti[1], Simona Achilli[2], Paolo D'Agosta[1], Alessio Orbelli Biroli[3], Guido Fratesi[2], Valeria Russo[1], Andrea Li Bassi[1], and Carlo Spartaco Casari[1] — [1]Department of Energy, Politecnico di Milano, I-20133 Milano, Italy — [2]Department of Physics, Università degli Studi di Milano, I-20133 Milano, Italy — [3]Department of Chemistry, Università di Pavia, I-27100 Pavia, Italy

Graphdiynes (GDYs) are novel carbon allotropes with mixed sp-sp^2 hybridization, characterized by tunable optoelectronic properties. This study investigates the temperature-dependent atomic-scale structure and vibrational properties of 1,4-bBEB-based GDY molecular wires frameworks synthesized via Ullmann coupling on Au(100) and Au(111) surfaces. Scanning Tunnelling Microscopy revealed the transition from ordered frameworks of densely packed and oriented 1D organometallic wires (OMF) at room temperature, to progressively more disordered covalent frameworks (COF) at high temperatures. Density Functional Theory calculations and in situ Raman spectroscopy measurements tracked the OMF-to-COF transition, assigning specific Raman features to both phases. Raman spectroscopy also revealed that surface orientation influences the wires-gold interaction, resulting in a lower temperature for the OMF-to-COF transition on Au(100) than on Au(111).

O 70: Poster Oxides and Insulator Surfaces: Adsorption and Reaction of Small Molecules

Time: Wednesday 18:00–20:00 Location: P2

O 70.1 Wed 18:00 P2

Nitrogen Doping of Cuprous Oxide Films: A Surface Science Perspective — Mina Soltanmohammadi and •Niklas Nilius — Carl-von-Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany

Nitrogen doping of Cu_2O films grown on Au(111) and Pt(111) supports was explored by a variety of surface-science techniques, including electron-diffraction, X-ray photoelectron-spectroscopy (XPS), scanning tunneling microscopy and photoluminescence spectroscopy (PL). The films were prepared by Cu vapor deposition and high-pressure oxidation at 50 mbar O_2. Nitrogen was inserted by adding N_2 to the reactive gas or via sputter doping. Only the latter resulted in a clear N1s signal in XPS, compatible with the insertion of N-atoms at O substitutional sites. The N-doping caused an overall degradation of the oxide lattice and suppressed the formation of the $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface reconstruction observed on pristine $Cu_2O(111)$. Moreover, the oxide Fermi level shifted from the valence-band top into the band gap, indicative for a reduced p-type conductivity of the sample upon doping. The N-dopants featured low thermal stability and largely desorbed at 500 K, leaving behind a pronounced 850 nm PL peak due to O vacancy emission. Our findings indicate that the N-atoms initially occupy O substitutional sites but get removed easily at moderate temperature, casting doubts whether N-doping is a suitable pathway to improve the conductance and luminescence behavior of Cu_2O.

O 71: Poster Plasmonics and Nanooptics: Fabrication, Characterization and Applications

Time: Wednesday 18:00–20:00 Location: P2

O 71.1 Wed 18:00 P2

Large area writing of In_3SbTe_2 metasurfaces for polarization optics and complex orbital angular momentum beams — •Maike Kreutz[1], Lukas Conrads[1], Andreas Mathwieser[2], Matthias Wuttig[1], Robert Schmitt[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen — [2]Fraunhofer IPT

Optical metasurfaces enable tailoring light-matter interaction for miniaturized optical elements with customized functionalities.The non-volatile reversible switching of phase-change materials (PCMs) has been applied for tunable optical metasurfaces [1]. The plasmonic PCM In_3SbTe_2 (IST) switches from an amorphous dielectric to a crystalline metallic state. IST has been exploited for the direct laser writing of metallic nanoantennas in a dielectric surrounding [2] and for geometric phase metasurfaces [3] including orbital angular momentum (OAM) beams with single singularities. Here, we investigate optical metasurfaces fabricated with the Nanoscribe Photonic Professional GT to shape OAM beams with multiple singularities. We show preliminary results regarding the optical programming of these OAM beams for possible applications in optical communications [4]. Additionally, metasurface polarization optics are explored, enabling plasmonic quarter-wave plates with large bandwidths in the infrared range. This work paves the way towards creating tailored reconfigurable metaoptics for the infrared without cumbersome fabrication techniques. [1] Wuttig et al., Nat. Photon. 11, 465 (2017), [2] Heßler et al., Nat. Commun. 12, 924 (2021), [3] Conrads et al. arXiv:2408.05044 (2024), [4] Shen, Y. et al. Light. Sci. Appl. 8, 90 (2019)

O 71.2 Wed 18:00 P2

Investigation of the plasmonic phase-change material In_3SbTe_2 in the near-infrared range — •Hristiyana Kyoseva, Lukas Conrads, Rebecca Rahmel, Gero von Plessen, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Phase-change materials (PCMs) provide a suitable platform for active nanophotonics and reconfigurable metasurfaces by enabling reversible switching between two phases with contrasting optical properties [1]. In_3SbTe_2 (IST) is a novel plasmonic PCM which can be switched between an amorphous (dielectric) and a crystalline phase (metallic in the whole infrared (IR) spectrum) with precise laser pulses [2]. The direct writing of micrometer-sized structures into a thin IST film with resonances in the mid-IR (above 5 μm) has been extensively demonstrated [3]; however, smaller structures have not been explored yet due to their challenging fabrication process. Here, we examine the smallest achievable sizes of structures written in IST by spatially overlapping crystallization and amorphization pulses. We investigate the resonances of sub-micrometer rod antenna arrays as they shift to shorter wavelengths (below 4 μm) with decreasing size. We also aim to identify its lower limit set by the refractive index of the surrounding media. Our work paves the way towards sophisticated antenna structures with resonances at shorter wavelengths, broadening the applications of IST as a versatile platform for active nanophotonics. [1] Wuttig et al. *Nat. Photon.* **11**, 465 (2017) [2] Heßler et al., *Nat. Com.* **12**, 924 (2021) [3] Heßler, Conrads et al., ACS Photon. **9**, 5 (2022).

O 71.3 Wed 18:00 P2

Laser pulse front tilt effects in the observation of SPPs using photoemission electron microscopy — •Hanno Christiansen[1], Tobias Eul[1], and Michael Bauer[2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

In recent years, PEEM has become an established technique for the investigation of surface plasmon polaritons (SPP). This technique allows, for example, the study of the propagation dynamics of these collective surface excitations with femtosecond resolution or the measurement of their dispersion relations with high spatial resolution. The characteristic signal measured in PEEM results from the coherent superposition of the exciting laser field and the emitted SPP. Based on simulations and experimental data we show in this contribution that the plasmonic PEEM signal is very sensitive to the pulse front tilt of the exciting laser pulse and thus represents a sensor for this often overlooked laser parameter.

O 71.4 Wed 18:00 P2

Surface plasmon polariton neuronal cell — •Emily Kruel[1], Christopher Weiss[1], Tobias Eul[2], Mario Pfeiffer[1], Benjamin Stadtmüller[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern- Landau, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, Germany — [3]Institute of Physics, University of Augsburg, Germany

Today, the classical electronic computer architecture is one of the limiting factors for fast and energy-efficient data processing. This has triggered the search for alternative hardware architectures to overcome these limitations. For instance, neuromorphic photonics has emerged as a novel research field for new classes of information processing devices that incorporate photonically integrated neural networks [1].

The hybrid nature of surface plasmon polaritons (SPPs) offers a concept for integrating neuromorphic photonics by combining photonic advantages such as high bandwidth and speed with strong electronic interactions. Here, we present an experimental approach to constructing essential components of an artificial neuron based on SPP interactions. We optimized the dimensions of individual components through a combination of finite-difference time-domain (FDTD) simulations and iterative experimental adjustments. The resulting plasmonic responses are imaged using a photoemission electron microscope (PEEM).

[1] Shastri, B.J., Tait, A.N., Ferreira de Lima, T. et al., Nat. Photonics 15, 102-114 (2021)

O 71.5 Wed 18:00 P2

Investigating Gel Electrolyte Compositions for Enhanced Switching Speed in PEDOT:PSS Electrochromic Devices and Switchable Metasurfaces — •Hoorieh Fallah[1], Dominik Ludescher[1], Jonas Herbig[1], Mario Hentschel[1], Andy Steinmann[1], Klaus Dirnberger[2], Junqi Lu[2], Semi Kim[2], Aldilene Santos Franca[2], Sabine Ludwigs[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Institute of Polymer Chemistry, University of Stuttgart

Switchable metasurfaces using the conductive polymer PEDOT:PSS have gained substantial interest over the last years. PEDOT:PSS can be switched from metallic to dielectric state for wavelengths > 1.3 μm using electrochemistry, with CMOS compatible voltages between -1V to +1V. Here, we report on the preparation and characterization of gel electrolytes for PEDOT switching with varying ratios based on polyethylene oxide (PEO), polyvinyl alcohol polymers (PVA), acetonitrile, and lithium perchlorate ($LiClO_4$). Our gel electrolytes are integrated with PEDOT:PSS, coated onto ITO substrates to evaluate their performance in electrochromic switching applications. By applying alternating voltage and laser light, we analyze the dynamic switching speed of the PEDOT layer as it transitions from a conductive to an insulating state. Our approach explores how PEO- and PVA-based electrolytes impact high-frequency, low-voltage switching in PEDOT:PSS systems. We have achieved switching rates up to 100 Hz. The results aim to enhance our understanding of the influence of the electrolyte composition on switching behavior.

O 72: Poster Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy

Time: Wednesday 18:00–20:00 Location: P2

O 72.1 Wed 18:00 P2

Implementation of a fiber-based cathodoluminescence detector system for a scanning electron microscope — •Filip Majstorovic[1], Paul H. Bittorf[1], and Nahid Talebi[1,2] — [1]Institute for Experimental and Applied Physics, Kiel University, Leibnizstraße 19, D-24118 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, Christian-Albrechts-Platz 4, D-24118 Kiel, Germany

Cathodoluminescence (CL) is the light emitted from materials irradiated with the electron beam, within the infrared to ultraviolet spectral range. CL recently has gained a major interest in analyzing quantum materials and emitters, thanks to its high spatial and temporal resolutions. In our study, inside a scanning electron microscope (SEM) high energy and broad bandwidth electron beams are generated. The CL emission is then collected with a detector, consisting of a multimode fiber attached to piezo stages, which allows for nanometer precision movement of the fiber near the sample. We present the variety of possible measurements such a system allows. One component of this is obtaining the spectrum of the emitted light, that for example enables the investigation of plasmonic resonances. Further this detector system provides a way to measure the emission profile by scanning the fiber three-dimensionally along the sample. Such emission profiles give information about the processes responsible for this radiation and show if coherent or incoherent CL are more dominant. Moreover, higher-order correlations unravel a superbunching effect in CL generated from semiconducting samples.

O 72.2 Wed 18:00 P2

Comprehensive Probing of Electron and Phonon Systems by Raman Scattering — •Jan Kutschera[1], Marc Herzog[1], Wouter Koopman[1], Felix Stete[1], and Matias Bargheer[1,2] — [1]Institut für Physik & Astronomie, Universität Potsdam, Potsdam, Deutschland — [2]Helmholtz Zentrum Berlin, Berlin, Deutschland

Inelastic processes in light-matter interactions are crucial for understanding energy transport within solid-state materials, where energy is distributed between electron and phonon systems. Investigating these interactions provides deeper insights into fundamental processes relevant to plasmonics, optoelectronics, and optoacoustics. However, knowledge about the energy transfer dynamics within each system is also essential for a complete picture. By extending Raman spectroscopy to ultrashort timescales, we aim at analyzing the transient population dynamics of phonon modes and the interplay of different electronic bands to ultimately establish ultrafast Raman Spectroscopy which directly probes electron-electron, electron-phonon, and phonon-phonon interactions. Here, we present an intraband emission of the conduction band electrons in gold nanoparticles, which is excited by interband absorption and appears as a continuous background in static Raman experiments. Pump-probe experiments can help further examine the origin of this emission and the interaction of different electronic subsystems. Moreover, we investigate the phonon modes of HfN and other materials as potential candidates for the catalysis of light-driven reactions.

O 72.3 Wed 18:00 P2

Adiabatic focusing of propagating Surface plasmon polaritons at gold nanotriangles — •Gregor Stockmann, Felix Stete, and Matias Bargheer — Institut für Physik und Astronomie, Universität Potsdam, Deutschland

Surface plasmon polaritons (SPPs) are the collective oscillations of surface-near charges at a dielectric-metallic interface. Due to the Coulomb force, these oscillations can propagate along the surface. This effect can be utilized to spatially separate the laser excitation and a chemical reaction site. In this work, we use gold nano-triangles, to focus SPPs from a μm-sized excitation spot to the tip at the nanometer scale. We investigate the influence of different parameters on the propagation behavior of SPPs. Key parameters are the particle dimensions, excitation wavelength and the light polarisation.

O 72.4 Wed 18:00 P2

Plasmon assisted catalysis of Ferricyanide by Gold-Nanoparticles with different sizes and light intensities. — •Kyra Peikert, Wouter Koopman, and Matias Bargheer — Institut für Astronomie und Physik Universität Potsdam, Potsdam, Deutschland

In recent years plasmonic catalysis emerged as promising new field in photocatalysis. However, to improve its efficiency, a better understanding of its governing principles is required. In this study we investigate the reaction kinetics of the light driven reduction of ferricyanide catalyzed by gold nanoparticles of different sizes. To refill the holes generated by electron transfer to ferricyanide the hole scavenger Ethanol (EtOH) is added to the solution. We compare this situation to reactions in a purely aqueous solution. The kinetics under different light intensities including dark conditions help to understand the mechanisms. The results show indications of a charging effect of the particles due to the presence of the hole scavenger, which speeds up the reaction rate.

O 72.5 Wed 18:00 P2

Single particle sample with gold nanorods for micro-spectroscopy — •Alexandra Faber — Institut für Physik und Astronomie, Universität Potsdam, Deutschland

Nobel metal nanostructures show great potential for photocatalytical applications due to their broadband plasmonic absorption across the visible spectrum. Chemical reactions taking place at surfaces can be accelerated by several effects, including charge transfer and local heating. As one important factor, the accumulation of charges on the particle during a reaction process, is expected to have a large influence on the charge transfer process. In order to better understand the effects of photocharging of gold nanorods (GNR), possible electron transfer between individual GNRs and the substrate, single nanoparticles are studied by optical micro-spectroscopy. The samples are investigated by dark-field as well as scanning electron microscopy and must therefore fulfill different requirements. This includes that the sample must provide the necessary criteria such as conductivity and light transmission in order to be observed with both microscopy methods. At the same time, it should be possible to rediscover individual GNRs and the distance between the particles has to be large enough to allow spectroscopy of individual GNRs. We show the development and improvement of the sample preparation procedure as well as first recorded dark-field scattering spectra and fluorescence spectra of single GNRs.

O 72.6 Wed 18:00 P2

Size effects on the plasmon resonance in silver cluster anions studied by energy-resolved photoemission — •Norman Iwe[1], Klara Raspe[1], Franklin Martinez[1], Lutz Schweikhard[2], Karl-Heinz Meiwes-Broer[1,3], and Josef Tiggesbäumker[1,3] — [1]Institute of Physics, University of Rostock, Germany — [2]Institute of Physics, University of Greifswald, Germany — [3]Department of Life, Light and Matter, University of Rostock, Germany

Numerous applications ranging from efficient solar cells to cancer treatment profit from the interaction between nanoparticles and light. In the case of metal clusters, one often takes advantage of collective resonances of the valence electrons, which lead to a strong increase of the cross section at a certain wavelength. Previous studies already showed, that the resonance energy can be tuned via size and charge state of the nanoparticles. However, systematic measurements to explore the development of the plasmonic resonance in free metal clusters so far concentrate on small sizes.

We conduct photoelectron spectroscopy on anionic silver clusters Ag_N^- in a size range $N = 7 - 300$. By extracting photodetachment cross sections, we gain insights into the collective resonances. At $N = 55$, we observe a transition from a blueshift to a general redshift of the plasmon energies with decreasing cluster size. However, the resonance energies for sizes below N = 55 are oscillating whereby the maxima are found at known electronic shell closures. On top, a splitting of the resonance is observed at a few smaller cluster sizes, hinting on a deformation of the particle.

O 72.7 Wed 18:00 P2

Anisotropic photoelectron emission from individual Ag nanoparticles on silicon — •Waqas Pervez[1,2], Kevin Oldenburg[1,2], Sylvia Speller[1,2], and Ingo Barke[1,2] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Life, Light & Matter, University of Rostock, Germany

Laser excitation of localised plasmons in nanoparticles can give rise to a vastly enhanced photoemission yield [1, 2]. Here we study detailed characteristics of the photoelectron emission process of size-selected nanoparticles with diameters around 10 nm, deposited from the gas phase onto silicon. To this end we employ femtosecond laser excitation with wavelengths around 800 nm and 400 nm, respectively, in a photoemission electron microscope (PEEM). The spatially resolved electron yield is investigated as a function of laser wavelength and polarisation. Furthermore, we report on photoelectron emission from individual, supported nanoparticles in reciprocal space. Upon resonant plasmon excitation we observe anisotropic electron yield that depends on the laser polarisation. The observed photon order, ranging from 2PPE to 5PPE, and the underlying excitation and emission mechanisms are discussed in view of the local near field distribution and the effect of the substrate.

[1] M. Rohmer et al., Phys. Stat. Solidi B 247, 1132 (2010)
[2] K. Oldenburg et al., J. Phys. Chem. C 123, 1379 (2019)

O 72.8 Wed 18:00 P2

Near-field Fano spectroscopy of MaPbI3 nanoparticles — Jinxin Zhan[1], Tom Jehle[1], Sven Stephan[1], •Sam Nochowitz[1], Ekaterina Tiguntseva[2], Sergey Makarov[2], Juanmei Duan[1], Petra Gross[1], and Christoph Lienau[1] — [1]Universität Oldenburg, D-26129, Germany — [2]St. Petersburg, Russia

Semiconducting halide perovskite nanoparticles support Mie-type resonances that confine light on the nanoscale in localized modes with well-defined spatial field profiles yet unknown near-field dynamics. We introduce an interferometric scattering-type near-field microscopy technique [1] to probe the local electric field dynamics at the surface of a single MAPbI3 nanoparticle [2]. The amplitude and phase of the coherent light scattering from such modes are probed in a broad spectral range and with high spatial resolution. In the spectral domain, we uncover a Fano resonance with a 2π phase jump. In the near-field dynamics, this Fano resonance gives rise to a destructive interference dip after a few femtoseconds. Mie theory suggests that the interference between electric quadrupole and magnetic dipole modes of the particle, with spectra affected by resonant interband absorption of MAPbI3, lies at the origin of this effect [3]. Our results open up a new approach for probing local near-field dynamics of single nanoparticles.

[1] Zhan, J., et al. Advanced Photonics 2020, 2 (04)
[2] J. Zhan et al., Nano Lett. 2024
[3] Tiguntseva, E. Y., et al. Nano Lett. 2018, 18 (2), 1185-1190.

O 72.9 Wed 18:00 P2

Energy and momentum distribution of surface plasmon-induced hot carriers — •Ellen Brennfleck[1], Christopher Weiss[1], Jannis Lessmeister[1], Tobias Eul[2], Benjamin Stadtmüller[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, Germany — [3]Institute of Physics, University of Augsburg, Germany

Are the spectroscopic properties of plasmon- and photon-induced carriers fundamentally different? This question is crucial for advancing plasmonic energy conversion. Initial studies have suggested characteristic energy and momentum distributions for the photoemission of both bulk plasmon resonances and surface plasmons. For surface plasmons, however, the separation of plasmon and photon-induced emission patterns by their inherent spatial and dynamics remains challenging [1].

To further characterize the electron emission pattern of surface plasmons, we combine a femtosecond laser system with a spatial light modulator to generate a

vector vortex beam to excite surface plasmon polaritons at an annular structure. Our photoemission electron microscope enables us to compare the spectroscopic properties of photoemitted electrons and those generated by plasmonic emission at the center of the structure, providing valuable insights into the distinct emission mechanisms.

[1] Hartelt et al., ACS Nano 15, 12 (2021), 19559–19569

O 72.10 Wed 18:00 P2

Self-organized plasmonic particles configurations in front of mirror — •Aleksei Overchenko and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Plasmonic particles and their field enhancement properties found wide applications in various fields. For example, they are used in Surface-Enhanced Raman Spectroscopy (SERS), plasmon-enhanced fluorescence, Photothermal Therapy and energy conversion. Field enhancement can be achieved by bringing two spheres into close proximity, placing a sphere on a mirror, fabricating bowtie antennas, or designing hybrid structures like particle-dielectric-mirror systems. In most cases, surface functionalization often requires complicated modification methods such as lithography and chemical binding, e.g., of DNA origami which leads to complicated and non-reconfigurable systems. Here, we deliberately manipulate induvial as well as multiple gold particles in front of a gold mirror by local laser-induced temperature fields generating thermo-osmotic flow. Multiple particle trapping is performed by focused laser that can divide in multiple independent beams via AOD. We characterize the resulting single, dimeric and higher order clusters, their plasmonic coupling and the coupling of the particles to a thin gold film by scattering spectroscopy. The distance between the film and particles is around 10 nm due to the second minimum of the DLVO-theory. Enhancement is described by sensing of biomolecules. The system is reconfigurable as no binding is required and analytes may be bound to the film to enable spatially resolved SERS.

O 72.11 Wed 18:00 P2

Optical resonance tuning of micro- and nanoparticles with phase change materials in the near-infrared and visible range — •Rebecca Rahmel, Hristiyana Kyoseva, Jonathan Müller, Lukas Conrads, Thomas Taubner, and Gero von Plessen — I. Institute of Physics (IA), RWTH Aachen University

Micro- and nanoparticles with scattering and absorption resonances promise interesting optical behaviour. These resonances are highly sensitive to the particle size, shape, and configuration, as well as the dielectric properties of both particle and surrounding medium [1]. Phase-change materials (PCMs) show high optical contrast when switched between their amorphous and crystalline phases [2], facilitating antenna resonance tuning based on a change in refractive index [3]. The novel plasmonic PCM In_3SbTe_2 (IST) can be locally optically switched between the dielectric amorphous and the metallic (in the infrared) crystalline phase, enabling a sign change in permittivity [4]. While antenna resonance tuning with PCMs has been studied extensively, locally addressing PCMs below single particles has not been demonstrated yet. Here, we investigate the optical response of single polysterene micro- and gold nanoparticles placed on thin films of IST and other PCMs and locally switch the PCMs to tune the particle resonances. Our work paves the way towards mode selection of nanoparticles beneficial for tuning of emitters and sensing applications.

[1] Dahmen et al. *Aust. J. Chem.* **60**, 447-456 (2007) [2] Wuttig et al. *Nature Photon* **11**, 465-476 (2017) [3] Michel et al. *Adv. Mater.* **31**, 1901033 (2019) [4] Heßler et al. *Nat. Com.* **12**, 924 (2021)

O 72.12 Wed 18:00 P2

Analytical Theory of the Optical Inter- and Intraband Response in Noble Metals — •Robert Lemke, Andreas Knorr, and Jonas Grumm — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The optical response of plasmonic noble metal nanostructures can be attributed to the interplay of electronic intra- and interband processes described by coupled Boltzmann-Bloch equations. In this set of coupled equations, the specific properties of the noble metal are addressed by an anisotropic electronic dispersion relation expanded in the vicinities of the X and L high symmetry points.

In order to address the dephasing of the inter- and intraband polarizations we consider near equilibrium electron-phonon scattering rates in random phase approximation to estimate relaxation timescales. Our approach allows to connect spectroscopic signatures directly to microscopic processes, not possible with simple Drude-Lorentz models.

O 72.13 Wed 18:00 P2

Kinetics of hydrogen molecules on Ag(111) by tip-enhanced Raman spectroscopy — Shuyi Liu[1,2], Jun Yoshinobu[3], Martin Wolf[1], Takashi Kumagai[4], and •Akitoshi Shiotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Huazhong University of Science and Technology, Wuhan, China — [3]University of Tokyo, Kashiwa, Japan — [4]Institute for Molecular Science, Okazaki, Japan

Surface diffusion is the first step for adsorbates to undergo characteristic chemical and physical phenomena such as self-assembly, catalytic reactions, and low-dimensional molecular transport. However, the characterization of highly diffusive molecules, such as physisorbed molecules, has been challenging even with scanning tunneling microscopy and its related techniques. In this study, we use tip-enhanced Raman spectroscopy (TERS) to sensitively detect hydrogen molecules physisorbed on Ag(111) at low temperatures around 10 K. Strong Raman peaks were observed only when the diffusive molecule entered the plasmonic tip-sample junction, while the peaks decayed by thermal desorption at higher temperatures. By monitoring the peak intensities and investigating its temperature dependence, we successfully analyzed the kinetics of hydrogen molecules on the surface. This demonstrates that TERS is useful for evaluating the dynamics of diffusive molecules.

O 73: Poster Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules

Time: Wednesday 18:00–20:00 Location: P2

O 73.1 Wed 18:00 P2

In-situ tritium contamination and decontamination of fusion-relevant materials — •Elizabeth Paine[1], Dominic Batzler[2], James Braun[2], Robin Grössle[2], Philipp Haag[2], Marco Röllig[2], Marie-Christine Schäfer[2], Marius Schaufelberger[2], and Kerstin Trost[2] — [1]Eindhoven University of Technology, The Netherlands — [2]Tritium Laboratory Karlsruhe, Karlsruhe Institute of Technology, Germany

Nuclear fusion could offer a solution to the growing global demand for clean, sustainable and abundant energy. The deuterium-tritium fusion reaction offers a high energy yield and feasibility at achievable temperatures. However, the scarcity and radioactive nature of tritium pose significant challenges for its handling in fusion reactors. Tritium adsorption onto surfaces leads to challenges in licensing, process control and maintenance. Ozone is a known decontaminant and may provide a viable solution for the decontamination of these tritiated surfaces. Due to its strong oxidising nature, ozone reacts with the adsorbed tritium, which can then be evacuated. This study aims to investigate tritium accumulation and decontamination on the fusion-relevant materials: beryllium, EUROFER97 and tungsten. These are selected for their critical roles in reactor components and tritium-processing systems. The findings will provide insights into the behaviour of tritium in these materials and assess the potential of ozone-based decontamination techniques compared to established methods. This contributes to the development of effective strategies for tritium handling, decontamination and inventory management in future fusion reactors.

O 73.2 Wed 18:00 P2

Role of the surface for adsorbate motors — •Bensu Günay Ramovic[1], Grant Simpson[1], Mats Persson[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — [2]Department of Chemistry, University of Liverpool, Liverpool L69 3BX, United Kingdom

Molecular motors have the ability to perform uni-directional rotation or translation. In addition to such motors in nature, for instance kinesin, artificial molecular motors have seen great developments in the last decades. They have been studied intensely in solutions by averaging methods, but these cannot resolve individual motors. We have studied molecular motors on metal surfaces by scanning tunneling microscopy under ultrahigh vacuum and cryogenic temperatures, allowing us to track the motion of single molecules. Metallic surfaces generally play an important role for physical/chemical processes in molecular adsorbates. Here, we investigate adsorbate motors [1] on different metal surfaces in order to elucidate the role of the substrate for the molecular motion. It turns out that even rather small differences - maintaining the same surface symmetry, but changing the elemental composition - strongly affects the molecular configuration and motion.

[1] Simpson, G. J., Persson, M., & Grill, L. (2023). Adsorbate motors for unidirectional translation and transport. Nature, 621(7977), 82-86.

O 73.3 Wed 18:00 P2

Poisoning resistance of GaPt SCALMS model systems — •Christoph Wichmann[1,2], Michael Moritz[2], Haiko Wittkämper[2], Tzung-En Hsieh[3], Johannes Frisch[3], Macus Bär[2,3,4], Hans-Peter Steinrück[2], and Christian Papp[1] — [1]FU Berlin, Germany — [2]FAU Erlangen, Germany — [3]Helmholtz-

Zentrum Berlin, Germany — [4]Helmholtz Institute Erlangen-Nürnberg Germany

Supported catalytically active liquid metal solutions (SCALMS) are a novel concept, where low amounts of a catalytically active transition metal is dissolved in another low melting metal, which acts as a matrix. The highly dynamic surface provides an interesting system offering high activity and remarkable stabilities for dehydrogenation reactions. For industrial applications, different challenges have to be met. One of them is the presence of catalytic poisons in the catalytic feed such as sulfur compounds. Therefore, a model system of a macroscopic GaPt droplet with a low Pt content (1 at.%) and nanoscopic GaPt particles were investigated during the exposure to thiophene as catalyst poison using X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum and near-ambient pressure (0.1-0.2 mbar) conditions. The formation of Ga-sulfides at the surface of the catalyst is observed, leading to an accumulation of Pt in / under this layer. For higher temperatures (>650 K), the dissolution of the formed Ga-sulfides into the liquid metallic Ga-matrix is observed. In all cases, no Pt-sulfide was formed, indicating a resistance of the active Pt sites towards sulfur poisoning of SCALMS.

O 73.4 Wed 18:00 P2

An XPS and molecular beam study of olefin adsorption on ultrathin ionic liquid films on Pt(111) — •Laura Ulm, Cynthia C. Fernández, Leonhard Winter, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Solid catalysts with ionic liquid layer (SCILL) promise improvements for a wide range of applications, e.g. an enhanced selectivity of the 1,3-butadiene hydrogenation to 1-butene by coating a heterogeneous catalyst with thin ionic liquid (IL) films. We studied hydrocarbon adsorption as central step of this reaction by X-ray photoelectron spectroscopy combined with a supersonic molecular beam. Ultrathin films of three different ionic liquids with thicknesses below 1 nm were deposited onto a Pt(111) crystal in UHV by physical vapor deposition and characterized with XPS. These films were exposed to 1,3-butadiene or 1-butene from a supersonic molecular beam at 180 K. The coverage-dependent sticking coefficients of the two olefins were measured using the King-and-Wells method. With increasing IL pre-coverage, the total amounts of adsorbed olefins decreased until further adsorption was completely suppressed by the IL layer. The minimum IL coverage needed for complete suppression of adsorption and the differences between the ionic liquids will be discussed in the context of IL-induced selective 1,3-butadiene hydrogenation.

Supported by the DFG through SFB 1452 (Project ID: 431791331).

O 73.5 Wed 18:00 P2

N heteroatom effects in large aromatic physisorbed adsorbates on metal surfaces: azabenzopyrene on Cu(111) — •Henry Thake[1], Matthew Stoodley[1,2], David A. Duncan[2,3], and Reinhard J. Maurer[1] — [1]University of Warwick, UK — [2]Diamond Light Source, UK — [3]University of Nottingham, UK

Conjugated molecules at metal surfaces are bound by a subtle balance of short- and long-range interactions including charge transfer and dispersion interactions. As such, they represent a challenging opportunity to improve approximations to density functional theory (DFT) where accurate structural and spectroscopic benchmark measurements exist. Accurate structural predictions of the large aromatic molecules naphthalene and pyrene have shown weak adsorption in a flat geometry on Cu(111). Here, we present a combined computational and experimental study of a closely-related molecule featuring a single nitrogen heteroatom - azabenzopyrene on Cu(111). Based on DFT calculations, x-ray standing wave (XSW) structural characterisation, x-ray photoelectron (XPS) and near-edge adsorption fine structure (NEXAFS) spectroscopy simulations, we study the effect of the heteroatom on the adsorption of the conjugated molecule. We develop a structural model consistent with XSW structure determination and simulate XPS and NEXAFS signatures of the sole nitrogen species in the molecule. Nitrogen 1s XPS and K-edge NEXAFS spectra present multiple coexisting chemical environments for the nitrogen species, for which we present a model hypothesis.

O 73.6 Wed 18:00 P2

Surface Charge Modification of Silver Substrates for Enhanced SERS Selectivity — •Georgiana Ion, Stefania Dana Iancu, and Nicolae Leopold — Faculty of Physics, Babes-Bolyai University, 400084, Cluj-Napoca, Romania

Surface-enhanced Raman spectroscopy (SERS) uses the plasmonic properties of metallic nanoparticles for sensitive detection in complex matrices. A key challenge is controlling the detection of specific species. This study developed solid-state SERS substrates with optimized surface properties for selective detection of anionic and cationic analytes.

Citrate-capped silver nanoparticles (cit-AgNPs) were synthesized via the Lee-Meisel method, while hydroxylamine-reduced silver nanoparticles (hya-AgNPs) followed the Leopold-Lendl method. Concentrated nanoparticles were dried into 2 μL droplets on cover glass to create solid substrates. Raman spectra were obtained by immersing the substrates in 2 mL analyte solutions (Nile Blue, Crystal Violet, fumaric acid) using a 532 nm laser.

We found that adding $Ca(NO_3)_2$ only impacts selectivity when added to the colloidal form before drying, making it crucial for developing both substrate types. This optimized cit-AgNPs for anionic detection, while hya-AgNPs, covered with Cl^- ions, selectively detected cationic analytes. Cationic detection can also occur on cit-AgNPs by adding NaCl to the solution. This work highlights how surface modifications enhance SERS substrate selectivity and provide a pathway for tailored systems for specific analyte detection in complex environments.

O 73.7 Wed 18:00 P2

Water adsorption on Bi(111) surfaces calculated from first principles — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth is a semimetal with unique electronic properties, including a strong spin-orbit coupling. Water adsorption on bismuth surfaces is interesting from both a scientific and technological point of view, since the material has numerous electrode applications ranging from analytical chemistry, environmental monitoring, and energy storage to seawater desalination. Surprisingly, relatively little and partially contradiction information is available on the interaction between Bi and water [1,2]. In the present contribution, density-functional theory is used to calculate the adsorption of single water molecules, water clusters and water thin films on Bi(111). We analyze in detail the molecule-molecule and molecule-substrate interaction and provide information on the diffusion characteristics. The calculations are discussed in the context of previous theory and experimental data.

[1] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).
[2] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 73.8 Wed 18:00 P2

Investigation of Na^+ ion solvation on the Cu(111) surface by STM — •Anna Shugai and Karina Morgenstern — Physical Chemistry I, Ruhr-Universität Bochum, Bochum, 44801, Germany

Sodium-ion (Na^+) batteries offer great potential as an energy storage, making them an attractive alternative to the lithium-ion batteries. However, the practical realization is currently restricted due to the instability of the electrode-electrolyte interface. To reveal the reasons for it, we need to understand the underlying mechanisms that govern the process of Na^+ ion on-surface solvation. In this project, we use low-temperature scanning tunneling microscopy (STM) to get the locally resolved structure of D_2O-solvated Na^+ ions that are supported on the Cu(111) surface. First, the small D_2O clusters, containing 10 to 20 molecules, were prepared on the Cu(111) surface. We compare them to the D_2O clusters deposited on the Na^+-pre-covered Cu(111) surface. The results show that there is strong interaction between the Na^+ ion and the D_2O solvent molecules. Accordingly, the solvation behaviour of Na^+ is more similar to that exhibited by the Li^+ ion, than to that of the Cs^+ ion.

O 73.9 Wed 18:00 P2

Adsorption of bifunctional methoxy butene on Si(001): the multiplicity of non-selective adsorption — •Jannick Peters, Sophie Göbel, and Michael Dürr — Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

Both, ether group and C=C double bond, adsorb on Si(001) via an intermediate state and with high reactivity. When combining these two functional groups in a bifunctional organic molecule, a variety of different adsorption configurations can be envisioned. However, selective adsorption via the ether group was found for allyl ethers on the Si(001) surface [1]. In the case of methoxy butene (MeBut), the functional groups are separated by an additional CH_2 group when compared to allyl ethers. Despite this seemingly small change in the molecules' structure, major differences in the reactivity on Si(001) were observed. At surface temperatures between 90 and 450 K, no selective reaction but a large variety of different adsorption configurations, which are bound either via ether cleavage, the C=C double bond, or both functional groups, was observed when studying intermediates and final products by means of XPS. Depending on the final configuration, the reactivity of the ether group was found to be either enhanced or reduced, which results in an increased temperature window for the reaction from intermediate to final state.

[1] T. Glaser, et al., J. Phys. Chem. Lett. 15, 7168 (2024).

O 73.10 Wed 18:00 P2

Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes. In this research, we have developed a Steel Mesh-Supported

SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.

O 74: Poster Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Wednesday 18:00–20:00 Location: P2

O 74.1 Wed 18:00 P2

Lithium adsorption on Cu(111) for anodeless lithium ion batteries — •Darius Hübner — Universität Ulm, Institut für theoretische Chemie, Oberberghof 7, 89081 Ulm

Anodeless batteries in which the anode is created upon the first charging are of strong current interest as they avoid processing and cost concerns as well as lead to an increased safety. In order to contribute to the understanding of the the viability of copper charge collectors in anodeless Lithium ion batteries, we studied the deposition of lithium on a Cu(111) substrate using periodic density functional theory calculations.

We find that the lattice mismatch between lithium and copper leads to the formation of a fcc lithium structure with fewer atoms per layer than the copper substrate. Additionally, this lithium structure shows remarkably lower surface diffusion barriers compared to a standard bcc lithium surface. As an enhanced surface mobility is supposed to suppress dendrite growth, this suggests a reduced formation of dendrites in the initial steps of the anode formation.

O 74.2 Wed 18:00 P2

Spin-State Switching of Indium-Pthalocyanine on Pb(100) — Niklas Ide, Arnab Banerjee, •Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Kiel, Deutschland

Indium(III) phthalocyanine chloride, deposited on Pb(100), is investigated using a scanning tunnelling microscope at cryogenic temperatures. The chloride ions dissociate, leaving behind indium phthalocyanine (InPc), which is observed in two distinct configurations: the metal ion oriented either towards (↓) or away from (↑) the substrate. The study reveals isolated molecules and islands which exhibit a $\sqrt{65}\times\sqrt{65}$, R ± 30° superstructure, characterized by a unit cell containing four inequivalent molecules, one in the InPc↑ state and three in the InPc↓ state at different sites. Variations in the conductance spectra of the lowest unoccupied molecular orbital are observed, depending on the adsorption sites and azimuthal orientations of the complexes. Notably, only the InPc↑ molecules within the islands exhibit Shiba states, signifying the presence of a localized spin. Electron extraction allows for the conversion of both isolated complexes and molecules in islands from the InPc↑ to InPc↓ state. This transition is accompanied by a change in their spin state, as evidenced by the disappearance of the Shiba states.

O 74.3 Wed 18:00 P2

On-surface fabrication of cesium tin halide nanostructures deviating from the perovskite ABX_3 structure — Madad Abbasli, Dina Wilks, Carsten Busse, and •Robin Ohmann — University of Siegen, Siegen, Germany

We demonstrate that evaporation of the precursor molecules CsBr and $SnBr_2$ onto an atomically clean gold surface not only leads to the expected stoichiometric $CsSnBr_3$ structure, but also yields a range of other distinct structures. The experiments were conducted in ultra-high vacuum and investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). When deposited on Au(111), we observe a flower structure with hexagonal symmetry tentatively assigned to Cs_2SnBr_6, a ladder structure, a stripe pattern, a honeycomb structure, and a large square structure. The emergence of these structures depends on surface coverage - either submonolayer or multiple monolayers - and on the relative proportions of the two precursor molecules. In contrast, on Au(100) these structures are not observed, suggesting that the interface is playing a crucial role. The structures are compared with those formed by depositing either CsBr or $SnBr_2$ on Au(111). While a honeycomb structure can also be formed with $SnBr_2$ alone, the other structures bear no resemblence to either pure component. Thus, they are assigned to structures involving specific ratios of Cs, Sn and Br deviating from the standard ABX_3 structure. The structural variability underscores the importance of precise deposition conditions and interface selection in the fabrication of perovskite materials.

O 74.4 Wed 18:00 P2

Band alignment at InP/TiO_2 interfaces from density-functional theory — Isaac Azahel Ruiz Alvarado[1], Christian Dressler[2], and •Wolf Gero Schmidt[1] — [1]Universität Paderborn, Germany — [2]TU Ilmenau, Germany

The natural band alignments between indium phosphide and the titanium dioxide polymorphs rutile, anatase and brookite as well as amorphous titania are calculated from the branch point energies of the respective materials. Type-I alignment is predicted, irrespective of the type of titania interfacing with InP. The actual band offset may differ, however, from the natural band alignment depending on the microscopic structure of the interface. Supercell calculations are performed for the interface between P-rich InP(001) surface and amorphous titania thin films. The valence band offset increases substantially compared to the natural band alignment, while the conduction band offset is reduced, resulting in nearly aligned conduction bands. Depending on the interface properties, both type-I and type-II interfaces are observed in the simulations. The results show that with careful control of the microscopic interface structure and the atomic order of the titania film a very wide range of band alignments becomes accessible.

O 74.5 Wed 18:00 P2

Structure of tellurium phases on Ni(111) and Ni(111)-(1 × 1)-2C (graphene) — •Alexander Wegerich, Gwyn R. Thomas, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Using quantitative LEED-IV analyses, STM and DFT, we examine Te on Ni(111) to understand the interactions and emerging structures. For Θ_{Te} = 0.33 ML a $\left(3\times\sqrt{3}\right)_{rect}$-2Te superstructure is identified. For Θ_{Te} = 0.40 ML this changes to a $\left(5\times\sqrt{3}\right)_{rect}$-4Te superstructure. As LEED-IV analyses reveal, these superstructures are identical to those that can be observed for the Te/Cu(111) system [1], albeit with different stacking and reduced Te-Metal bond length.

In addition, we also present our first results regarding Te on the well-known Ni(111)-(1 × 1)-2C (graphene) structure [2, 3]. The presence of Te reduces the thermal stability of the graphene on Ni(111). At annealing temperatures above 570 K the graphene begins to dissolve and structures for the Te/Ni(111) system emerge. In the course of our studies, we also determined the Ni(111)-(1 × 1)-2C (graphene) structure by LEED-IV analysis and obtained picometer accuracy by virtue of a low Pendry R-factor of R = 0.10.

[1] T. Kißlinger et al., Phys. Rev. B **104**, 155426 (2021)
[2] J. Lahiri et al., New J. Phys. **13**, 25001 (2011)
[3] Y. Gamo et al., Surface Science **374**, 61-64 (1997)

O 74.6 Wed 18:00 P2

An atomistic analysis of the carpet growth of KCl across Ag(111) step edges — •Anna Juliana Kny[1], Adam Sweetman[2], and Moritz Sokolowski[1] — [1]Clausius Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [2]School of Physics and Astronomy, University of Leeds, UK

Thin alkali halide (AH) films of 2-3 atomic layer thickness, grown on metal substrates, are widely used for studying decoupled molecules by scanning tunneling microscopy. For many combinations of AH and metal surface, a continuous growth of the AH layer across step edges of the substrate is observed, which is called carpet growth. Here, we report a first atomistic analysis of the layer distortions in the carpet growth region of KCl layers at Ag(111) step edges.[1] STM measurements were performed at room temperature and with Cl anions decorated W-tips which yield a high atomic resolution. We find that the AH layer distorts locally and in a non-uniform manner within a short lateral distance of four unit cells, when it grows across the Ag step. Furthermore, we find that the Ag(111) surface adapts to the AH layer, as the carpet growth is accompanied by a straightening of the Ag steps along the <110> direction and a splitting of higher Ag steps into multiple mono-atomic ones. These mono-atomic Ag steps allow for the carpet growth if the distance between them is larger than 13 Å, while a carpet growth across higher or closer Ag steps was not observed.[1]

Supported by the DFG through the research training group 2591, the Royal Society, and the ERC.

[1] A.J. Kny et al., J. Phys. Chem. Letters (2024), under revision.

O 74.7 Wed 18:00 P2

Epitaxial growth of bismuthene-based transition metal compounds — •Holger Diehm, Bing Liu, Simon Moser, Jörg Schäfer, and Ralph Claessen — Würzburg-Dresden Cluster of Excellence ct.qmat and Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany

This work explores the fabrication of alloy phases between bismuthene - a fully planar honeycomb structure of bismuth atoms on a silicon carbide (0001) sub-

strate - and 3d transition metals (TMs).

Bismuthene is a promising candidate for quantum spin Hall (QSH) effect at room-temperature [1] that shows interacting 1D spin-polarized electrons in a metallic edge channel [2]. While topological protection of the edge channels can be lifted by edge coupling [3], interfacing it with ordered TM-rich phases could locally introduce magnetic moments. This provides a novel platform to explore the effects of broken time-reversal symmetry and its potential impact on the topological phase.

Our work focusses on epitaxially grown bismuthene, garnished with manganese, chromium or cobalt. While bismuthene on silicon carbide shows a rt(3) x rt(3) surface reconstruction in low energy electron diffraction (LEED), incorporation of transition metals causes an additional 3 x 3 phase. In addition, scanning tunneling microscopy (STM) is used to analyze the surface structure on an atomic level.

This study paves the way for both fundamental research and application-oriented development in spintronics.

[1] Science 357, 287 (2017); [2] Nat. Phys. 16, 47 (2020); [3] Nat. Commun. 13, 3480 (2022).

O 75: Poster Focus Session Chemical Imaging for the Elucidation of Molecular Structure (joint session O/BP)

Time: Wednesday 18:00–20:00 Location: P2

O 75.1 Wed 18:00 P2

Imaging of structure, conformation, and assembly of biological molecules by scanning probe microscopy (SPM) — •Joshua Holloway, Márkó Grabarics, Banjamin Mallada, Alejandro Lynch Gonzalez, Lukas Eriksson, and Stephan Rauschenbach — University of Oxford, Oxford, UK

Direct imaging of (bio)molecules by scanning probe microscopy (SPM) is a powerful approach for molecular structure elucidation. Sample preparation presents a challenge: an analyte must be taken into the gas phase, and intactly deposited on the sample surface. Because many biological molecules we wish to study are incompatible with sublimation, we employ electrospray ion beam deposition (ES-IBD). A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Q Exactive UHMR) allows for mass-filtered, soft-landed deposition onto atomically flat metal crystals for high-performance SPM imaging.

Here we present the workflow of mass spectrometry, selection, deposition, and imaging for several examples of biological molecules. In particular we explore the imaging of molecular assemblies of biomolecules with large and small ligands, formed in the gas-phase and/or on the surface.

O 76: Poster Focus Session Atomic Scale Investigation of Magnetic 2D Materials

Time: Wednesday 18:00–20:00 Location: P2

O 76.1 Wed 18:00 P2

Unconventional magnetic response in epitaxial-grown single-layer Cr_2S_3-2D — •Affan Safeer[1], Calisa Carolina Oliveira[2], Mahdi Ghorbani-Asl[3], Jörg Schöpf[1], Wouter Jolie[1], Amilcar Bedoya-Pinto[2], Arkady V. Krasheninnikov[3], Thomas Michely[1], and Jeison Fischer[1] — [1]Universität zu Köln, Köln, Germany — [2]University of Valencia, Paterna, Spain — [3]Institute of Ion Beam Physics and Materials Research, Dresden, Germany

We studied the magnetic ordering in epitaxially-grown single-layer Cr_2S_3-2D on Gr/Ir(110) using X-ray magnetic circular dichroism (XMCD), scanning tunneling microscopy (STM) and spectroscopy (STS). Prior characterization of the 2D material structure via low-energy electron diffraction (LEED), STM, and density functional theory (DFT) calculations confirmed that single-layer Cr_2S_3-2D has a NiAs-type structure. DFT calculations further predicted that the ground state could be either A-type antiferromagnetic or ferromagnetic, depending on the Hubbard parameter. Differential conductance STS measurements as a function of the out-of-plane magnetic field at 1.7 K show a hysteresis behavior with a switching field of about 4T, indicating a ferromagnetic ordering. In contrast, XMCD measurements on the same sample revealed no signal, indicating zero net magnetic moment, suggesting antiferromagnetic behavior.

O 76.2 Wed 18:00 P2

Atomically thin $MnBr_2$ grown by molecular-beam epitaxy on graphene/Ir — Oktay Güleryüz, Affan Safeer, Nicolas Georgopoulos, Thomas Michely, and •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We report on the growth of potentially magnetic manganese dibromide ($MnBr_2$) films on graphene/Ir substrates using molecular-beam epitaxy. $MnBr_2$ is evaporated as a single compound from an effusion cell onto the graphene/Ir. Low-electron energy diffraction analysis reveals that the hexagonal lattice constant of $MnBr_2$ amounts to 0.390 ± 0.005 nm, consistent with calculated 0.3885 nm and bulk 0.3873 nm values.

Our scanning tunneling microscopy study reveals that the best growth conditions to form large, compact monolayers involve deposition at elevated temperatures (400 K). Growth at low temperature on graphene/Ir(110) leads to the formation of small islands with a distribution of orientations. A new moiré superstructure is formed, which reflects the interaction of the $MnBr_2$ lattice with the corrugated graphene/Ir(110) moiré.

Low-temperature scanning tunneling spectroscopy at 1.7 K of monolayer $MnBr_2$ further reveals a significant band gap of approximately 5 eV. Additionally, isolated polarons are observed, which can be manipulated, created, and destroyed by the STM tip.

O 76.3 Wed 18:00 P2

The Nickelocene as an STM Atomic-Spin Sensor via cotunnelling theory — •Andres Pinar Sole[1,2], Manish Kumar[1], Diego Soler-Polo[1], Oleksandr Stetsovych[1], and Pavel Jelinek[1] — [1]Czech Institute of Physics, Cukrovarnicka 10, Prague 6, 16200 (Czech Republic) — [2]Center for Quantum Nanoscience (QNS) Research Cooperation Building Ewha Womans University, 03760 Seoul, (Republic of Korea)

Functionalization of a scanning microscopy probe with a single nickelocene attached to the tip allows reproducible spin-sensitive measurements of magnetic systems on surfaces. As a S=1 molecule, the triplet ground state of the nickelocene tip gives rise to a inelastic electron spin-flip excitation which changes upon interactions with spin systems on the surface. Some advantages of nickelocene functionalization compared to spin-polarized tips include tip passivation, enabling data acquisition at close tip-sample distances and well defined spin and tip apex. These features enable us to determine the local spin moment on the surface with atomic-scale precision.

While the interactions between the nickelocene spin and the magnetic centers has been modelled using a two-site Heisenberg Hamiltonian, we complement it to include the tunnelling current as an electronic transport phenomenon via cotunneling theory. It allows understanding the absence of transitions that are not allowed according to the selection rules or have relatively weaker intensity. We cover S = 1/2, 1, and 3/2 systems, as well as 2D magnetic materials and compare the simulations with experimental results.

O 77: Poster Vacuum Science Technology: Theory and Applications

Time: Wednesday 18:00–20:00 Location: P2

O 77.1 Wed 18:00 P2

An apparatus of preparing frozen solution samples for ultra-high vacuum experiments — •Jiadong Guo, Xinmeng Liu, and Ying Jiang — International Center for Quantum Materials, School of Physics, Peking University, Beijing, China

Here we develop an apparatus for preparing frozen solution samples, which can be characterized by surface science techniques under ultra-high vacuum (UHV) condition. When a temperature-variable substrate is approached to contact the frozen solution at 77 K, the surface of the frozen solution is locally melted and then refreeze with the substrate. By detaching the substrate from the frozen so-

lution in high vacuum, the frozen solution is cleaved and transferred onto the substrate. Applying this method, we demonstrate transferring NaCl and $LiNO_3$ frozen solutions onto the Au substrate, and directly image the crystallization of NaCl and $LiNO_3$ using atomically resolved atomic force microscopy (AFM) in UHV at 5 K.

This apparatus provides a new approach to transfer solution samples in their glassy states into the UHV environment while maintaining the cleanliness of the samples, laying the foundation for further research related to solution environment, such as crystallization, hydration, chemical reaction, materials synthesis and bioimaging.

O 77.2 Wed 18:00 P2

Investigating Nanoscale Hydrophobic Polymer Coatings for the use in the Einstein Telescope — •Maike Kühler, Achim Stahl, Charlotte Benning, and Oliver Pooth — III. Physikalisches Institut B, RWTH Aachen

With 120 km pipes of 1m diameter, the ultra-high vacuum (UHV) system of the Einstein Telescope is going to be one of the largest vacuum systems in existence. It will need an enormous input of innovation and optimization. This work explores superhydrophobic coatings for the vacuum chambers of the Einstein Telescope. Hoping to achieve faster pumpdown times and eventually lower bake out temperatures to reach sufficient pressure regimes. This poster presents a coating based on reactive silyl anchor units and functionalised with a long perfluoropolyether/organofluorine chain. The coating has been investigated for its performance and compatibility with UHV conditions. Its compatibility with the vacuum system of the Einstein Telescope was evaluated through molecular flow simulations.

O 77.3 Wed 18:00 P2

Tritium Induced Exchange Reaction of Hydrogen Isotopes — •James O'Callaghan, Robin Grössle, Simon Niemes, and Robin Holzwarth — Tritium Laboratory Karlsruhe (TLK), Institute of Astroparticle Physics (IAP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Tritium (T), the heaviest isotope of hydrogen, is used for experiments in astroparticle physics and is essential as fuel for fusion reactors. It comes with many challenges due to its radioactivity. Isotopic exchange is one such challenge, Hydrogen-1 (H) and Deuterium (D) can be left in an idealised vessel and will practically not react with each other; the concentrations of H2, D2 and HD will remain unchanged and will not reach the thermal equilibrium in practical time scales. This is not the case with tritium. In the presence of tritium, the radioactive decay induces chemical reactions and therefore the concentrations will shift towards the chemical equilibrium. Most prominently in a fusion reactor context, starting with mixtures of homonuclear molecules (H2, D2, T2), the production of potentially undesirable heteronuclear molecules (HD, HT and DT) up to the chemical equilibrium is facilitated by the decay of tritium. This needs to be understood for designing fuel cycle components for a fusion reactor. In this contribution first efforts for a data driven development of an empirical model to describe the reactions rates in tritiated mixtures is given.

O 78: Overview Talk Manish Garg

Time: Thursday 9:30–10:15 Location: H24

Topical Talk O 78.1 Thu 9:30 H24

Imaging Electronic and Atomic Motion in Molecules — •Manish Garg — Max Planck Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart 70569

The capability to capture electronic and atomic motions at their natural length (Ångstrom-scale) and time-scales (attoseconds to femtoseconds) is a long-standing goal in modern science. In my talk, I will show you how electron dynamics in molecules can be locally probed with angstrom-scale spatial resolution and sub-femtosecond temporal resolution simultaneously, at the single orbital-level with the help of a scanning tunnelling microscope (STM), defying the previously established fundamental space-time limits [1-3].

Quantum decoherence of the excited electronic states and dipole-dipole interactions between molecules can now be imaged in real-space and real-time. We have recently imaged electronic excitation transfer dynamics between donor and acceptor kind of molecules. Excitons locally excited in a donor molecule exchanges energy by coherent dipole-dipole interaction with a neighboring acceptor molecule [4].

Atomic motions in a single molecule can be directly imaged by realizing coherent anti-Stokes Raman spectroscopy in an STM [5-8]. These recent developments pave the way towards direct real space-time imaging of chemical reactions and phase transformations in two-dimensional materials.

O 79: Ultrafast Electron Dynamics III

Time: Thursday 10:30–12:30 Location: H2

O 79.1 Thu 10:30 H2

Hybrid Exciton Orbital Tomography in 2D-organic interfaces — •Christian Simon Kern[1], Michele Capra[2], Marco Gruenewald[3], Torsten Fritz[3], Mirko Cinchetti[2], Peter Puschnig[1], and Giovanni Zamborlini[1] — [1]Institute of Physics, University of Graz, Austria — [2]Department of Physics, TU Dortmund University, Germany — [3]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Organic molecules adsorbed on semiconducting 2D substrates pose an interesting class of interfaces for optoelectronic applications. Here we investigate the interface of pentacene and a transition metal dichalco-genide layer with many-body perturbation theory. In particular, we compare those results to optical spectroscopy and demonstrate the connection of excitons to their experimentally observable photoemission signatures in pump-probe spectroscopy. The latter approach— exciton photoemission orbital tomography [1]—especially allows for the unambiguous characterization of the excitons' hole and electron configuration, and is extended to the case of hybrid interlayer excitons.

[1] C. S. Kern, A. Windischbacher, and P. Puschnig, Photoemission orbital tomography for excitons in organic molecules, PRB 108, 085132 (2023)

O 79.2 Thu 10:45 H2

Ultrafast table-top three-dimensional photoemission orbital tomography — •G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Thi Lan Dinh[2], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Lennart Weinhagen[1], Bent van Wingerden[1], Fabio Frassetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russell Luke[2], and Stefan Mathias[1] — [1]University of Göttingen, I. Physikalisches Institut, Göttingen, Germany — [2]University of Göttingen, Institute of Numerical and Applied Mathematics, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, 35131 Padova, Italy

In photoemission orbital tomography (POT), molecular orbitals can be imaged with femtosecond resolution. Also, when combined with photon-energy-dependent measurements, POT is, so far, the only method that can probe the orbitals of adsorbed molecules in 3D. However, the study of, e.g., hybridization in organic/inorganic heterostructures [Bennecke *et al.*, arXiv:2411.14993 (2024)] by 3D-POT is extremely challenging due to the demanding nature of the experiment. Here, we present a table-top approach for 3D POT: By combining a photoelectron momentum microscope with a pulse-preserving monochromator for laser-generated extreme ultraviolet light, we speed up data acquisition. Moreover, we developed a new reconstruction algorithm that reduces the sampling requirements by about an order of magnitude [Dinh *et al.*, New J. Phys. 26 043024 (2024)]. Our first results achieved on PTCDA/Ag(110) highlight the potential for ultrafast femtosecond time-resolved 3D-POT.

O 79.3 Thu 11:00 H2

Exciton wave function signatures from time-resolved photoemission tomography of an organic molecular layer — •Siegfried Kaidisch[1], Marcel Theilen[2], Monja Stettner[3], Eric Fackelman[3], Galit Cohen[4], Amir Kleiner[4], Christian Simon Kern[1], Andreas Windischbacher[1], Sivan Refaely-Abramson[4], Frank Stefan Tautz[3], Ulrich Höfer[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Fachbereich Physik, Philipps-Universität Marburg — [3]PGI-3, FZ Jülich & RWTH Aachen University — [4]Weizmann Institute of Science, Israel

Oriented layers of organic molecules adsorbed on passivated metal surfaces are a promising class of interfaces for studying electron dynamics at femtosecond timescales. In particular, time-resolved photoemission tomography promises to reveal information about the electron distribution in optically excited states. Using the example of sexithiophene (6T) multilayers adsorbed on Cu(110)-p(2x1)O, we observe photoemission patterns for the low-energy excited states. These measured momentum maps exhibit signatures that cannot be explained by a mere population of the lowest unoccupied molecular orbital of 6T. To analyze the source of these features, we perform GW/BSE (Bethe-Salpeter equation)

calculations on multiple levels of theory (gas-phase, cluster, embedded and periodic calculations). Using the framework of photoemission orbital tomography for excited states, we also simulate the photoemission patterns and thereby shed light on the nature of the exciton wave function of the lowest optically allowed state.

O 79.4 Thu 11:15 H2

Quenching Strong-Field Recollisions at Nanotapers with Strong Bias Fields — •Rasmus Lampe, Germann Hergert, and Christoph Lienau — Institut für Physik, Carl-von-Ossietzky Universität, 26129 Oldenburg, Germany

Recollisions of intensively accelerated electrons with the parent are a well-known effect in strong-field photoemission of electrons, leading to photoemission spectra showing a recollision plateau with a cut-off energy of ten times the ponderomotive energy. It has recently been demonstrated that such a recollision plateau also arises in multiphoton photoemission from metallic nanostructures, showing that recollisions are much more fundamental to photoemission than anticipated [1].

We analyze electron recollisions from strongly biased tungsten nanotapers illuminated by few-cycle near-infrared laser pulses. We demonstrate significant changes in the photoelectron spectra in the strong-field regime by applying static electric fields on the order of the optical near-field driving the photoemission. A continuous transition of a horizontal recollision plateau into triangularly shaped spectra is observed.

Stronger static fields increase the acceleration of the electrons away from the apex, such that the ponderomotive acceleration by the near-field is not sufficient to drive the electrons back to the surface, ultimately suppressing recollisions. This enables the control of the electron motion with bias fields, which has an immediate importance for ultrafast low-energy electron microscopy allowing to maintain few fs time resolution of the electron beam over mesoscopic distances.

[1] B. Bánhegyi et al., Phys. Rev. Lett. 133, 033801 (2024)

O 79.5 Thu 11:30 H2

Time-resolved photoemission orbital tomography of 6T on Cu(110)-(2×1)O — •Marcel Theilen[1], Monja Stettner[2], Eric Fackelman[2], Francois C. Bocquet[2], Alexa Adamkiewicz[1], Sarah Zajusch[1], Siegfried Kaidisch[3], Christian Kern[3], Robert Wallauer[1], Peter Puschnig[3], F. Stefan Tautz[2], and Ulrich Höfer[1,4] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [3]Institut für Physik, Universität Graz — [4]Fachbereich Physik, Universität Regensburg

For ordered molecular layers, photoemission orbital tomography (POT) is a powerful technique for imaging the electron distribution of molecular orbitals in momentum space. When combined with laser pump-probe techniques, time-resolved photoemission orbital tomography (tr-POT) offers the ability to track the population dynamics of the excited molecular states on a femtosecond time scale[1].

In this talk, I will discuss our recent results obtained through tr-POT for three distinct, well-ordered layers of sexithiophene (6T) on a Cu(110)-(2×1)O surface: a monolayer, a bilayer and a multilayer. The focus will primarily be on the dynamics of the populated 6T LUMO via an optically HOMO-LUMO transition. For instance, a comparison between the individual layers reveals a significant extension of the LUMO lifetime with increasing layer thickness. Specifically, we find that the lifetime for the monolayer is less than 50 fs, while it increases to more than 600 fs for the multilayer.

[1] R. Wallauer *et al.*, Science **371**, 1056 (2021).

O 79.6 Thu 11:45 H2

Understanding the ultrafast electron dynamics and CDW transition in $LaTe_3$ using machine learning — •Gesa Siemann[1], Davide Curcio[1], Paulina Majchrzak[1], Charlotte Sanders[2], Jenny Rigden[2], Yu Zhang[2], Deepnarayan Biswas[3], Leslie Schoop[4], Emma Springate[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]Diamond Light Source, UK — [4]Department of Chemistry, Princeton University, USA

The rare-earth tritelluride $LaTe_3$ hosts a unidirectional charge density wave (CDW) with a high transition temperature of 670 K. Recently, it has been suggested that exposing the system to a short light pulse not only suppresses this primary CDW but also induces a second CDW in the perpendicular direction[1]. An open question is, how these structural dynamics affect the electronic structure, and if fingerprints of the second CDW can be found in corresponding data obtained by time- and angle-resolved photoemission spectroscopy. Here, we explore this question, studying the frequency-dependent coherent response of the system, and the time-dependent evolution of the Fermi surface topology, which we compare to predictions by a simple tight-binding model. We support our analysis using k-means clustering, a machine learning technique, in order to identify different dynamics throughout the Brillouin zone. This reveals varying relaxation times across the Fermi surface, as well as multiple frequencies that can be ascribed to coherent excitations. [1]A. Kogar *et al.*, *Nat. Phys.* 16, 159*163 (2020).

O 79.7 Thu 12:00 H2

Following charge-transfer between plasmonic NPs and adsorbed molecules by time-resolved IR spectroscopy — •Daniel Sandner[1], Katrin Schulz[1], Andrei Stefancu[2], Reinhard Kienberger[1], Emiliano Cortes[2], and Hristo Iglev[1] — [1]Lehrstuhl für Laser- und Röntgenphysik E11, TUM, James-Franck Str 1, 85748 Garching — [2]Fakultät für Physik, LMU München

Plasmonic Nanoparticles can efficiently convert light in a broad range into hot charge carriers, which can be subsequently transferred to molecules or semiconductors for photocatalytic processes. The role of charge-carrier-mediated or thermal reaction pathways is still under debate. Here, we use time-resolved IR spectroscopy between 1200-3000 cm-1 as a sensitive probe for free charges and study the dynamics of different molecules attached to silver NPs. Charge transfer is only observed for resonant excitation of the plasmon resonance and in the presence of attached molecules. Furthermore, we find a correlation between the lifetime of transferred charges and the chemical reactivity.

O 79.8 Thu 12:15 H2

Ultrafast Photoexcitation of Semiconducting Photocathode Materials: An Ab Initio Study — •Hilde Bellersen, Michele Guerrini, and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

Cs-based semiconductors like Cs_3Sb and Cs_2Te are currently used as photocathode materials in particle accelerators. Their performance as electron sources critically depends on their response to the intense laser radiation impinging them. In this work, we investigate from first principles the time-dependent response of Cs_3Sb and Cs_2Te to ultrafast laser pulses of varying intensities, ranging from 1 GW/cm^2 to 100 TW/cm^2. Nonlinear effects, including high harmonic generation and multiphoton absorption, emerge at thresholds of 400 GW/cm^2 for Cs_3Sb and 500 GW/cm^2 for Cs_2Te. Beyond these intensities, the energy uptake and number of excited electrons saturate, with renewed increases observed beyond 10 TW/cm^2. These findings provide new insights into the nonlinear optical properties of Cs_3Sb and Cs_2Te, contributing to the optimization of these materials for the development of next-generation photoinjectors.

O 80: Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I

Time: Thursday 10:30–12:30 Location: H4

O 80.1 Thu 10:30 H4

CISS in single heptahelicene molecules on Fe bilayers on W(110) — •Daniel E. Bürgler[1], Mohammad Reza Safari[1], Frank Matthes[1], Karl-Heinz Ernst[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut, Forschunschungszentrum Jülich, Germany — [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600, Dübendorf, Switzerland

We reproduce and extend our single-molecule studies of CISS [1,2] to an alternative substrate system. Heptahelicene molecules are sublimed onto a multidomain Fe bilayer film on W(110) instead of single-domain Co bilayer nanoislands on Cu(111). Using spin-polarized low-temperature scanning tunneling microscopy, the current flow through single *(M)*-enantiomers chemisorbed on neighboring and oppositely magnetized domains of the Fe bilayer film is mapped in the constant-height mode, where the tip is scanned at constant height above the Fe surface. The CISS magnetoresistance reaches up to 18% at 5 K and shows a strong dependence on the bias voltage. A comparison is drawn with the data obtained on Co nanoislands.

[1] M.R. Safari, F. Matthes, V. Caciuc, N. Atodiresei, C.M. Schneider, K.-H. Ernst, D.E. Bürgler. Adv. Mater. **36**, 2308666 (2024)

[2] M.R. Safari, F. Matthes, C.M. Schneider, K.-H. Ernst, D.E. Bürgler, Small **20**, 2308233 (2024)

O 80.2 Thu 10:45 H4

STM topography and photoluminescence of three different Eu complexes — •Adrian Ebert[1], Lukas Gerhard[1], Julia Feye[2], Senthil Kumar Kuppusamy[3], Mario Ruben[3], Peter Roesky[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Organic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

We explore the self-assembly and luminescence properties of three distinct Europium (Eu) complexes *Eu(tta)$_3$(H$_2$O)$_2$, Eu(btfa)$_3$(bpy), and Eu(tta)$_3$(bpy)* on a Au(111) surface. Utilizing Scanning Tunneling Microscopy (STM), we explore the molecular topography and the ordered structures formed by these complexes, providing insight into their surface interactions. The Europium Eu^{3+} ion, a member of the lanthanide series, is renowned for its unique photophysical properties, particularly its sharp emission lines and long-lived luminescence, which make it a valuable component in light-emitting devices, bio-imaging, and sensing applications.

O 80.3 Thu 11:00 H4

First-Principles Modeling of Mixed-Dimensional Heterostructures: A Path Forward — •Jannis Krumland and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Inorganic/organic interfaces between transition-metal dichalcogenides and organic adsorbates are promising candidates for future opto-electronic applications, leveraging and combining the unique strengths of the two different types of materials. The first-principles description of such interfaces, however, remains challenging because methods based on density-functional theory are unreliable for their simulation [1]. This is a result of the mixed dimensionality of the interface, with molecules being zero-dimensional while surfaces are two-dimensional. The mixed dimensionality moreover poses challenges in the analysis of the results, as molecules are usually described in terms of energy levels, whereas surfaces are characterized by band structures. Here, we present a methodological study establishing pragmatic yet accurate simulation approaches for the calculation of energy-level alignments [2]. In addition, we highlight unfolding techniques as a key tool for gaining a deeper understanding of the interactions and hybrid-state formation occurring at such interfaces [3].

[1] J. Krumland and C. Cocchi, Phys. Stat. Sol. A 221, 2300089 (2024)
[2] J. Krumland and C. Cocchi, J. Phys. Chem. Lett. 15, 5350-5358 (2024)
[3] J. Krumland and C. Cocchi, Electron. Struct. 3, 044003 (2021)

O 80.4 Thu 11:15 H4

Photo-induced force microscopy of organic molecules on thin van der Waals substrates — •Markus Kratzer[1], Mohamad Khan[1], Simon Leitner[1], Aleksandar Matkovic[1], Olivier Siri[2], Conrad Becker[2], and Christian Teichert[1] — [1]Chair of Physics, Montanuniversität Leoben, Franz-Josef Straße 18, 8700 Leoben, AUT — [2]Aix Marseille Univ., CNRS, Cinam, 13288 Marseille, FGrance

Photo-induced force microscopy (PiFM) is an atomic force microscopy based technique for obtainiung infrared spectroscopic data with a spatial resolution down to a few 10 nm. Here, we utilized PiFM to investigate nano and microstructures comprising small organic molecules like para-hexaphenyl or dihydrotetraaza-acene (DHTA7) on exfoliated thin layers of van der Waals materials as hexagonal boron nitride (hBN). It is notices that the PiFM spectra systematically vary with van der Waals substrate thickness. Further PiFM spectra of upright standing molecular structures and flat lying structures are copared. PiFM turned out to be sensitive even for single molecular layers, which are only about 2 nm thick. Similarities and differences between thin film and bulk infrared data are discussed.

O 80.5 Thu 11:30 H4

Engineering Optical Properties through Polymorphism — •Nina Kainbacher[1,2], Peter Puschnig[1], and Oliver T. Hofmann[2] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Austria

Molecular monolayers on a supporting substrate can order in different configurations, i.e. polymorphs. Owing to variations of the intermolecular coupling between the transition dipole moments, we expect that different polymorphs exhibit also distinctly different optical properties due to changes in transition energies and oscillator strengths. In this study, we computationally study the impact of polymorphism of organic molecular monolayers on optical absorption spectra. Specifically, we investigate influencing factors, such as geometric distortions upon adsorption, interactions between transition dipole moments, changing selection rules due to the symmetry of different polymorphs, and particularly, effects arising from the potential delocalization of the wave functions. As an example, we predict the polymorphism of the dipolar organic molecule nitropyrene-amine on NaCl(100) using machine learning-based structure search and calculate its optical properties based on density functional theory and the RPA approximation. Specifically, we find two distinctly different polymorphs, where the excitation energies differ by approximately 0.2 eV which we attribute to a combination of the above-mentioned effects.

O 80.6 Thu 11:45 H4

Imaging the occupied states of multilayers of α-sexitiophene (6T) on Cu(110)-p(2x1)O using orbital tomography — •Monja Stettner[1,2], Andrey Matetskiy[1], Eric Fackelman[1,2], Siegfried Kaidisch[3], Serguei Soubatch[1], François C. Bocquet[1], Peter Puschnig[3], Christian Kumpf[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), FZ Jülich, Germany — [2]RWTH Aachen University, Germany — [3]Institute of Physics, University of Graz, Austria

Deposition of α-sexithiophene (6T) on an oxygen-reconstructed Cu(110)-p(2x1)O surface results in a well ordered, close-packed monolayer structure, and at higher coverages in layer-by-layer growth. Note that even beyond a monolayer, 6T retains its orientation along the [001] direction of Cu. We investigated samples with coverages of up to eight layers using ARPES and - in particular - orbital tomography. For the latter, experimental momentum maps are compared to simulated maps which are calculated for a single free molecule and for extended layers of 6T. We found a good resemblance for several occupied molecular states, e.g., the HOMO. However, in the binding energy range of several deeper orbitals, the momentum maps clearly show signatures of a sizable intermolecular dispersion that cannot be explained by a superposition of the single gas phase maps. The orbitals rather form dispersing bands, which indicates a significant intermolecular hybridization.

O 80.7 Thu 12:00 H4

Electronic structure of molecular and crystalline benzene on an MoS_2 monolayer — •Jan-Phillip Topmöller and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

TMDCs show great potential in terms of their applicability in optical electronics. Due to their large surface, molecules can easily bind to the TMDC and affect its electronic properties. Here we investigate molecular benzene and its bulk crystal as prototypical systems.

We use DFT (GGA) and DFT-D3 to determine the most stable adsorption position of both the molecule and the bulk crystal on MoS_2. Subsequently, we use many body perturbation theory to calculate the electronic spectrum of the adsorbate system and its individual components (MoS_2 and the benzene molecule/crystal) in order to investigate the effect of the molecule on the MoS_2 electronic and optical spectrum.

O 80.8 Thu 12:15 H4

Contact-dependent electronic properties of anthracene-MoS_2 heterostructures — •Hsin-Mei Ho and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Flexible nanodevices composed of atomically thin layers have revolutionized fundamental and applied sciences. Based on density functional theory (DFT), we consider the organic-inorganic heterostructures: anthracene molecules adsorbed on monolayer MoS_2. Our investigations of the adsorption geometries and the energy band dispersions demonstrate that the contact between the organic and inorganic layers greatly affects the electronic properties. Anthracene thin films give rise to different shifts of the frontier energy levels, and consequently, variations in the band alignments when the molecules are in the perpendicular and parallel orientations on MoS_2. As anthracene is known for ordered structures when grown on substrates, we find in the present study that the bandgap of an anthracene film reduces when the interactions between molecules increase. This suggests that how the molecules are packed also plays a critical role. Our study provides detailed insights regarding the advances of oligoacene-TMDs layers for both theoretical and experimental sides.

O 81: Heterogeneous Catalysis III

Time: Thursday 10:30–12:30 Location: H6

O 81.1 Thu 10:30 H6

Cu Oxide Nanoparticles for Virus Inactivation — •Daniel Silvan Dolling[1,2], Miguel Blanco Garcia[1,2], Mona Kohantorabi[1], Mohammad Ebrahim Haji Naghi Tehrani[1,2], Jan-Christian Schober[1,2], Ming-Chao Kao[1,2], Jagrati Dwivedi[1], Arno Jeromin[1], Thomas F. Keller[1], Olof Gutowski[3], Dimitry V. Novikov[3], Andreas Stierle[1,2], and Heshmat Noei[1] — [1]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

TiO_2 is known to inactivate SARS-CoV-2 photocatalytically under UV light. Recently, it has been shown that Cu oxide on Titania shifts the photoactivty into the visible light region. The specific oxidation state of Cu is paramount for the photocatalyst efficiency. Here, we use single crystalline TiO_2 to investigate the effects of growth conditions of Cu nanoparticles (NPs). To this cause, we em-

ploy X-ray diffraction (XRD) and scanning electron microscopy (SEM), revealing a temperature-dependent morphology. Subsequently, we analyze the short- and long-term oxidation behavior with X-ray photoelectron spectroscopy (XPS) and scanning Auger microscopy (SAM). Finally, we investigate the interaction of the NPs with asparagine amino acid using reflection-absorption infrared spectroscopy (IRRAS) and grazing-incidence small-angle scattering (GISAXS).

O 81.2 Thu 10:45 H6

Charting Catalysis: Unveiling Regime Boundaries in Kinetic Phase Spaces Through Concentration Profiles — •Maryke Kouyate, Gianmarco Ducci, Frederic Felsen, Christian Kunkel, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

In an industrial context, optimizing process variables is a critical step in ensuring optimal performance of catalytic reactors. Selecting the relevant process variables not only aids in meeting precise requirements but also in streamlining reactions and thus saving time and costs. Robust kinetic rate laws capable of accurately describing experimental data allow for predictive modelling in reactor design, optimization, and control. Specialized profile reactors efficiently yield the required data to derive kinetic models by providing access to spatio-temporally resolved chemical information along the reactor axis. Depending on the range of experimental conditions and the catalytic reaction, the kinetic phase space can exhibit sub-regions of smooth kinetic behavior, separated by transitional regions characterized by sudden qualitative changes of the kinetic behavior. These kinetic phase transitions carry important information about the catalytic reaction network. To pinpoint distinct sub-regions and corresponding models within a kinetic phase diagram, we propose an automated system capable of systematically exploring the design space. This algorithm manages the experimental reactor and iteratively suggests new experiments through model-based design of experiments.

O 81.3 Thu 11:00 H6

Mechanistic Probes for Photocatalysis: Gas Phase Reactions of Tertiary Alcohols on Titania in a Micro-Photoreactor — •Martin Tschurl[1], Clara Aletsee[1], Paula Neumann[1], Ib Chorkendorff[2], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]SurfCat Section for Surface Physics and Catalysis, Department of Physics, Technical University of Denmark, 2800 Kgs Lyngby, Denmark

The lack in mechanistic understanding still hinders the rational design of efficient photocatalyst for various applications. To gain more comprehensive insights into the fundamental effects in photocatalysis, we analyze the gas phase photoreactions of tertiary alcohols on titania powder in a micro-photoreactor in a well-defined environment under the exclusion of oxygen. The parallels of the observed reaction properties to studies performed on a rutile single crystal in vacuum suggest similar mechanistics, which is in contrast to the generally assumed reaction model under such conditions. Furthermore, the time resolution of the micro-reactor setup allows the determination of the alcohol surface coverage, which excludes the existence of liquid films and evidences a gas phase reaction. In addition to the scientific insights on photocatalysis on titania, these results demonstrate the use of tertiary alcohols as suitable probe reactants for mechanistic studies.

O 81.4 Thu 11:15 H6

Selectivity trends in CO hydrogenation over transition metal surfaces — •David Degerman[1,2], Patrick Lömker[1], Markus Soldemo[1], Fernando Garcia-Martìnez[3], Robin Yoël Engel[1,2], Martin Beye[1,2,3], and Anders Nilsson[1,2] — [1]Department of Physics, Stockholm University, 114, 21, Stockholm, Sweden — [2]WISE - Wallenberg Initiative Materials Science for Sustainability, Department of Physics, Stockholm University, 114, 21, Stockholm, Sweden — [3]Deutsches Elektronen Synchrotron, DESY, Photon Science, Notkestraße, 22607, Hamburg, Germany

Understanding the selectivity of heterogeneously catalyzed CO hydrogenation is increasingly important for the transition towards a sustainable chemical industry. While theoretical studies yielded a model based on the competition of various elementary surface reactions, we need experimental observation of the surface's chemical state to verify the mechanistic origin of the selectivity. Here, we compare in-situ x-ray photoelectron spectra over operating single crystal catalysts (200 to 325 °C, 150 mbar) of Fe, Rh, Ni, Co and Cu and infer from the observed trends which mechanistic steps decides the product distribution for each material. In particular, we find that the chemisorption energies of C and O (commonly used descriptors for activity and selectivity) qualitatively predicts the rate-limiting step of catalysts, but fails when the reaction mechanism of Ni and Fe is fundamentally altered due to reaction-induced carburization. This work emphasizes that the complete chemical overview provided by photoemission spectroscopy is required to understand the selectivity of CO hydrogenation.

O 81.5 Thu 11:30 H6

Exploration of Explicit Solvation Effects in Heterogeneous Catalysis Using Machine Learning Interatomic Potentials — •Maciej Baradyn and Johannes T. Margraf — University of Bayreuth

The presence of solvent affects many aspects of modeling elementary reactions involved in heterogeneous catalysis, such as stabilization of adsorbed species, the nature of interaction with the surface, as well as energetics and reaction rates, to name just a few. Unfortunately, treating solvent effects in atomistic simulations is a great challenge, since the solvent adds many additional degrees of freedom to the calculation. In first-principles calculations, implicit solvation models are often used to approximately include these effects with moderate computational effort. However, they do not take into account the explicit solvent-surface and solute-solvent interactions, and are therefore known to fail, e.g. when hydrogen bonding is important. More importantly, the solvent molecules can sometimes play a decisive role in the reaction's mechanism (e.g. as proton shuttles), which cannot be captured by implicit models, where solvent is treated as a continuous medium. In this contribution, we explore the efficiency of machine learning potentials based on the MACE-MP-0 foundation model for describing explicit solvation at catalytic interfaces. These potentials are used to capture the kinetic and thermodynamic parameters of small organic molecules interacting with metallic surface in an explicit water bath. Implications for our understanding of the underlying catalytic reaction network and improved design of catalysts will be discussed.

O 81.6 Thu 11:45 H6

Reducibility of Sm-doped ceria islands on Ru(0001) — •Raquel Sanchez-Barquilla, Rudi Tschammer, Lars Buss, Carlos Morales, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Germany

The interaction between metal and oxide is critical when considering the hydrogenation of CO_2 to hydrocarbons. In this context, the inverse oxide/metal catalysis architecture allows for achieving better catalytic performance due to strong oxide-metal interactions. In particular, in cerium-based inverse catalyst systems, the Ce^{3+} cations have been demonstrated to play an active role in methanol synthesis, suggesting that the activity can be enhanced by promoting those through alloying with trivalent, catalytically active rare-earth metals, such as Sm. Here, we present a low-energy and X-ray photoemission electron microscopy (LEEM/XPEEM) investigation that shows how the reducibility of CeO_2(111) islands on Ru(0001) is highly enhanced when doped with Sm. After post-annealing with Sm, intensity-voltage (I-V) LEEM curves show an immediate reduction of the islands at the surface. Exposure to low H_2 pressures efficiently reduces the islands to a (3×3) superstructure formed by ordered oxygen vacancies, as evidenced by characteristic IV-LEEM spectra and low-energy electron diffraction patterns. Furthermore, annealing at high temperatures shows the further reduction of the Sm-ceria islands, with features characteristic of the hexagonal Ce_2O_3(0001) phase. While this reduction takes about one hour for pure ceria, this transition is virtually immediate for the Sm-doped ceria islands at comparable conditions.

O 81.7 Thu 12:00 H6

Interaction of single cobalt co-catalyst atoms with the $SrTiO_3$(001) surface — •Aji Alexander[1], Pankaj Kumar Samal[1], Llorenç Albons[1], Jan Škvára[1], Dominik Wrana[2], Viktor Johánek[1], Josef Myslivecek[1], and Martin Setvin[1] — [1]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland

Perovskite surfaces attract attention in the catalysis community due to their promising chemical properties, ability to separate electron-hole pairs for light harvesting, and ferroelectricity in various phases. Understanding metal clusters, specifically their electronic structure and atomic utilization efficiency, is crucial for developing more efficient and sensitive catalysts.

This work focuses on the atomic structure of doped $SrTiO_3$(001) perovskite surface and the potential to modify its catalytic activity by the presence of extrinsic metals, with the main focus on cobalt. Combined STM/AFM, LEED, and XPS show a combination of cobalt clustering and dispersion within an ordered reconstruction. We will highlight how cobalt interacts with perovskite surfaces at different reducing conditions and explain the various phases of the supported cobalt as a function of temperature.

The work was supported by projects MSMT LL2324, GACR 20-21727X, and GAUK 10/252122. The work was supported by projects GAUK 10/252122, GACR 20-21727X, and GAUK Primus/20/SCI/009.

O 81.8 Thu 12:15 H6

Machine Learning Assisted Realistic Description of Mo-V Mixed Oxide Surfaces — •Kyeonghyeon Nam, Y. Song, L. Masliuk, T. Lunkenbein, A. Trunschke, K. Reuter, and C. Scheurer — Fritz-Haber-Institut der MPG, Berlin

The activity and selectivity of realistic heterogeneous catalysts can be noticeably altered by subtle changes in factors such as bulk composition, dopants, defects, and reaction conditions. These effects are intricately interrelated. To systematically unravel them, we aim to understand their impact on the evolution of catalyst surfaces. Specifically, we focus on the M1 structural modification of $(Mo,V)O_x$ and $(Mo,V,Te,Nb)O_x$ as selective catalysts for the oxidative dehydrogenation of ethane to ethylene.

The large primitive cell of the M1 catalyst poses challenges for a detailed study of its surface terminations using conventional first-principles calculations. To overcome this, we trained machine learning interatomic potentials (MLIPs) using a staged training method from motifs to surfaces. By combining density-functional tight-binding (DFTB) calculations with simulations employing MLIPs, such as molecular dynamics and *ab initio* thermodynamics (AITD), we elucidated the influence of niobium and tellurium doping on enhanced surface structure stability and catalytic activity during the thermal activation. This was supported by experimental *quasi-operando* scanning transmission electron microscopy (STEM) images.

O 82: Plasmonics and Nanooptics: Fabrication, Characterization and Applications II

Time: Thursday 10:30–12:30 Location: H8

O 82.1 Thu 10:30 H8

Femtosecond Direct Laser Writing of Conductive and Electrically Switchable PEDOT:PSS Optical Nanostructures — •Dominik Ludescher[1], Pavel Ruchka[1], Leander Siegle[1], Yanzhe Huang[2], Philipp Flad[1], Monika Ubl[1], Sabine Ludwigs[2], Mario Hentschel[1], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]IPOC - Functional Polymers, Institute of Polymer Chemistry, University of Stuttgart, Germany

Conducting polymers, exemplified by PEDOT:PSS, exhibit distinctive electronic and polymeric attributes. When subjected to CMOS-compatible voltages (-3 V and +2 V), PEDOT:PSS transitions between insulating and metallic states via an intrinsic electrochemical redox reaction. Consequently, this conducting polymer is suited perfectly for AR/VR applications, advanced display technologies, dynamic sensors, and integration with printed optics. The latter application requires a robust foundation in fabrication and the ability to combine 3D printed optics with switchable materials to open the route to dynamic miniaturized optics. We present an alternative fabrication method based on the photon-induced solubility modulation that combines conventional, static photopolymer structures (IP-S) with the dynamic behavior of PEDOT:PSS. Additionally, we demonstrate that the electrical, optical, and dynamic material properties remain even after structuring based on direct laser writing, present the resolution limit at 400 nm structure width, and investigate the switching speed and sample longevity.

O 82.2 Thu 10:45 H8

Revolutionizing OLED Performance and Efficiency with Core-Shell Nanoparticles in HTL and Carbon Dots in ETL Layers — •Zoi Georgiopoulou[1,2], Apostolis Verykios[1], Theodoros Triadis[1], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Center for Scientific Research *Demokritos* — [2]Solid State Physics Section, Department of Physics, National and Kapodistrian University of Athens

The development of efficient organic light-emitting diodes (OLEDs) is essential for advancing modern displays and flexible electronics. This presentation explores two methodologies to enhance OLED performance through innovative material integration. The first involves incorporating core-shell nanoparticles into the hole transport layer (HTL). Metal nanoparticles (M-NPs) are encapsulated in a tungsten polyoxometalate (POM) compound and embedded in the PEDOT:PSS layer, leveraging the Localized Surface Plasmon Resonance (LSPR) effect. Analyses, including UV-Vis spectroscopy, atomic force microscopy, and electrical measurements, reveal enhanced optoelectronic properties with POM-M-NP integration. The second approach enhances OLED efficiency by combining carbon dots and a porphyrin layer in the electron transport layer (ETL). Carbon dots improve electron mobility and reduce recombination losses, while the porphyrin layer facilitates charge injection and blocks backflow. This synergy optimizes charge balance, lowers operating voltage, and improves luminous efficiency. These strategies underscore the importance of advanced material engineering in OLED development

O 82.3 Thu 11:00 H8

Engineered disorder metasurfaces for near-field light shaping — •Luca Schmid[1], Julian Schwab[1], Chi Li[2], Stefan Maier[2], Harald Giessen[1], Haoran Ren[2], and Mario Hentschel[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]School of Physics and Astronomy, Monash University, Clayton, Victoria, Australia

Plasmonic and dielectric nanophotonic building blocks allow for shaping the flow of light at boundaries and interfaces. They have opened the field of metasurfaces, which until now mostly allow for the creation of nearly arbitrary far-field intensity distributions in the far field. Drawing inspiration from this concept, we introduce metasurfaces for near-field light shaping. Desired near-field intensity distributions can be created by engineering the distribution of individual scatterers on metallic surfaces and hence the interference of the individually launched surface plasmons. Using this ansatz, we demonstrate engineered-disorder metasurfaces which enable to direct, focus, and demultiplex incident light. We implement these structures by a peel-off process from molds, which results in ultra-smooth metallic surfaces, maximizing the plasmon propagation length. Far-field measurements based on a k-space spectroscopy setup allow us to image the local near-field and show excellent agreement with modelling and simulation. We envision that the creation of nearly arbitrary near-field distributions will enable nanoscale routing and sorting of light based on polarization, orbital angular momentum, and wavelength, as well as help realize novel coupling schemes to emitters and nanoscale systems.

O 82.4 Thu 11:15 H8

Strong polarization-tuned optical nonlinearity via femtosecond-laser plasmonic nanolithography in lithium niobate — •Han Zhu[1,2], Shengqiang Zhou[1], and Feng Chen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Shandong University, Jinan 250100, China

Despite the advantages of lithium niobate (LN)-based photonic integration platforms in various applications, the inherently weak third-order nonlinear optical response of conventional materials limits the miniaturization and energy efficiency of nonlinear optical devices in compact optical systems. Localized surface plasmons (LSPs) provide a promising solution to this miniaturization challenge by confining and enhancing light fields at deep subwavelength scales. However, due to nanofabrication limitations, strongly coupled single-crystal LN-LSP structures have yet to be realized. Here, we demonstrate Au nanorod-LN hybrid plasmonic structures assembled via plasmonic nanolithography. By leveraging plasmon-mediated energy deposition and photon momentum transfer under femtosecond laser irradiation, the nanoparticles within the single-crystalline region are formed from implanted elements. With plasmons excited in distinct axial directions, the resulting nanorod-LN hybrid plasmonic material exhibits polarization-dependent nonlinearity, with the nonlinear absorption coefficient for long-axis polarized light augmented by five orders of magnitude compared to the pure LN. Utilizing this feature, we develop a Q-switched laser exhibiting pronounced polarization-dependent behavior.

O 82.5 Thu 11:30 H8

Nonlocal Substrate Influence on the Plasmon of a Supported Silver Nanoparticle — Kevin Oldenburg, Karl-Heinz Meiwes-Broer, and •Ingo Barke — ELMI-MV, Department *Life, Light & Matter*, and Institute of Physics, University of Rostock

The effect of a substrate on a particle plasmon (Localized Surface Plasmon Resonance, LSPR) is often considered to be of local nature, where the substrate primarily affects the plasmon at short distances [1]. Here we present spatially resolved plasmon excitation probabilities of a single 11 nm silver nanoparticle deposited from the gas phase onto a narrow rim of a carbon substrate ("cliffhanger"), thus providing a cross-sectional view. We employ electron energy loss spectroscopy (EELS) with a scanning transmission electron microscope (STEM) where we find the strongest substrate effect, i.e., the largest red shift, when the plasmon is excited farthest away. As will be discussed, this non-local substrate influence is a consequence of the simplicity and size of the system. These results are corroborated by simulations based on the boundary element method (BEM), which also help extract the full mode structure from the experimental data. Furthermore, we observe pronounced symmetry breaking, lifting the threefold degeneracy of the dominating dipole modes, potentially resolving long-standing discrepancies in the literature regarding plasmon energies of silver clusters in this size regime [2].

[1] S. Mazzucco, et al., Nano Letters 12, 1288 (2012).
[2] H. Haberland, Nature (2013), 494 E1-E2; A. Campos et al., Nature Physics (2019), 15, 275

O 82.6 Thu 11:45 H8

Dynamic beam switching using individually adressable plasmonic gratings made from switchable metallic polymer in planar technology — •Jonas Herbig, Dominik Ludescher, Monika Ubl, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

The ability to steer light in an optical system is vital for light detection and ranging (LiDAR) applications as required for autonomous driving and technology based on artificial intelligence (AI). One relevant drawback of conventional LiDAR platforms is their large size, making them unsuitable for integration into compact devices. Here, we demonstrate a compact and programmable electrode nanopattern utilizing the structuring of indium tin oxide (ITO) layer in conjunction with the conducting polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). This structure demonstrates the individ-

ual addressability of multiple subgratings, enabling switching between different superlattice periods with CMOS-compatible voltages, resulting in multiple diffraction angles of up to 26° at a wavelength of 2150 nm. This work lays the foundation for adaptive optics as well as single addressable pixels necessary for advanced display systems and other active devices, such as spatial amplitude and phase modulators exceeding 1000 l/mm.

O 82.7 Thu 12:00 H8

Disorder-driven localization of surface plasmon resonances in disordered assemblies of gold nanoparticles — •Kristina Weinel[1,2,3], Johannes Schultz[1], Mohammed Fayis Kalady[1], Daniel Wolf[1], Leonardo Agudo Jácome[3], and Axel Lubk[1,2] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Dresden, Germany — [2]Technical University Dresden (TUD) Dresden, Dresden, Germany — [3]Federal Institute of Materials Research and Testing (BAM), Berlin, Germany

The general wave phenomenon of Anderson localization, which is the absence of diffusion of waves in disordered systems, is studied for surface plasmon waves in two-dimensional disordered systems. To that end disordered assemblies of plasmonic gold nanoparticles (NPs) on an insulating silicon oxide substrate were synthesized by a newly developed synthesis method where an electron beam in a scanning electron microscope is used to heat a gold microparticle precursor until evaporation and deposition of the gold atoms on the substrate forming NPs of varying sizes. To reveal the surface plasmons and their localization behavior, electron energy loss spectroscopy in the transmission electron microscope is applied and compared with self-consistent dipole model simulations. Disorder-driven spatial and spectral localization of the hybridized localized surface plasmon modes was found experimentally and via simulation. Moreover, the localization exhibits a characteristic thickness dependency determining the localization length dependency on the plasmon energy.

O 82.8 Thu 12:15 H8

Nanophotonics of ultra-thin gold flakes — •Gayathri Haridas, Farid Aghashirinov, Julian Schwab, Bettina Frank, and Harald Giessen — 4-th Physics Institute, University of Stuttgart, Germany

In our work, we focus on fabricating ultrathin single-crystalline gold platelets using an electrochemical synthesis approach. This process involves the reduction of gold atoms from the electrode surface to form gold ions, which then nucleate as seeds and grow into well-defined crystalline platelets. By systematically adjusting and controlling the growth parameters, we aim to optimize the synthesis conditions to achieve reproducible and stable fabrication of platelets with precise control over their lateral size and thickness. The characterization of the synthesized platelets is carried out using spectroscopic techniques such as Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), to understand the surface morphologies and height profiles of the crystals.

The primary objective is to reduce the thickness of platelets to the single-digit nanometer scale while maintaining their lateral sizes. At this regime, the gold platelets exhibit unique optical and electrical properties that are highly sensitive to their size. This arises from the quantization of electronic states. We are particularly interested in probing these quantum effects, which can give rise to further research in the field of quantum plasmonics and thereby establishing gold as a suitable platform for it.

O 83: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

O 83.1 Thu 10:30 H11

Charge ordered phases in the hole-doped triangular Mott insulator 4*Hb*-TaS_2 — •Byeongin Lee[1], Junho Bang[1], Hyungryul Yang[1], Sunghun Kim[2], Dirk Wulferding[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, Ajou University, Suwon 16499, Republic of Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Republic of Korea

4*Hb*-TaS_2 has a unique layered structure, featuring a heterojunction between a 2D triangular Mott insulator and a charge density wave metal. Since a frustrated spin state in the correlated insulating layer is susceptible to charge ordering with carrier doping, it is required to investigate the charge distribution driven by interlayer charge transfer to understand its various phases. In this study, we utilize scanning tunneling microscopy and spectroscopy (STM/S) to examine the charge-ordered phases of 1*T*-TaS_2 layers within 4*Hb*-TaS_2, explicitly focusing on the non-half-filled regime. Our STS findings reveal an energy gap that exhibits an out-of-phase relation of the charge density. We attribute the emergence of the charge-ordered insulating phase in a doped triangular Mott insulator to the interplay between on-site and nonlocal Coulomb repulsion.

O 83.2 Thu 10:45 H11

Superlattice engineering in graphene and 1T-$NbSe_2$ heterostructures — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I. Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering has become a major branch of condensed matter research, not at least due to the variety of exotic states observed twisted in van der Waals heterostructures. We here present a new method to periodically modulate graphene by stacking it on 1T/2H-$NbSe_2$. By tuning the twist angle, we realized two near-commensurate superlattices: $\sqrt{3}\times\sqrt{3}$ and 2×2 aligned with the charge density wave (CDW) of 1T-$NbSe_2$. Using scanning tunnelling microscopy, we visualized local stacking configurations for these two superlattices. We applied a newly developed symmetry analysis method to track rotational symmetry breaking as a function of bias. In the 2×2 superlattice, C_3 rotational symmetry was preserved. However, in the $\sqrt{3}\times\sqrt{3}$, a strong strip phase occurs. This symmetry breaking is explained by our tight-binding model. Our findings highlight a mechanism for superlattice-induced symmetry breaking that hints towards exotic states of matter.

O 83.3 Thu 11:00 H11

Influence of Edge Termination on the Electronic Structure of Single Layer MoS_2 on Graphene/Ir(111) — •Alice Bremerich[1], Marco Thaler[2], Thais Chagas[1], Borna Pielic[1], Laerte Patera[2], and Carsten Busse[1] — [1]Universität Siegen, Deutschland — [2]Universität Innsbruck, Österreich

MoS_2 is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic edge state that induces partial charge accumulation at its edges, resulting in band bending effects. This 1D state acts as a barrier to electron transport across the edge and contributes significantly to quantum confinement effects in TMDC islands. In this study, we tune the edge state and the associated band bending by altering the edge termination of MoS_2/gr/Ir(111) and investigate the resulting changes in the electronic structure by Scanning Tunneling Microscopy and Spectroscopy (STM and STS) at 8 K.

Quasi-freestanding MoS_2 is grown on gr/Ir(111) by Molecular Beam Epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). We vary the chemical potential of sulfur and thereby modify the chemical environment of the boundaries. The partial charge at the perimeter depends on edge type as well as edge chemistry. In consequence, also the upward bending of both valence and conduction band shows distinct variations.

O 83.4 Thu 11:15 H11

magnetic-field-induced dimensionality transition of charge density waves in strained 2H-NbSe2 — •Ryo Ichikawa[1], Yukiko Takahashi[2], Eiichi Inami[3], and Toyo Kazu Yamada[1,4] — [1]Department of Material Science, Chiba University — [2]National Institute for Material Science, Tsukuba — [3]School of system Engineering, Kochi University of Technology — [4]Molecular Chirality Research center, Chiba University

Layered transition metal dichalcogenides (TMDs) exhibit various correlated phases, including charge density waves (CDW), superconductivity, and magnetic orders. Bulk 2H-NbSe2 (2H niobium diselenide) is one of the most extensively studied TMDs, showing a triangular (3Q) incommensurate CDW with a 3a period in real space (3 * 3, TCDW ~ 33 K). Electric and magnetic fields have been used to manipulate spatial or time inversion symmetry, while the CDW in 2H-NbSe2 remains robust even under large magnetic fields on the order of tens of Tesla. However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe2, where a weak magnetic field of approximately 30 mT can switch the electronic phase within the thin film, resulting in a supercurrent diode effect. This study investigates the strained 2H-NbSe2 exhibiting the 2*2 CDW phase. We utilize low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) in ultrahigh vacuum (UHV). STS maps reveal the coherence of the 2*2 CDW patterns. However, applying an out-of-plane magnetic field induces a dramatic transformation akin to that observed in 1T-NbSe2, shifting the metallic 2D CDW pattern to a 1D CDW pattern.

O 83.5 Thu 11:30 H11

Ultrafast phonons dynamics of monolayer transition metal dichalcogenides — •yiming pan and fabio caruso — Kiel University, Germany

Valley degrees of freedom in transition-metal dichalcogenides influence thoroughly electron-phonon coupling and its nonequilibrium dynamics. Here we present a time-resolved ab-initio study of the ultrafast dynamics of chiral phonons following carrier excitation with circularly-polarized light. By investigating the valley depolarization dynamics of monolayer MoS_2 and WS_2, we find that a population imbalance of carriers distributed at K and K′ can lead to valley polarized phonons persisting beyond 10 ps, and characterized by a distinctive chirality [1]. Additionally, we find that strain can be exploited as a tool to control the phonon emission and the relaxation channels of hot carriers [2]. Finally, we briefly discuss available opportunities for experimental detection of these phenomena

[1] Y. Pan and F. Caruso, Nano Lett. 23, 7463 (2023)
[2] Y. Pan and F. Caruso, npj 2D Mater. Appl. 8, 42 (2024)

O 83.6 Thu 11:45 H11

Probing Excitonic Properties and Structural Effects in WS_2-Graphene Heterostructures Using EELS and DFT-BSE Modeling — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Robin Günkel, Badrosadat Ojaghi Dogahe, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the excitonic properties of WS_2 epitaxially grown on graphene by metal-organic chemical vapor deposition. We focus on understanding the effects of structural changes, such as variations in the number of WS_2 layers. Using monochromatic electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), we observe in the monolayer region of WS_2 an excitonic spectrum with excitonic peaks at 2.0 eV and 2.4 eV, as well as additional spectral features at higher energies. Measurements in the bilayer region show a small redshift of these features due to the additional layer. Complementary density functional theory and Bethe-Salpeter calculations show that this redshift in the K-valley excitons is due to both a change in quantum confinement and a change in the WS_2 lattice constant, with the latter being the dominant effect. Using STEM, this lattice distortion can be attributed to the heteroepitaxial alignment of the lower WS_2 layer to the graphene substrate, while the upper layer is relaxed. This study provides valuable insights into the relationship between atomic structure and optical properties in complex material systems, providing essential knowledge for the design and optimization of 2D heterostructures for advanced device applications.

O 83.7 Thu 12:00 H11

Optical excitations in 2H-MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]University of Münster, Institute of Solid State Theory, Münster, Germany — [2]University of Münster, Institute of Physics and Center for Nanotechnology, Münster, Germany

Theoretical and experimental investigations have shown several changes in the optical spectrum of the 2H-MoS_2 bilayer under pressure [1].

By using density functional theory (DFT) and many-body perturbation theory in combination with linear elasticity, our computational investigations show an effective shift of the A exciton under pressure. It is strongly connected to the behavior of the direct band gap at the K point, which shifts in energy under pressure. The direction of this shift depends on the stress condition. While a hydrostatic pressure leads to a blueshift, a suppression of the in-plane contraction, as it appears in diamond anvil cell-experiments due to the interaction between the sample and the substrate, shows a redshift.

Moreover, we observe a similar behavior for the interlayer exciton, whereas the shift rate is smaller than that of the A exciton, which results in a decreasing A-IL splitting for an increasing pressure.

[1] P. Steeger, J. Graalmann et al., Nano Lett., 23, (2023)

O 83.8 Thu 12:15 H11

Visualizing and controlling charge states of metal nanoislands on a two dimensional semiconductor — •Junho Bang[1], Byeongin Lee[1], Jian-Feng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul, Korea — [2]Department of Topological Quantum Chemistry, Max Planck Institute for Chemical Physics of Solids, München, Germany

Nanoscale objects show unique electronic behaviors when weakly coupled to electrodes. Coulomb blockade (CB) can occur in such systems, where the repulsive Coulomb interaction between electrons prevents additional electrons from entering the quantum dots, hindering their flow. Single electron tunneling occurs by these correlated electron transports, leading to the discrete charge states of objects in double barrier tunneling junctions. Despite enormous progress, challenges remain in precisely controlling the interplay between objects' charge states and tunneling dynamics under varying conditions. Here, we visualize the charge states and their spatial variation on the random array of the indium islands on two-dimensional semiconductor black phosphorus using scanning tunneling microscopy and spectroscopy. Our spatially resolved tunneling spectra reveal that the junction capacitance varies across the islands. Furthermore, we find that the CB features are visible outside the islands, which is attributed to the remote gating of the islands. Our work advances the manipulation of electron transport at the nanoscale, which will be helpful in the application of nanoscale object-based single-electron devices.

O 84: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: H24

O 84.1 Thu 10:30 H24

CO cryo-sorption on a FeNC catalyst as a spectroscopic probe of the active site density — •Benedikt P. Klein[1,3], Beomgyun Jeong[1], Hafiz Ghulam Abbas[2], Geunsu Bae[2], Adith R. Velmurugan[2], Chang Hyuck Choi[4], Geonhwa Kim[5], Dongwoo Kim[5], Ki-jeong Kim[5], Byeong Jun Cha[6], Young Dok Kim[6], Frederic Jaouen[7], Reinhard J. Maurer[3], and Stefan Ringe[2] — [1]Korea Basic Science Institute, Daejeon, ROK — [2]Korea University, Seoul, ROK — [3]University of Warwick, Coventry, UK — [4]POSTECH, Pohang, ROK — [5]PAL, Pohang, ROK — [6]Sungkyukwan University, Suwon, ROK — [7]University of Montpellier, France

To quantify the number of active sites in a catalyst is a crucial necessity for the evaluation of its performance. A possible quantification approach is the adsorption of a gas molecule to the catalytically active sites as a probe. If the adsorbed molecules can be reliably detected, their surface density can be determined by using spectroscopic techniques and the active site density of the catalyst can be obtained. For this approach it is necessary to identify the probe molecules according to their spectroscopic features, a task much helped by the computational simulation of spectra. In this the NAP-XPS and NAP-NEXAFS study, we present direct spectroscopic evidence for the adsorption of CO on an iron-nitrogen-carbon (FeNC) catalyst. The well defined spectroscopic features enable us to determine the active site density using by experimental data combined with state-of-the-art DFT based spectroscopy simulation.

O 84.2 Thu 11:00 H24

Nano-optical imaging of grating-coupled waveguide modes in 3R-MoS_2 — •Fabian Mooshammer[1], Xinyi Xu[2], Chiara Trovatello[2], P. James Schuck[2], and D. N. Basov[3] — [1]Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]Department of Mechanical Engineering, Columbia University, New York, USA — [3]Department of Physics, Columbia University, New York, USA

Waveguide modes in thin slabs of van der Waals crystals serve as reliable probes of the anisotropic dielectric response of the material and also hold great potential for the implementation of on-chip optical elements. Here, we show that near-field imaging can resolve the propagation patterns of waveguide modes, which encode the birefringence of transition metal dichalcogenides. We use a laser patterning procedure to write grating structures into 3R-MoS_2 crystals with grooves as sharp as 250 nm. Spatial maps of the scattered electric field in the vicinity of the gratings reveal a directional, polarization-splitting outcoupling of waveguide modes, which is in line with finite element simulations. Experiments over a range of near-infrared photon energies provide key parameters for waveguide second-harmonic generation. The latter is finally demonstrated by grating-coupling femtosecond pulses into the slabs. In the future, nano-optical imaging may be used to directly capture the frequency conversion process during the propagation of the modes. Our work demonstrates the feasibility of compact frequency converters and examines the tunings knobs that enable optimized coupling into layered waveguides.

O 84.3 Thu 11:30 H24

Imaging Infrared Materials Excitations with Sum-Frequency Spectro-Microscopy — •Niclas S. Mueller[1], Alexander Fellows[1], Richarda Niemann[1,2], Andrew E. Naclerio[2], Ryan A. Kowalski[2], Ben John[1], Katayoun Gharagozloo-Hubmann[3], Soeren Wasserroth[1], Guanyu Lu[2,4], Joshua D. Caldwell[2], Piran R. Kidambi[2], Martin Wolf[1], Martin Thaemer[1], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Vanderbilt University, Nashville, TN, USA — [3]Freie Universitaet Berlin, Berlin, Germany — [4]Northwestern University, Evanston, IL, USA

Nonlinear optical microscopy and spectroscopy are powerful tools to characterize interfaces and lower-dimensional materials. Here, I show two examples how we use infrared + visible sum-frequency generation (SFG) to image mid-infrared

materials excitations with wide-field optical microscopy. The techniques provide combined spatial and spectral information, with sub-diffractional spatial resolution. 1. We visualize the propagation of infrared phonon polaritons in a metasurface of silicon carbide [1]. Through a combination of microscopy and spectroscopy, we observe the hybridization and strong coupling of propagating and localized polaritons, as well as the activation of edge states. 2. We visualize monolayers of hexagonal boron nitride, which are usually optically invisible. Resonant infrared excitation of phonons and heterodyne sum-frequency imaging enable us to image, both, the local topography and crystal orientation with unprecedented detail.

[1] Niemann, Mueller et al. Advanced Materials 36, 2312507 (2024)

O 84.4 Thu 12:00 H24

Towards Understanding Surface Restructuring: Automatic Process Exploration and Local Environment Analysis — •Patricia Poths, King Chun Lai, Francesco Cannizzaro, Christoph Scheurer, Sebastian Matera, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

The formation of surface oxides on the Pd(100) surface is a prototypical example of catalyst surface restructuring under *operando* conditions. Despite extensive investigation of this process, its mechanism and corresponding time scales remain unknown. By combining a Machine-Learned Interatomic Potential with our newly-developed Automatic Process Explorer (APE) [1], we study the O-induced restructuring of the Pd(410) vicinal surface as an example for step-edge initiation of oxide formation. We identify ~3,000 unique elementary processes. Taking first steps towards a comprehensive mechanism, we analyze this rich library of processes utilizing a fuzzy classification methodology [2]. Many identified pathways involve non-intuitive complex collective motion of several atoms. These pathways can explain experimentally-observed restructuring, such as step bunching or microfaceting. Furthermore, the time scales of the majority of restructuring pathways are comparable to those of catalytic processes, implying significant coupling between surface restructuring and catalysis [3].

[1] Lai *et al.*, ChemRxiv, DOI:10.26434/chemrxiv-2024-jbzr7 .
[2] Lai *et al.*, J. Chem. Phys. **159**, 024129 (2023).
[3] Poths *et al.*, ChemRxiv, DOI:10.26434/chemrxiv-2024-36l28 .

O 84.5 Thu 12:30 H24

band engineering via metal substitution in porphyrin-graphene hybrid systems — •feifei xiang[1], yanwei gu[2], amogh kinikar[1], nicolò bassi[1], andres ortega-guerrero[1], carlo a. pignedoli[1], giovanni bottari[3], tomás torres[3], klaus müllen[2], pascal ruffieux[1], and roman fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Synthetic Chemistry, Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [3]Departamento de Química Orgánica Universidad Autónoma de Madrid Madrid 28049, Spain

Graphene and its derivatives serve as a versatile platform for finely tuning physical properties across a wide range. Expanding the potential applications of graphene to optoelectronics and gas sensing has driven the development of new materials including hybrid molecular systems that integrate porphyrins with graphene. On-surface synthesis provides a viable approach to achieving such well-defined hybrid structures. Here, we present the synthesis and characterization of porphyrin-graphene hybrid systems (chemrxiv-2024-z9rgh), in which the porphyrin units feature varying metal substitutions. The strong electronic coupling between porphyrin and tailored graphene nanostructures enables the metal center to play a significant role in modulating the band structure through charge doping, and to generate new hybrid states arising from d-π interactions, which allows long range spin coupling between magnetic metal centers. Such robust hybrid molecular systems hold promise in applications in p-n heterojunctions and paves the way towards achieving coherent control of spin chains.

O 85: New Methods: Theory

Time: Thursday 10:30–12:45 Location: H25

O 85.1 Thu 10:30 H25

Quantifying the conductance of molecular structural variables using machine learning — •Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

In single molecule electronics, where individual molecules are placed between two nanoscale electrodes, conductance depends critically on the geometry at the junction. Atomistic simulations using DFT-NEGF are ideally suited to address this, but their computational cost restricts their use to only few junction geometries. In experiments, however, molecular geometry is thought to change significantly since measurements are often carried out at room temperature.

Here we use an approximate method to calculate molecular conductance within DFT for thousands of geometries [1]. The method uses small Au-molecule-Au clusters and is thus computationally very efficient, yet reproduces DFT-NEGF conductance well. Combined with MD simulations of the junction, we compute for thousands of geometries the variation in conductance arising from thermally-induced conformational changes in the molecule.

We use machine-learning methods to identify which of the molecular structural parameters, all of which are changing continuously and simultaneously during the MD simulations, have a greater impact in conductance. This elucidates how molecular conformational changes contribute to the width of the conductance signal in single molecule junctions.

[1] H. Vazquez, J. Phys. Chem. Lett. 13 9326 (2022)

O 85.2 Thu 10:45 H25

Efficient implementation of charge-equilibration schemes for fourth-generation machine learning potentials — •Moritz R. Schäfer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department of Physics, University of Basel, Switzerland

Fourth-generation high-dimensional neural network potentials (4G-HDNNPs) are a modern technique to compute energies and forces with close to ab initio accuracy for conducting extensive molecular dynamics simulations of complex systems. They are based on global information and include long-range charge transfer, electrostatics and atomic energies to describe the interactions in a system. A central component of 4G-HDNNPs is a charge equilibration (Q_{eq}) step, which due to its non-local nature dominates the computational costs. Here, we discuss efficient implementation strategies, and show their performance on selected benchmark systems.

O 85.3 Thu 11:00 H25

Real-time Bethe-Salpeter Equation for optical properties of molecules – Implementation and benchmark calculations — •Štěpán Marek, Maximilian Graml, and Jan Wilhelm — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Regensburg, Germany

We present an implementation of a real-time version of the Bethe-Salpeter equation (RT-BSE) in CP2K, offering new capabilities for investigating electron dynamics in molecules under laser excitation. The RT-BSE implementation is tested on Thiel's molecular benchmark set - a set of organic molecules of various types. We evaluate the accuracy and performance of the RT-BSE approach for the determination of absorption spectra of molecules, with respect to the Casida-BSE approach. We discuss the scaling of the method to show its potential for studying optical properties of large molecules and complex materials.

O 85.4 Thu 11:15 H25

Extension of FLAPW method FLEUR to phonon calculations of polar solids using DFPT — •Friedrich Hanrath[1,2], Thomas Bornhake[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Physics Department, RWTH Aachen University, Aachen, Germany

Phonons play a pivotal role in determining important properties of solids. In polar materials, phononic vibrations are altered by the interaction of macroscopic electric fields in the limit of long wavelengths. This gives rise to the characteristic splitting of longitudinal and transversal optical phonon frequencies. Density function perturbation theory (DFPT) is a state-of-the-art approach to calculate many essential physical properties of solids from first principles. By using an ionic displacement perturbation, it has previously been employed in order to calculate phonons in the framework of the full-potential linearized augmented plane-wave method FLEUR [1, 2]. — In this talk, this method is extended to a macroscopic homogeneous electric field perturbation allowing the calculation of static dielectric properties, Born effective charges and hence LO-TO-splitting. We present the current results for the static dielectric tensor for various semiconductors and insulators by comparing them with experimental results.

This work was supported by the CoE-MaX (EuroHPC JU, Grant No. 101093374) and DFG through CRC 1238 (Project C01).

[1] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de
[2] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).

O 85.5 Thu 11:30 H25

Efficient treatment of long-range electrostatics in charge equilibration approaches — •Kamila Savvidi, Ludwig Ahrens-Iwers, and Robert Meissner — Hamburg University of Technology, Hamburg, Germany

We present a charge equilibration (QEq) method in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) based on real-space Gaussians of width η_i as charge densities. This implementation builds on the `ELECTRODE` package, which already supports Gaussian charge densities [1]. In addition, an efficient particle-particle particle-mesh k-space solver [2] is used, which significantly improves the computational performance compared to existing QEq implementations in LAMMPS. We validate our approach with the test cases of Ti/TiO_x and SiO_2 polymorphs. In the limit of very narrow Gaussians, we were able to show that our algorithm converges to EEM results for the case of Ti/TiO_x. By fitting the Coulomb energy of two isolated Gaussian charge distributions to the repulsion between two Slater-type orbitals, optimized widths for Si and O were obtained that led to results in good agreement to previous studies using STOs instead of Gaussians.

[1] Ludwig J. V. Ahrens-Iwers, Mathijs Janssen, Shern R. Tee, Robert H. Meißner; ELECTRODE: An electrochemistry package for atomistic simulations. J. Chem. Phys. 28 August 2022; 157 (8) [2] Ahrens-Iwers LJV, Meißner RH. Constant potential simulations on a mesh. J Chem Phys. 2021 Sep 14;155(10)

O 85.6 Thu 11:45 H25

Machine Learning for Polaronic Materials: TiO_2(110) at the nanoscale — •Firat Yalcin[1], Simon Trivisonne[1], Viktor Birschitzky[1], Carla Verdi[2], and Michele Reticcioli[1,3] — [1]University of Vienna, Austria — [2]University of Queensland, Australia — [3]CNR-SPIN L'Aquila, Italy

The combination of machine learning (ML) with density functional theory accelerates material simulations, expanding both spatial and temporal scales. However, current ML methods struggle to address polaron trapping. We present a novel machine learning force field (MLFF) approach that incorporates polaron trapping descriptors, enabling large-scale studies of polaronic materials. Using TiO_2(110) as a case study, we reveal how Nb dopants and oxygen vacancies affect polaron configurations and drive catalytic CO adsorption. Additionally, our method captures the dynamic evolution of polarons with unprecedented statistical robustness. This work advances fundamental understanding of defect-polaron interactions while offering a fully-automated and efficient computational suite for the study of polaronic materials.

O 85.7 Thu 12:00 H25

Uncertainty quantification for DFT calculations — •Teitur Hansen[1], Thomas Bligaard[2], and Karsten W. Jacobsen[1] — [1]DTU Physics, Kongens Lyngby, Denmark — [2]DTU Energy, Kongens Lyngby, Denmark

Density functional theory (DFT) is widely used for understanding material properties and chemical reactions. DFT simulations use approximations which result in errors when comparing to experiments. There are errors in different types of energies, lattice constants and other properties. Quantitative uncertainty estimates would be helpful for DFT simulations to highlight which results are trustworthy. Quantifying uncertainties not only improves trust in calculations but also identifies high-uncertainty predictions that can subsequently be revisited and reanalyzed.

We propose a method to model uncertainties using a probability distribution over exchange-correlation functionals. The probability distribution is trained on experimental values of molecular atomization energies, cohesive energies of solids, reactions energies, heat of formations, and lattice constants. The optimized probability distribution is then used to define an ensemble method which can be used to estimate the bias and variance on simulated materials properties. I will demonstrate that the method gives systematic improvements in error estimates over the Bayesian error estimation class of functionals (BEEF).

The proposed method is general enough to be applied to any simulation methodology where accurate reference benchmarks exist.

O 85.8 Thu 12:15 H25

Assessment of the Accuracy of Equation-of-motion Coupled- cluster band gaps in the Bulk Limit — •Evgeny Moerman[1], Alejandro Gallo[2], Andreas Irmler[2], Andreas Grüneis[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI- MPG, Berlin — [2]Institute for Theoretical Physics, TU Wien, Vienna

As a highly regarded theoretical framework in molecular quantum chemistry, coupled-cluster (CC) theory is expected to yield reliable and systematically improvable results for both ground-state and ex cited state properties of materials. One major obstacle to obtaining converged CC results for periodic solids is the often slow convergence with respect to system size. We have investigated the finite-size convergence behaviour of band gaps in equation-of-motion CC (EOM-CC) theory and revealed a direct relation to the GW approximation [1]. Based on these findings, a GW-aided scheme to reliably estimate the size-converged EOM-CC band gap has been developed and tested [2], allowing to assess the true accuracy of the widely used EOM-CCSD method in the periodic case. We find that the accuracy of EOM-CCSD band gaps sensitively depends on the magnitude of orbital relaxation effects, suggesting that such low-order truncation methods as EOM- CCSD may not be sufficiently accurate even for simple materials and that higher orders of correlations seem to be necessary. - This work received support from the European Union's Horizon 2020 research and innovation program under Grant Agreement No.740233.

[1] Moerman et al., arXiv:2409.03721 (2024)
[2] Moerman et al., to be published

O 85.9 Thu 12:30 H25

Full periodic real-time TD-DFTB implementation for solids and low-dimensional materials — •Carlos R. Lien-Medrano[1], Franco P. Bonafé[2], Matías Berdakín[3], Cristián G. Sánchez[4], and Michael Sentef[1,2] — [1]University of Bremen, Bremen, Germany — [2]MPSD, Hamburg, Germany — [3]Universidad Nacional de Córdoba, Córdoba, Argentina — [4]Universidad Nacioanl de Cuyo, Mendoza, Argentina

The current real-time time-dependent density functional tight-binding (TD-DFTB) dynamics implementation in the DFTB+ package [1] employs the length gauge of the electric field. In this work, we introduce an implementation of the vector potential within the velocity gauge framework. This approach enables the extension of real-time dynamics simulations to periodic systems along arbitrary spatial directions, making it applicable to photo-induced dynamical processes in bulk, low-dimensional materials, and surfaces. To demonstrate its potential, we present proof-of-concept applications, including the inhomogeneous optical absorption around the K point in graphene, light absorption in bulk materials, and prospective applications in the field of valleytronics.

[1] Hourahine, B., et al. (2020). DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. The Journal of Chemical Physics, 152(12), 124101.

O 86: Electronic Structure of Surfaces: Spectroscopy, Surface States II

Time: Thursday 15:00–17:30 Location: H2

O 86.1 Thu 15:00 H2

Low temperature STM/AFM detection of 2D electronic gas on reduced $SrTiO_3$ surface — •Akash Gupta, Marcin Kisiel, Remy Pawlak, and Ernst meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Perovskite such as $SrTiO_3$ ubiquitous to host various reconstruction with fine tuning of the annealing temperature. At 1050˚C, in oxygen poor conditions, a $\sqrt{5}\times\sqrt{5}$ surface reconstruction is formed with oxygen vacancies. These oxygen vacancies result in compactly confined electrons as two-dimensional electron gas (2DEG) system. The 2DEG is confirmed as filled surface states in Low Temperature (4 K, UHV) Scanning Tunneling Spectroscopy (STS). Additionally, Image Potential States (IPS) emerges at lower energies than vacuum level, revealing work function, as well. The charging of this 2DEG system can be induced with capacitively coupled tip of Atomic Force Microscope, and it results in giant dissipation peaks as signature of surface charging with change in the tip-sample voltage. Furthermore, quantum capacitance is calculated as function of the gate voltage. The evolution of dissipation peaks were observed with tip-sample distance. The Force-Distance curves confirm the 2DEG charging and is used to determine the tunneling rate of the charging within 2DEG system.

O 86.2 Thu 15:15 H2

Tunneling Spectroscopy of RuO_2(110): Electronic Structure, Correlation Effects and Substrate Interactions — •Philipp Kessler, Andreas Feuerpfeil, Hendrik Hohmann, Matteo Dürrnagel, Armando Consiglio, Jonas Erhardt, Michael Sing, Ralph Claessen, Ronny Thomale, and Simon Moser — Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The (110) surface of RuO_2 hosts a flat band surface state (FBSS) close to the Fermi level that is prone to Fermi surface instabilities and can be readily observed in angle resolved photoemission. A local spectroscopic investigation of this FBSS to study such instabilities is, however, still outstanding. In this talk, we present the synthesis of high quality RuO_2(110) surfaces, enabling systematic scanning tunneling spectroscopy (STS) measurements across wide defect free domains. We observe hints of correlation effects, manifesting in signatures of a charge density wave and a zero-bias anomaly. Furthermore, we offer preliminary evidence suggesting that the electronic structure of RuO_2 depends on the oxide film thickness and immediate screening environment within the substrate. These findings illuminate the interplay between the Ru metal substrate and the RuO_2 oxide, advancing this topical material.

O 86.3 Thu 15:30 H2

Quasi-particle interference studies on ultra-thin films of Cu(111) — •Jungin Yeo — Chung-Ang University, Seoul 06974, Republic of Korea

Recently, ultra-thin crystalline Cu(111) film has been successfully grown on a sapphire substrate through the atomic sputtering epitaxy (ASE). In-depth studies were conducted to explore the crystal growth mechanism and the oxidation process. Ultra-thin film without grain boundary (GB) shows hidden intrinsic nature such as transport by hole carriers. Meanwhile, twin boundaries (TB) appear inevitably during the growth even such an atomically high-quality film. As two orientations adjacent to a TB satisfy the symmetry operation exactly, TBs are expected to show different electronic properties from GBs. The unique electronic properties resulting from the two-dimensional nature and the presence of TBs are currently under investigation. For our study, we utilized scanning tunneling microscopy (STM) to examine 20 nm thick ASE-grown Cu(111) films. The STM topography revealed an atomically flat surface with an indication of twin boundaries. We performed quasi-particle interference (QPI) measurements across TBs. The surface states of Cu(111) and quantum-confined states within the film thickness were successfully resolved. By analyzing the QPI data, we were able to reconstruct the electronic dispersion near the Fermi energy, both at the surface and within the bulk of 20 nm thick. The transmission probability across TBs will be discussed.

O 86.4 Thu 15:45 H2

Electronic structure of the correlated topological metals $CoTe_2$ and $NiTe_2$ — Abhijeet Shelke[1], Chien-Wen Chuang[2], Truc Ly Nguyen[1], Yo-Xun Chen[1], Masato Yoshimura[1], Nozomu Hiraoka[1], Satoru Hamamoto[3], Masaki Oura[3], Chia-Nung Kuo[4], Chin-Shan Lue[4], Atsushi Fujimori[5,1], and •Ashish Chainani[1] — [1]National Synchrotron Radiation Research Center, Hsinchu 300092, Taiwan — [2]Dept. of Physics, Tohoku University, Sendai 980-8578, Japan — [3]RIKEN SPring-8 Center, Hyogo 679-5148, Japan — [4]Dept. of Physics, NCKU, Tainan 70101, Taiwan — [5]Dept. of Physics, The University of Tokyo, Tokyo 113-0033, Japan

The transition-metal(TM) tellurides $CoTe_2$ and $NiTe_2$ are known to exhibit topological semi-metallic Dirac bands from ARPES studies. We carry out core level and valence band measurements using hard x-ray photoemission spectroscopy(HAXPES), x-ray absorption spectroscopy(XAS) and TM $2p-3d$ resonant photoemission spectroscopy(R-PES) to study electronic structure of $CoTe_2$ and $NiTe_2$. The R-PES spectra show clear evidence of TM LVV Auger two-hole correlation satellites. Using the Cini-Sawatzky method, we estimate an on-site Coulomb energy, U_{dd}~3 eV for Co in $CoTe_2$, and U_{dd}~4 eV for Ni in $NiTe_2$. Using these values in charge-transfer cluster model calculations, we simulate the TM $2p$ HAXPES core level and L-edge XAS spectra of $CoTe_2$ and $NiTe_2$. The electronic parameter analyses indicate a negative charge transfer energy Δ for both $CoTe_2$ and $NiTe_2$. The results indicate a p-type metal in terms of the Zaanen-Sawatzky-Allen phase diagram for $CoTe_2$ and $NiTe_2$.

O 86.5 Thu 16:00 H2

Visualizing topological ladder in $PtTe_2$ — •Mohammed Qahosh[1], Gustav Bihlmayer[2], Jakub Schusser[3], Muthu Masilamani[3], Friedrich Reinert[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]PGI-1/IAS-1 Forschungszentrum-Jülich — [3]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg

We have examined the topological ladder [1] and band inversions in $PtTe_2$ using spin-polarized angle-resolved photoemission (spin-ARPES) with two-dimensional momentum imaging. Examining such spin images allows in-depth insight into the topological properties, not accessible by routine methods. We mapped extended momentum-space regions and visualized distinct topological ladder states, notably a surface Dirac cone at $E_B \sim 2.3$ eV, as well as states at $E_B \sim 1.0$ eV, $E_B \sim 1.6$ eV, and near the Fermi level. By comparison to *ab initio* calculations, we demonstrate a significant correlation between the measured and the initial state spin polarization. We discuss interatomic phase shifts [2] for orbitals mixed between Pt and Te sites as well as spin-orbit scattering that leads to additional spin polarization in spin-ARPES. [1] Nature Materials 17, 21 (2018). [2] Phys. Rev. Lett. 130, 146401 (2023).

O 86.6 Thu 16:15 H2

Origin of the Spin-Polarized Fermi Surface of a Tl Bilayer on Ag(111) — •Sven Schemmelmann[1], Yuichiro Toichi[2], Peter Krüger[3], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan — [3]Institut für Festkörpertheorie, Universität Münster, Germany

ARPES measurements have shown that the Fermi surface of a Tl bilayer grown on Ag(111) exhibits two hexagonal-shaped states [1]. While the inner one is fully spin polarized, the outer one appears to be unpolarized. Spin-resolved inverse photoemission experiments of the unoccupied states reveal the origin of this peculiar behavior. We observe two downward dispersing states which are both spin split. The two spin branches of the one state are responsible for the two states observed forming the Fermi surface. Interestingly, the spin up branch coincides with the spin down branch of the other downward dispersing state. This is the reason why this state appears to be unpolarized.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675 (2023)

O 86.7 Thu 16:30 H2

Analyzing excitonic contributions to reflection anisotropy spectra — •Max Grossmann[1], Kai Daniel Hanke[2], Chris Yannic Bohlemann[2], Thomas Hannappel[2], Wolf Gero Schmidt[3], and Erich Runge[1] — [1]Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Fundamentals of Energy Materials, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany

Reflection anisotropy spectroscopy (RAS) is a powerful optical tool for probing semiconductor surfaces. However, the interpretation of RA spectra is challenging due to the complex interplay of features caused by surface states and so-called surface-induced bulk anisotropy, as well as the significant influence of excitonic effects. Overcoming these challenges requires a close collaboration between experiment and theory. In this work, we combine high-quality low-temperature RAS measurements with state-of-the-art *ab initio* calculations in the framework of many-body perturbation theory to study the RAS of arsenic-terminated Si(100) surfaces. The excitonic contributions to the RAS are studied in detail through a thorough analysis of the results from a solution of the Bethe-Salpeter equation. Our approach aims to combine experimental observations with theoretical insights to decipher the complex effects that shape RAS spectra and to advance the understanding of the optical properties of semiconductor surfaces.

O 86.8 Thu 16:45 H2

Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY Hamburg

Beta-phase gallium oxide is a wide-gap semiconductor with a band gap of 4.85eV and promising prospects in high-power electronics. The electric breakdown field can be increased by alloying the oxide with aluminum, further enhancing its properties.

The present work discusses structural and electronic properties of β-$(Al_xGa_{1-x})_2O_3$ thin films and bulk crystals with Al content of up to 33 %. Their Al content was determined by X-ray photo-electron spectroscopy (XPS) and compared to the values estimated from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, the thin films have been investigated by XPS depth profiling, i.e., XPS combined by sequential Ar^+ sputtering, revealing lower aluminum content at the sample surface, which points to possible surface segregation of gallium during annealing. Furthermore, the band gap was determined by electron loss spectra from XPS and optical absorbance measurements and correlated to the Al content estimated for both thin films and bulk crystals.

O 86.9 Thu 17:00 H2

Higher-order van Hove singularities in Kagome metal RbV_3Sb_5 — •Gahee Lee — Department of Physics, Chung-Ang University, Seoul 06974, Republic of Korea

The divergence of the density of states (DOS) near the Fermi energy is crucial for enhancing electron correlations. Van Hove singularities (vHS) commonly cause this DOS divergence, with their properties determined by the dimensionality of electron dispersion. The atomic arrangement on the surface of layered materials can influence the effective dimensionality of electron dispersion, thereby shaping the characteristics of vHS. In V-based Kagome metals RbV_3Sb_5 (A = K, Rb, and Cs), the saddle-shaped dispersion results in two-dimensional vHS. Interestingly, the surface arrangement of atoms in a Kagome lattice can modify the effective dimensionality of electron dispersion, affecting the strength of electron correlations. In this study, we present a novel approach to enhancing electron correlation by arranging the surface Rb atoms. The resulting higher-order vHS significantly enhances the divergence of DOS and strengthens charge density waves in V-based Kagome metals.

O 86.10 Thu 17:15 H2

Single Hemisphere & Time-of-Flight Hybrid Photoelectron Momentum Microscopy — •Olena Tkach[1], Matthias Schmitt[2,3], Deepnarayan Biswas[2], Olena Fedchenko[1], Jieyi Liu[2], Hans-Joachim Elmers[1], Michael Sing[3], Ralph Claessen[3], Tien-Lin Lee[2], and Gerd Schönhense[1] — [1]JGU Mainz, Germany — [2]DIAMOND, Didcot, United Kingdom — [3]Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

The 2ns pulse period of the photon beams from most synchrotrons is too short for pure time-of-flight (ToF) photoelectron spectroscopy. With the use of a hemispherical analyzer (HSA) as a pre-filter, ToF momentum microscopy becomes possible at such high pulse rates. The first hemisphere & ToF hybrid MM

is operated at the soft X-ray branch (photon energies from 105 eV to 2 keV) of beamline I09 at DIAMOND. The HSA reduces the transmitted energy band to typically 0.5 eV, which is then dispersed by ToF recording. In the first experiments the total efficiency gain when switching from the standard 2D (k_x, k_y) to the 3D (k_x, k_y, E_{kin}) hybrid mode was about 25. It is determined by the number of resolved kinetic energies (here 12) and the transmission factor of the electron optics due to the higher pass energy (500 eV) of the HSA in hybrid mode. The α^2- term and the transit time spread due to different path lengths in the HSA are numerically corrected. The performance was validated by studying the well-known electronic structure of Au(111) and Cu(111), including circular dichroism (CDAD) measurements. The high efficiency was exploited in a series of measurements on the Kagome metal CsV_3Sb_5.

O 87: Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy I

Time: Thursday 15:00–17:30 Location: H4

O 87.1 Thu 15:00 H4

Nonlinear plasmonic near– and far fields in the context of Babinet's Principle — •Valentin Dichtl, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth

The third-order nonlinear material response of noble metals enables the formation of the third-harmonic near field around a plasmonic nanostructure [1]. The corresponding spatial emission pattern of the third-harmonic hot spots changes drastically when the fundamental wavelength is slightly tuned over a linear resonance of the nanorod.

However, third harmonic generation (THG) also leads to high temperatures in the structure and its surroundings. These temperatures are usually high enough to destroy more complex samples. Therefore, structures with the same emission properties but a higher ratio of THG to temperature are needed.

To overcome this, we are inspired by the Babinet principle. In this sense, a rod antenna can be replaced by a slit in a thin layer of gold. The surrounding gold should now dissipate heat more effectively than a single rod. This talk compares the (non-linear) emission properties of plasmonic nanostructures and their complementary counterparts, highlighting the applicability of Babinet's Principle.

[1] Wolf, D. *et al.* Shaping the nonlinear near field. *Nat. Commun.* 7:10361 (2016). doi: 10.1038/ncomms10361

O 87.2 Thu 15:15 H4

Beyond-dipole, self-consistent light-matter coupling in plasmonic cavities from first principles — •Franco Bonafe[1], Carlos Bustamante[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]MPI for Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York, USA

The theoretical treatment of light-matter coupling of molecules in complex electromagnetic (EM) environments is key for making progress in the area of modified matter properties in cavities and strong coupling. While several semiclassical methods can treat the coupling of molecules with EM environments, no method has yet considered the combined effects of self-consistent radiative coupling of molecule and environement, and beyond-electric-dipole interactions to account for the effects of inhomogeneous EM fields. This multiscale problem is now possible to address using our full minimal coupling Maxwell-TDDFT framework [1], implemented in the Octopus package. In this talk, we show how the effects of self-consistent light-matter coupling for different systems. On the one hand, we report the spectral Lamb-like shifts of plasmonic dimers described from first principles when radiation-reaction is considered. Moreover, we discuss the effects of transverse and longitudinal field inhomogeneity in the spectral properties of molecules in plasmonic environments described by a Drude response, including retardation effects. Finally, outlooks on self-consistent coupling of electrons, phonons and structured light are discussed. [1] F.P. Bonafé, A. Rubio, H. Appel et al. arXiv:2409.08959v2 (2024)

O 87.3 Thu 15:30 H4

Polarisation-dependent Mie void resonances — •Serkan Arslan[1], Shaban B. Sulejman[2], Sebastian Klein[1], Jonathan Haehner[2], Dominik Ludescher[1], Tim Davis[1,2], Lukas Wesemann[2], Ann Roberts[2], Harald Giessen[1], and Mario Hentschel[1] — [1]Univesity of Stuttgart, 4th Physics Institute, Germany — [2]University of Melbourne, School of Physics & TMOS, Australia

Over the last decade, researchers in nanophotonics have extensively studied the properties and applications of high refractive index dielectric nanoresonators that support subwavelength Mie resonances. Recently, it was demonstrated that similar resonances also occur in wavelength- and subwavelength-sized holes in high refractive index dielectrics, now known as Mie voids. These Mie voids efficiently confine light within air and support resonances spanning from the IR to UV wavelengths, thereby providing a new building block and expanding the parameter space of dielectric nanophotonics.

Until now, only circular Mie voids have been investigated. Here, we present the first study of non-isotropic Mie voids, including elliptical and rectangular shapes. We numerically and experimentally investigate the polarisation dependence of the resonances and reflection spectra, paving the way for polarisation-dependent structural colors and optical security features. Specifically, we demonstrate polarisation-dependent color patterns and micrometer-sized color prints. Anisotropic Mie voids also allow for the design of Mie void metasurfaces based on a generalised geometric phase.

O 87.4 Thu 15:45 H4

Using strong coupling to control plasmonic catalysis — •Jakub Fojt, Paul Erhart, and Christian Schäfer — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Plasmonic excitations decay within femtoseconds, leaving nonthermal (often referred to as "hot") charge carriers behind that can be injected into molecular structures to trigger chemical reactions that are otherwise out of reach – a process known as plasmonic catalysis. In this contribution, we demonstrate that strong coupling between resonator structures and plasmonic nanoparticles can be used to control the spectral overlap between the plasmonic excitation energy and the charge injection energy into nearby molecules. Our atomistic description couples real-time density-functional theory self-consistently to an electromagnetic resonator structure via the radiation-reaction potential. Control over the resonator provides then an additional knob for nonintrusively enhancing plasmonic catalysis, here more than 6-fold, and dynamically reacting to deterioration of the catalyst – a new facet of modern catalysis.

O 87.5 Thu 16:00 H4

Photoemission electron microscopy of Exciton-Polaritons in thin WSe_2 waveguides — •Tobias Eul[1], Victor DeManuel-Gonzalez[1], Miwan Sabir[1], Florian Diekmann[1], Kai Rossnagel[1,2,3], and Michael Bauer[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Ruprecht Haensel Lab, 22607 Hamburg, Germany

Exciton-polaritons emerging from the interaction of photons and excitons in the strong coupling regime are intriguing quasi-particles for the potential exchange of energy during light-matter interaction processes such as light harvesting. This coupling causes an energy anti-crossing in the photon dispersion centered around the exciton resonance, i.e. a Rabi-splitting between a lower and upper energetic branch. The size of this splitting correlates to the coupling strength between the exciton and the photonic modes. In this work, we investigate this coupling between excitons and photonic waveguide modes excited simultaneously in thin-film flakes of the transition-metal dichalcogenide WSe_2. Using a Photoemission electron microscope, we are able to extract the dispersion of the TE- and TM-modes propagating through these flakes as well as extract the energy splitting. Ultimately, our findings precipitate the investigation of the propagation of exciton-polaritons in the time-domain via time-resolved photoemission.

O 87.6 Thu 16:15 H4

Surface-mediated ultra-strong cavity coupling of two-dimensional itinerant electrons — Christian Eckhardt[1,2], Andrey Grankin[3], Dante Kennes[2,1], Michael Ruggenthaler[1], Angel Rubio[1], •Michael Sentef[4,1], Mohammad Hafezi[3], and Marios Michael[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [3]Joint Quantum Institute, Department of Physics, University of Maryland — [4]Institute for Theoretical Physics, University of Bremen

Engineering phases of matter in cavities requires effective light-matter coupling strengths that are on the same order of magnitude as the bare system energetics, coined the ultra-strong coupling regime. For models of itinerant electron systems, which do not have discrete energy levels, a clear definition of this regime is outstanding to date. Here we argue that a change of the electronic mass exceeding 10% of its bare value may serve as such a definition. We propose a quantitative computational scheme for obtaining the electronic mass in relation to its bare vacuum value and show that coupling to surface polariton modes can induce such mass changes. Our results have important implications for cavity design principles that enable the engineering of electronic properties with quantum light.

O 87.7 Thu 16:30 H4

Photoheating nanoscale Pd to temperatures exceeding attached Au nanoparticle antennas — Felix Stete[1], Shivani Kesarwani[2], Charlotte Ruhmlieb[2], Florian Schulz[2], Marc Herzog[1], Holger Lange[1,2], and •Matias Bargheer[1,3] — [1]Universität Potsdam — [2]Universität Hamburg — [3]Helmholtz-Zentrum Berlin

In the non-equilibrium following optical excitation, energy transfer processes at the nanoscale can exhibit extraordinary and surprising phenomena such as heat transport without heating and dominant phonon heat transport in the noble metal gold. Here we present transient absorption experiments on a systematic and well-characterized series of gold nanoparticles with a Pd satellite shell. Modeling the fluence dependence of the entire series of hybrid structures with a fixed set of thermophysical parameters shows that we can create hybrid nanophoto-catalysts that concentrate light energy into the catalytically active Pd. We can make a few Pd satellites efficiently collect nearly all photothermal energy deposited by plasmonically enhanced absorption in gold and heat up the Pd by 180 K while the gold core remains cold. Consequently, highly active catalytic sites emerge which can enhance light driven molecular transformations. The tailoring and modeling of such unexpected nanoscale energy transfer phenomena is backed up by ultrafast x-ray diffraction experiments that provide a material-specific direct measure of the crystal lattice response to energy in phonons and electrons of each material in heterostructures and nanocomposites.

O 87.8 Thu 16:45 H4

Investigation of light-matter coupling in tight binding models — •Jonas Reimann[1,2], Michael Ruggenthaler[1,2], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Center for Computational Quantum Physics, The Flatiron Institute, New York, NY, USA

The theoretical and mathematical foundations for light-matter interactions in a continuum theory are well-established. With the Pauli-Fierz Hamiltonian as the basic building block there is a starting Hamiltonian with all the required properties to study systems containing both matter and light. This can for example be used in the arising field of cavity material engineering where the interplay of light and matter is utilized to design new material properties.

How to imprint these mathematical properties onto tight-binding models describing such materials is at the center of a long-ongoing discussion. A widely deployed approach in this context is the Peierls substitution, coupling light to the hopping elements of the matter Hamiltonian. In this contribution we investigate the reliability of the Peierls substitution in terms of fundamental light-mattter coupling properties within the context of cavity material engineering.

O 87.9 Thu 17:00 H4

Revealing the crystallization dynamics of phase-change materials in vicinity of metallic nanostructures with multiphysics simulations — •Luis Schüler[1,2], Lukas Conrads[2], Sebastian Meyer[2], Yingfan Chen[2], Lina Jäckering[2], Matthias Wuttig[2], Thomas Taubner[2], and Dmitry Chigrin[1,2] — [1]DWI - Leibniz Institute for Interactive Materials, Aachen — [2]I. Institute of Physics (IA), RWTH Aachen University, Aachen

Optical metasurfaces composed of metallic or dielectric scatterers (meta-atoms) promise a powerful way of tailoring light-matter interactions. Phase-change materials (PCMs) are prime candidates for non-volatile resonance tuning of metasurfaces based on a change in refractive index. Precise resonance control can be achieved by locally applying laser pulses to crystallize a PCM, modifying the dielectric surrounding of meta-atoms. However, the complex crystallization kinetics of PCMs in the vicinity of metallic meta-atoms have not been studied yet. Here, we investigate metallic dimer antennas on top of the PCM $Ge_3Sb_2Te_6$ and address these nanoantennas with laser pulses to crystallize the PCM below. Our study reveals inhomogeneous crystallization caused by the absorption and heat conduction of the metallic nanoantennas. A self-consistent multiphysics model, including electromagnetic, thermal, and phase-transition processes, is employed to simulate the crystallization and predict the resulting resonance shift of the antennas. This model enables the optimization of the laser parameters and the geometry of the meta-atoms to achieve an optimal resonance shift, thereby improving the efficiency of metasurfaces.

O 87.10 Thu 17:15 H4

How accurate is the pole expansion of the scattering matrix? — •Elias Fösleitner[1], Adrià Canós Valero[1], Egor Muljarov[2], and Thomas Weiss[1] — [1]Department of Theoretical Physics, University of Graz, Graz, Austria — [2]School of Physics and Astronomy, Cardiff University, Cardiff, United Kingdom

Optical metasurfaces are flat arrangements of nanostructures with different subwavelength sizes and orientations, which allow tailoring the light propagation in a layer of subwavelength thickness. Such metasurfaces are often described using their resonant states. These states, also known as quasi-normal modes, serve as the foundation for the pole expansion of the optical scattering matrix, providing a more efficient and insightful alternative to conventional full-wave simulations. Existing formulations of such an expansion have, however, limitations, particularly in terms of accuracy, efficiency, and convergence. The aim of this study is to compare different approaches for pole expansions and identify their advantages and limitations. Moreover, we discuss how the choice of basis functions of the scattering matrix influences its complex pole structure and the resulting pole expansion. Overall, these findings will allow for a faster prediction of optical properties by choosing the best suited resonant expansion and also provide additional insight that is necessary for many applications such as nanophotonic sensors.

O 88: 2D Materials: Stacking and Heterostructures (joint session O/HL)

Time: Thursday 15:00–17:45 Location: H6

O 88.1 Thu 15:00 H6

Systematic Study of Interlayer Interactions in Transition Metal Dichalcogenide Bilayers Using microARPES — •Thomas Nielsen[1], Chakradhar Sahoo[1], Alfred Jones[1], Zhihao Jiang[1], Kenji Watanabe[2], Takashi Taniguchi[2], Suman Chakraborty[4], Prasana Sahoo[4], Jill A. Miwa[1], Yong P. Chen[1,3], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan — [3]Department of Physics, Purdue University, USA — [4]Materials Science Centre, Indian Institute of Technology, India

Stacked transition metal dichalcogenide monolayers are emerging as a platform to study correlated phases such as Mott insulators or Wigner crystallization. Spatially resolved ARPES can potentially visualize the moiré bands and hybridization effects in the electronic structure underpinning these correlated phases. Observing these phenomena in ARPES in a reproducible way remains challenging, motivating systematic studies of interlayer interactions in twisted TMD bilayers. 20 different heterobilayers of WSe_2, WS_2, $MoSe_2$, and WS_2, as well as homobilayers of WSe_2 are fabricated with varying twist angles. Their electronic properties are measured using the microARPES branch at the ASTRID2 synchrotron at Aarhus University. Band alignments and hybridization effects are tracked as a function of material composition and twist angle. The used dry-transfer fabrication techniques do not yield the direct observation of flat bands from moiré effects in the valence band. Based on this work future avenues for reproducibly attaining moiré effects in photoemission from TMDs are discussed.

O 88.2 Thu 15:15 H6

Gate-Tunable miniband dispersion in twisted graphene superlattices near the magic angle measured with MicroARPES — •Alfred J. H. Jones[1], Zhihao Jiang[1], Dongkyu Lee[2], Youngji Park[2], Kimberly Hsieh[1], Paulina Majchrzak[1], Chakradhar Sahoo[1], Thomas S. Nielsen[1], Kenji Watanabe[3], Takashi Taniguchi[3], Philip Hofmann[1], Jill A. Miwa[1], Yong P. Chen[1,4], Jeil Jung[2], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, University of Seoul, Korea — [3]National Institute for Materials Science, Japan — [4]Department of Physics and Astronomy, Purdue University, USA

Twisted superlattices of mono- and bilayer-graphene are emerging as powerful tools to explore quantum many-body effects such as unconventional superconductivity and Mott insulating states. Access to the momentum-resolved electronic structure simultaneous to changing the carrier concentration and displacement field within a twisted superlattice device can directly provide key information on the miniband dispersion tunability that underpins the correlated phenomena.

Here, we present microARPES measurements from SGM4 at ASTRID2 on two-terminal "near-magic-angle" twisted bilayer (TBG) and double-bilayer graphene (TDBG) devices. Our findings for the two systems are strikingly different: On TBG, we find a filling factor-dependent bandwidth change of the flat moiré bands, whereas on TDBG the effect of tuning the doping and displacement field leads to non-monotonous bandwidth changes and tunable gap opening effects.

O 88.3 Thu 15:30 H6

Topological magnetic Moiré heterostructures — •Aymeric Saunot[1,3], Sebastien E. Hadjadj[2], Tonica Valla[1], Maxim Ilyn[3], and Ilya I. Klimovskikh[1] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastían, Basque Country, Spain. — [2]Materials Physics Center (MPC), Paseo Manuel de Lardizabal N5,b20018 Donostia, Spain. — [3]Departamento de Física de Materiales UPV/EHU, San Sebastían, Spain.

Over the last few years Moiré superlattices have become a hot topic in condensed matter, thanks to the experimental success of magic angle twisted graphene. Moiré superpotentials arise from either twist or atomic mismatch at the interface between van der Waals materials, leading to a rich physics of strongly correlated electrons. Intriguingly, creation of Moiré pattern on the surface of 3D topological insulator (TIs) is theoretically expected to lead to, among others, topological superconductivity, high Chern number systems and non-trivial magnetic textures.

Here, we present Moiré heterostructures made from 3D TIs and novel 2D magnetic insulators transition metal dihalides. We investigate the heterostructure's surface by means of STM, ARPES, XMCD, and LEED. Our results show that the Moiré periodicity and the symmetry of the potential, can be tuned based on the ratio between the lattice parameters of the heterostructure's layers. Band structure measurements excitedly show the main Dirac cone surrounded by several Dirac cone replicas creating new Dirac minicones at the crossing points, opening a whole new platform to study topological Moiré physics.

O 88.4 Thu 15:45 H6

SNOM of lateral TMDC heterojunctions — •Philipp Schwendke[1], Samuel Palato[1], and Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG

Two transition metal dichalcogenide monolayers, joined together laterally, form a one-dimensional heterojunction where charge transfer with associated space charge region and current rectification have been shown experimentally [1]. Furthermore, there are unique local electronic properties determining the excitonic response in the boundary region. Nanoscale spectroscopic methods are needed for the observation of such local optical properties. We use scanning near-field optical microscopy (SNOM) in combination with a continuous wave (cw) light source at 633 nm, as well as a pulsed laser tunable in a wide range from 250 nm to 1300 nm. We employ pseudo-heterodyne modulation for noise suppression and optical phase information, and quadrature-assisted discrete demodulation in order to use the tunable light source at kHz repetition rates. Resonant SNOM measurements show a quenching near the WS_2-MoS_2 boundary, which can be indicative of local energy shifts or electronic states specific to the boundary region. This is complementary to previous measurements which show quenching of photoluminescence [2], attributing it to exciton recombination. In addition, the agreement of results acquired with cw and pulsed light sources paves the way towards time-resolved near-field measurements.

[1] Li et al., Science, vol 349, p 524 (2015)
[2] Chou et al., Nanoscale, vol 14, p 6323 (2022)

O 88.5 Thu 16:00 H6

Charge density wave interactions in bilayer 1T-TaSe2 — •Robert Drost, Ziying Wang, Büşra Arslan, Adolfo Fumega, Jose Lado, and Peter Liljeroth — Aalto University, Department of Applied Physics

Van der Waals materials offer splendid opportunities for quantum material engineering through stacking and heterostructure formation. While well-proven for many essential two-dimensional materials, these techniques are less explored for correlated materials. The 1T phase of TaSe2 is a two-dimensional Mott insulator and and excellent model system for correlations in reduced dimensions. The correlation gap in 1T-TaSe2 is highly sensitive to the thickness of the material, suggesting that electron-electron interactions between the charge density waves play an important role in determining the electronic properties of few-layer TaSe2. We also observe and additional site dependence of the gap size, showing that the stacking order may be equally important. These effects hint at the possibility of using charge density wave stacking as a design element in new quantum materials.

O 88.6 Thu 16:15 H6

Giant Zeeman effect at a magnetic topological van der Waals interface — Tobias Wichmann[1,2], Keda Jin[1,3], Jose Martinez-Castro[1,3], Tom G. Saunderson[4,5], Honey Boban[6], Lukasz Plucinski[6], Yuriy Mokrousov[4,5], Markus Ternes[1,3], F. Stefan Tautz[1,2], and •Felix Lüpke[1,7] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]Institut für Experimentalphysik IV A, RWTH Aachen University — [3]Institut für Experimentalphysik II B, RWTH Aachen University — [4]Institute of Physics, Johannes Gutenberg University Mainz — [5]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich — [6]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [7]II. Physikalisches Institut, Universität zu Köln

We report giant Zeeman effects with Landé g-factors up to $g \approx 230$ at the interface of graphene and the van der Waals (vdW) ferromagnet Fe_3GeTe_2 (FGT). They arise from orbital moments generated by the non-trivial band topology of the FGT and cause a huge asymmetric level splitting when a magnetic field is applied. By exploiting the inelastic phonon gap of graphene, we can directly access the vdW interface to the FGT underneath by scanning tunnelling microscopy and spectroscopy. By analyzing the Faraday-like screening of the tunnelling tip by the graphene, we are able to quantify the electric field at the vdW interface.

O 88.7 Thu 16:30 H6

Nanoscale band-gap modulation and dual moiré superlattices in the weakly-coupled h-BN/graphite heterostructure — Fábio J. R. Costa[1,2], Luiz F. Zagonel[1], Tin S. Cheng[3], Jonathan Bradford[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergei V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Klaus Kuhnke[2], Klaus Kern[2,6], and •Anna Rosławska[2] — [1]Unversity of Campinas, Brazil — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Nottingham, United Kingdom — [4]Laboratoire Charles Coulomb, Montpellier, France — [5]Institut Universitaire de France, Paris, France — [6]EPFL, Lausanne, Switzerland

Van der Waals materials, such as hexagonal boron nitride (h-BN), and their heterostructures are highly promising for novel nanophotonic and electronic devices. In such stacks, moiré patterns arise and modulate the electronic properties of the material at the scale of typical superstructure periods (approx. 10 nm), and as such are challenging to probe. Here, we investigate the moiré superlattices in the weakly coupled h-BN/graphite heterostructure at the atomic scale. Scanning tunneling microscopy (STM) imaging reveals extensive moiré unit cells on the surface, while spectroscopic measurements demonstrate significant modulation in the work function and band gap across the periodic supercell. Additionally, we identify a dual moiré superlattice in twisted bilayers of h-BN on graphite, providing an extra degree of freedom to tune the heterostructure's properties.

O 88.8 Thu 16:45 H6

Impact of point defects and grain boundaries on sulfur diffusion and memristive properties of MoS_2 single sheets — •Aaron Flötotto[1], Jules Oumard[1], Benjamin Spetzler[2], Martin Ziegler[2], Erich Runge[1], and Christian Dressler[1] — [1]Technische Universität Ilmenau, Germany — [2]Christian-Albrechts-Universität zu Kiel, Germany

The memristive properties of transition metal dichalcogenides, such as MoS_2, are currently the subject of intense research and have recently been traced back to the dynamics of sulfur vacancies [1, 2]. In this theoretical work, we employ molecular dynamics to determine the sulfur vacancy diffusion coefficients in the vicinity of various point defect structures and grain boundaries in single sheet MoS_2. To address the necessity of large cell sizes and long time scales, we utilize machine learning force fields, applying both Gaussian approximation potential and equivariant graph neural networks. We then compare the accuracy of these force fields and discuss the results in regard to the memristive properties of MoS_2. Our findings indicate a reduction in energy barriers for sulfur vacancy diffusion as the size of vacancy clusters increases and highlight the importance of certain interstitial sites in these vacancy clusters.

[1] Li, D., et al. (2018). ACS Nano, 12(9), 9240-9252. doi.org/10.1021/acsnano.8b03977
[2] Spetzler, B., et al. (2024). Adv. Electron. Mater., 10, 2300635. doi.org/10.1002/aelm.202300635

O 88.9 Thu 17:00 H6

Machine-Learning the Electronic Structure of Twisted Bilayer Graphene — •Lenz Fiedler[1], Agnieszka Kuc[1], Florian Arnold[2], and Attila Cangi[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Dresden, Deutschland — [2]Technische Universität Dresden, Dresden, Deutschland

Twistronics, i.e., the study of twodimensional materials in which individual layers are twisted w.r.t.öne another, has the potential to significantly propel technological progress. Twisted bilayer materials, e.g., graphene, may exhibit a significant change in electronic structure and electrical properties based on twist angle. Their computational treatment with density functional theory (DFT) proves difficult, as small twist angles affect the periodicity of the cell and can only be simulated with large unit cells. In this talk, the recently introduced Materials Learning Algorithms (MALA) - a framework for accelerating DFT calculations based on machine learning - is applied to twisted bilayer graphene. Bilayer graphene serves as a proxy for the larger field of twistronics itself. It is shown how the electronic structure, including electronic density of states and electronic charge density, can be predicted from a small number of twist angles for a range of twisted bilayer graphene structures. Since the MALA framework uses the local density of states to encode the electronic structure on a numerical grid, predictions can be made on much larger length scales than with standard DFT calculations. This work demonstrates how machine learning can be used to computationally model twisted bilayer structures where standard first-principles methods are not viable.

O 88.10 Thu 17:15 H6

High-throughput *ab initio* screening of 2D heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], Roman Kempt[1], and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Duke University, Durham, USA

Heterostructure interfaces produced by stacking two-dimensional (2D) materials facilitate the development of advanced electronic functionalities down to the atomic level. The efficient autonomous creation and computational study of these systems is, however, a challenge due to the general incommensurability of the 2D monolayers. This often results in large unit cells with hundreds to thousands of atoms.

Here, we present an extensive *ab initio* screening of heterostructures made of 2D systems. The approach makes use of the AFLOW-Hetbuilder – a newly developed tool that automates the heterotructure generation based on coincidence lattice theory [1,2]. It is fully integrated into the AFLOW framework [3,4]. We study the binding energy of a large set of heterostructures and also analyse their structural, electronic, and magnetic properties [5]. The presented efficient workflow can enable the systematic data-driven design of 2D heterostructures.

[1] D. S. Koda *et al.*, J. Phys. Chem. C **120**, 10895 (2016).

[2] https://zenodo.org/record/4721346.
[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[4] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[5] A. Nihei *et al.*, manuscript in preparation (2024).

O 88.11 Thu 17:30 H6

Size-Dependent Diffusion of Radioactive Alcohols Through CNMs — •Neita Khayya, Andre Beyer, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Conventional membranes frequently struggle to achieve both, high permeance and high selectivity. On the other hand, two-dimensional membranes demonstrated remarkable progress. For example, nanometer-thin carbon nanomembranes (CNMs) from self-assembled monolayers of terphenylthiol molecules combine rapid water permeation with a rejection of ethanol in pressure-driven experiments as well as ultrahigh ionic exclusion in ion conductivity measurements. Although there has been great progress in understanding the distinctive characteristics of CNMs, more work is required to fully understand their transport characteristics, which requires complementary approaches. In this work, we employed the radio-active tracer diffusion method to study the size-depended concentration-driven permeation of different alcohols, namely [14C] CnH2n+1OH (n = 1*3) through thickness-varied CNMs from biphenylthiol (BPT), terphenylthiol (TPT) as well as quaterphenylthiol (QPT) molecules. Our findings align with vaporous alcohol pressure-driven permeation measurements regarding the size exclusion through CNMs. Interestingly, our results indicate an increased permeation rate in the liquid phase, which can be rationalized by hydrogen bonds created inside the membrane between the water molecules and diffused alcohols.

O 89: Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Thursday 15:00–17:45 Location: H8

O 89.1 Thu 15:00 H8

From Unit Cells to Diffraction Patterns: `celltools`, a Python Toolkit for Structural Modeling — •Sebastian Hammer[1] and Bradley J. Siwick[2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Departments of Physics and Chemistry, McGill University, Montreal H3A 0B8, Canada

The coupling of lattice and electronic system crucially determines the properties of modern materials. This interaction is at the heart of many emergent phenomena, such as charge-density wave formation, polaron dynamics, and transient metal-insulator transitions, which have peaked the interest of researchers.

While electronic properties can often be reliably described by quantum chemical methods, capturing structural changes is computationally more demanding. Hence, diffraction experiments are the usual method of choice to investigate structural distortions. However, extracting atomic positions from diffraction data is tedious and not straight forward.

In this contribution, I introduce the python package `celltools`, a versatile tool for constructing and manipulating unit cells as well as simulating their diffraction patterns. Using the case study of excimer formation in the prototypical molecular semiconductor zinc-phthalocyanine investigated with ultra-fast electron diffraction [1], I demonstrate how this tool enables the extraction of momentary atomic position from time-resolved diffraction datasets.

[1] S. Hammer *et al.*, *PNAS* (2024)

O 89.2 Thu 15:15 H8

Automation of data acquisition and measurement evaluation in LEED $I(V)$ — •Florian Dörr[1], Michael Schmid[1], Lutz Hammer[2], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Solid State Physics, FAU Erlangen, Germany

We designed a system capable of acquiring and evaluating quantitative low-energy electron diffraction [LEED $I(V)$] data, the Vienna Package for Erlangen LEED (ViPErLEED). The system contains three parts: One part performs data acquisition and is discussed in this contribution. The other two parts focus on the extraction of LEED-$I(V)$ curves from image series [1] and simulation of $I(V)$ spectra for quantitative structure optimization [2].

The data acquisition package consists of open-source hardware for controlling the LEED electronics and software for calibration and the actual measurements. Compared with previous solutions, the package contains functions that improve data quality, such as low-noise measurement of the beam current I_0, automatic calibration of the beam energy, and analysis of the response time of the LEED controller. On the image acquisition side, the software corrects for deficiencies of the camera, such as hot or dead pixels. We will discuss issues that affect the accuracy and duration of LEED-$I(V)$ measurements; this is especially important for sensitive samples that easily degrade.

[1] https://doi.org/10.48550/arXiv.2406.18413
[2] https://doi.org/10.48550/arXiv.2406.18821

O 89.3 Thu 15:30 H8

X-ray reflectivity of μm-samples — •Steffen Tober[1], Wieland Corts[1,2], Steven Leake[3], Toka Matar[1,2], Lisa Randolph[1], Breno Saraiva[4,5], Vedran Vonk[4], Andreas Stierle[4,5], and Hans-Georg Steinrück[1,2] — [1]Forschungszentrum Jülich, Institute for Sustainable Hydrogen Economy (INW), Jülich — [2]RWTH Aachen, Institute of Physical Chemistry, Aachen — [3]ESRF, Grenoble — [4]Deutsches Elektronen-Synchrotron (DESY), Centre for X-Ray and Nanoscience (CXNS), Hamburg — [5]University of Hamburg, Physics Department, Hamburg

X-ray reflectivity (XRR) non-destructively probes electron density profiles of surfaces and interfaces with sub-nm resolution. Large beam footprints in grazing-incidence geometries commonly limit XRR to mm-sized, flat samples because the beam spillover for smaller samples significantly reduces the signal to noise ratio. To probe samples such as individual particles in electrodes or catalysts, a significant reduction of the footprint is needed. As demonstrated for crystal truncation rods [1], the nm-sized X-ray beams of modern synchrotron sources can be used for XRR on μm-sized samples with reduced footprint. We present first proof-of-principle studies comparing XRR of mm- and μm-sized thin-film samples measured with 80 and 400 nm X-ray beams at ESRF ID01 and the necessary optimisation of alignement- and scan procedures [2]. Our results show the general feasibility of nm-beam XRR to be adapted for future *in situ/operando* studies.

[1] J. Stubbs et al., Clays Clay. Miner. 69, 688 (2021)
[2] S. J. Leake et al., J. Synchrotron Rad. 26 571 (2019)

O 89.4 Thu 15:45 H8

How a quartz crystal microbalance reacts to a thermal load — Martina Fellinger[1], Eduardo Pitthan[2], Christian Cupak[1], Friedrich Aumayr[1], Daniel Primetzhofer[2], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Department of Physics and Astronomy, Uppsala University, Sweden

The most common technique for measuring deposition rates in vacuum is the quartz crystal microbalance (QCM). QCMs are also employed for the determination of sputter yields; further applications are in chemistry and biology. In all these applications, the response of the resonance frequency f to temperature is important. Apart from the crystal's sensitivity to a homogeneous temperature [the $f(T)$ curve], the influence of the thermal stress on the frequency has to be taken into account. In contrast to standard AT-cut crystals, SC-cut (stress-compensated) crystals are insensitive to radial stress. Therefore, SC-cut crystals are used for high-precision measurements or if the power dissipated on the crystal is high (e.g., for sputter yield measurements). Nevertheless, stress effects must be taken into account if the heat source is not exactly centered. The static $f(T)$ response and the effects of local heating, including stress effects, lead to a superposition of a fast response (within $\lesssim$ 1 s) and a slow frequency change over several minutes; the latter being related to the thermal resistance between the crystal and the crystal holder. Examples of finite-element simulations for a localized heat source will be shown and compared to experimental data of SC-cut crystals irradiated by MeV ions with up to 70 mW power, causing a temperature increase by up to 100 K.

O 89.5 Thu 16:00 H8

Bilayer Formation of Tl on Ag(111): Spatial and Electronic Structural Insights — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan

Ultrathin thallium films on Ag(111) have become a model system for studying the spatial and electronic properties of atomic-layer systems [1-3]. In this study, we focus on investigating the formation of bilayer Tl on Ag(111), leveraging Auger electron spectroscopy, low energy electron diffraction (LEED), and inverse photoemission (IPE) to investigate both spatial and electronic structure. LEED studies indicate that the Tl layers are rotated with respect to the substrate, with the angle of rotation depending on the Tl coverage and deposition temperature. Furthermore, IPE measurements reveal distinct unoccupied electronic states for both the monolayer and the bilayer. With increasing deposition time, the intensity of the monolayer-related state is reduced, while the intensity of the bilayer-related state increases. These results provide insight into the bilayer growth mechanism of Tl on Ag(111) and offer experimental criteria for differentiating between mono- and bilayer.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)

[2] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[3] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)

O 89.6 Thu 16:15 H8

Capping of terbium silicide nanostructures on Si(111) — •Markus Bachler[1], Milan Kubicki[1], Hüseyin Çelik[2], Sören Selve[3], Martin Franz[1], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623, Germany — [3]Zentraleinrichtung Elektronenmikroskopie (ZELMI), Technische Universität Berlin, 10623, Germany

Rare earth silicide films on Si surfaces are of great interest because of their appealing properties, such as extremely low Schottky barrier heights on *n*-type Si, abrupt interfaces, and the formation of two- and three-dimensional films or one-dimensional nanowires. However, a protective layer is required for further utilisation of these properties, and capping by Si has the further advantage of no lattice mismatch to the substrate and the opportunity to form three-dimensionally stacked nanostructures. For this purpose, rare earth silicides on Si(111) with their very low to no lattice mismatch to Si are very promising for epitaxial capping.

Here we studied capping of thin Tb silicide layers on the Si(111) surface with Si by using scanning tunneling microscopy, cross-sectional high-resolution transmission electron microscopy as well as cross-sectional scanning transmission electron microscopy with energy dispersive X-ray analysis. We observed that overgrowth of the Tb silicide layers with amorphous and crystalline Si leads to intact double layers, demonstrating the stability of the Tb silicide layer upon capping.

O 89.7 Thu 16:30 H8

Exploring surface properties of hexagonal Si and Ge — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1,3] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Sultan Qaboos University, Muscat, Oman — [3]Ruhr Universität Bochum, Germany

We present ab initio calculations, using density functional theory in a slab geometry, that explore structural and electronic properties of the surfaces of hexagonal silicon and germanium, which are novel materials for active optoelectronic applications. We study the relaxed 1 × 1 a, m, c and r-plane facets, who's surface energies allow the creation of Wulff constructions of Si and Ge nanocrystals and wires. Our focus lies on understanding surface stability and its implications on material and device design, as well as the effects of the relaxation on the electronic properties. The comparison with experimental findings offers practical insights for substrate selection for thin film growth and the construction of heterostructures.

O 89.8 Thu 16:45 H8

Strong electron doping of single-layer MoS_2 on an oxidized contact — •Marco Bianchi[1,2], Charlotte Sanders[3], Davide Curcio[4], Daniel Lizzit[5], Paolo Lacovig[1], Ezequiel Tosi[6], Jill Miwa[2], Silvano Lizzit[1], and Philip Hofmann[2] — [1]Elettra Sincrotrone Trieste S.C.p.A., Trieste, IT — [2]Dep. of Physics and Astronomy, iNANO, Aarhus University, DK. — [3]Artemis Program, UK Central Laser Facility, Harwell, STFC, UK — [4]IOM, Consiglio Nazionale della Ricerca, Trieste, IT — [5]DPIA - University of Udine, IT — [6]Instituto de Ciencia de Materiales de Madrid (ICMM - CSIC), ES

One of the major obstacles for the use of two-dimensional semiconductors in devices continues to be the high contact resistance to metallic conductors and the associated losses. Promising results have recently been obtained by using group V semimetals as contact materials. The obtained low contact resistance was explained partly by the a degenerate doping of the two-dimensional semiconductor. Here we study the band alignment and structure of such a system, a single-layer of MoS_2 on Au(111) with an intercalated layer of Bi. We investigate the electronic structure and growth by angle-resolved photoemission spectroscopy, X-ray photoemission spectroscopy, low energy electron diffraction and scanning tunneling microscopy. Our results show no evidence for an occupation of the MoS_2 conduction band when the material is brought into close contact with Bi. Surprisingly, however, a subsequent oxidation of the intercalated Bi gives rise to an extremely strong electron doping of the conduction band with a carrier density on the order of 10^{13} cm^{-2}.

O 89.9 Thu 17:00 H8

Growth of two-dimensional Ta-S structures from TaS_3 nuclei to TaS islands — •Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Abdus Samad[2], Udo Schwingenschlögl[2], Carsten Busse[1], and Thais Chagas[1] — [1]Department Physik, Universität Siegen, D-57072 Siegen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia

Transition metal dichalcogenides (TMDCs) are emerging as promising 2D materials, known for their unique physical and electronic properties. Despite the rapid growth of research in this field, the exact mechanisms governing their growth remain largely speculative, especially when compared to more well-understood systems, such as metal-on-metal growth.

In this study, we employ Scanning Tunneling Microscopy (STM) to investigate the growth process of ultrathin tantalum sulfide (Ta-S) phases. We observe the evolution from embedded TaS_3 nuclei to Ta_3S_6 islands, and ultimately to TaS islands. These findings provide new insights into the growth dynamics of Ta-S phases, revealing the underlying processes.

Furthermore, these structural observations are supported by Density Functional Theory (DFT) calculations, which compare the energies of various structures, offering additional validation of the experimental results.

O 89.10 Thu 17:15 H8

Ab initio surface phase diagram of $(Al_xGa_yIn_{1-x-y})_2O_3$ — •Qaem Hassanzada[1], Yuanyuan Zhou[1,2], and Matthias Scheffler[1] — [1]The Fritz Haber institute, Berlin, Germany — [2]The Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Group III sesquioxides with ultra-wide bandgaps are the most promising candidates for high-power electronics. Numerous efforts have been made to grow group-III sesquioxides, however, the fundamental understanding of growth process is still shallow. The prerequisite to understand growth process is detailed information about the surface geometry and stoichiometry under growth conditions. This can be provided in surface phase diagrams. In this study, we explore the surface phase diagram of Group III sesquioxides, $(Al_xGa_yIn_{1-x-y})_2O_3$, for the entire compositional range, using ab initio atomistic thermodynamics [1, 2] and the sure-independence screening and sparsifying operator (SISSO) [3] machine learning methods. We predict the most probable phases under the corresponding growth conditions. For instance, in the Ga-rich region, we predict the formation of a Ga monolayer, which may be related to the experimental hypothesis of Ga adlayer formation at a lower O/Ga ratio [4] reminiscent of the phenomena in GaN.

[1] Scheffler, M. Studies in Surface Science and Catalysis, Vol. 40; Elsevier: 1988, pp 115−122. [2] Reuter, K.; Scheffler, M. Phys. Rev. B 2001, 65, 035406. [3] Ouyang, R. et al. M. Phys. Rev. Mater. 2018, 2, 083802. [4] Chou, T. et al. AIP Advances 2021, 11, 115323.

O 89.11 Thu 17:30 H8

Ultrathin NiO(100) films on Ag(100): Pitfalls in understanding growth using intensity-voltage low-energy electron diffraction — •Jan Lachnitt[1], Shuvankar Das[2], Krishnakumar S. R. Menon[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Surface Physics & Material Science Division, Saha Institute of Nuclear Physics, Kolkata, India

Ultrathin NiO films have prospective applications in heterogeneous catalysis, microelectronics, and spintronics and are thus an object of active research. In model systems, the Ag(100) surface is frequently used as support for these films, as its cubic lattice parameter is only 2.2% smaller than that of NiO, enabling pseudomorphic growth for very small thicknesses. Interestingly, the early-stage growth of NiO films on Ag(100) turns out to be complex compared to other simple oxide systems, such as MgO/Ag(100). We have grown pseudomorphic NiO(100) films of well-defined average thickness in steps of 0.5 monolayer (ML), up to 3 MLs, and studied them with intensity-voltage low-energy electron diffraction (IV-LEED). We have also employed density-functional theory (DFT) calculations to gain additional insights. Our IV-LEED results indicate a deviation from layer-by-layer growth, expected to take place from 2 MLs onwards [1], and the detailed analysis of the oxide-metal system has turned out to be tricky. We discuss the pitfalls and limitations of common IV-LEED procedures and compare the results with our DFT calculations and existing literature.

[1] J. Wollschläger et al., Thin Solid Films 400 (2001) 1.

O 90: Spins on Surfaces at the Atomic Scale II

Time: Thursday 15:00–17:30 Location: H11

O 90.1 Thu 15:00 H11

Relativistic Orbital Effects in Hyperfine Splittings on Surfaces — •Katharina Lorena Franzke, Wolf Gero Schmidt, and Uwe Gerstmann — University of Paderborn Warburger Str. 1 33098 Paderborn

The recent combination of electron spin resonance and scanning tunneling spectroscopy (ESR-STM) provide a new platform to access single spins of atoms and molecules on surfaces [1, 2]. Characteristic hyperfine (hf) splittings due to the interaction between the electronic spin and the magnetic moments of the nuclei can be measured and compared with theoretical predictions from density functional theory (DFT). In comparison with defects in bulk material, however, the calculated data deviates considerably from the experimental values. Limited accuracy of the xc functionals or the direct influence of the electric field of the STM-tip have been discussed as possible reasons.

Large parts of the observed discrepancies however stem from a relativistic effect, the suppression of orbital quenching at surfaces. We developed a fully relativistic method that allows the calculation of this orbital contribution for complex structures [3]. For Pb ions as well as PbPc molecules on the MgO/Ag(111) substrate, this orbital part leads to additional hf splittings in the GHz range and is thereby required to achieve overall accuracy in predicting the hf interactions of single spins in 2D nanostructures.

[1] S. Baumann, et al., Science 350, 417 (2015) [2] L. Farinacci et al., Nano Letters 22, 8470 (2022) [3] K.L. Franzke, et al. J. Phys.: Conference Series. 2701, 012094 (2024)

O 90.2 Thu 15:15 H11

Electric Control of Molecular Spins on a Surface — •Paul Greule[1], Wantong Huang[1], Máté Stark[1], Kwan Ho Au-Yeung[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Christoph Wolf[2], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Korea

Single electronic spins hosted by atoms or molecules are candidates for future quantum technologies. To utilize them as functional building blocks in quantum information processing it is necessary to gain local control of their quantum properties. Lately, electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) was demonstrated as a versatile method to access atoms and molecules on a surface [1]. For single Ti atoms it was shown that the Zeeman energy of electron spins can be tuned via the applied bias voltage in the tunnelling junction [2] constituting an atomic-scale electric field control. In our work, we present a voltage-dependent shift of the ESR frequency for two different molecular spin systems, Iron-phthalocyanine (FePc) and FePc-Fe ferrimagnet complexes. Intriguingly, we observe a strong non-linearity in the shift connected to the molecular orbital of FePc. We rationalize this theoretically by many-body interactions with the exchange bias field of the tip. Moreover, we show how the bias voltage control can be used to detune Rabi oscillations in pulsed ESR experiments. [1] Y. Chen et al., Adv. Mater. 2022, 2107534 [2] P. Kot et al., Nat Commun 14, 6612 (2023)

O 90.3 Thu 15:30 H11

Coherent control of a single Er electron spin on surface — Dasom Choi[1,2], Yaowu Liu[1,3,4], Stefano Reale[1,3], Jeongmin Oh[1,2], We-hyo Seo[1,3], Andreas Heinrich[1,2], Soo-hyun Phark[1,3], and •Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Korea — [2]Physics Department, Ewha Womans University, Korea — [3]Ewha Womans University, Seoul, Korea — [4]Department of Energy, Politecnico di Milano, Milano, Italy

Electron spins on surface provide an atomic scale qubit platform for quantum information science using scanning tunneling microscopy (STM) [Phark et al. ACS Nano 17, 14144 (2023), Wang et al. Science 382, 87 (2023)]. A bottleneck of this new platform lies in the decoherence stemming from the strong interaction with the environments. Lanthanide atoms, with their highly localized 4f electrons, offer a potential solution to this issue and make them as strong candidates of single atomic spin qubits on surfaces with a high quality factor $Q = 2\Omega T_2$ (Ω = Rabi rate, T_2 = coherence time). In this talk, we present a recent advance in the qubit quality factor, achieved using erbium (Er) atoms on a MgO surface [Reale et al. Phys. Rev. B 107, 045427 (2023)]. We performed a coherent control of the Er atoms using pulsed electron spin resonance (ESR), sensed by a nearby Ti spin [Reale et al. Nat. Commun. 15, 5289 (2024)]. Notably, a single Er spin showed a fivefold improvement in the qubit quality factor compared to the prototypical Ti spin on the same substrate [Yang et al. Science 366, 509-512 (2019)]. This result represents a step towards implementing quantum processes into atomic spin qubits on surfaces.

O 90.4 Thu 15:45 H11

Spin interactions at the periphery between atomic and condensed-matter physics — •Dmitriy Borodin, Andrés Pinar Solé, Merve Ercelik, and Andreas J. Heinrich — IBS Center for Quantum Nanoscience, Seoul, South Korea

Exchange interactions are essential for the formation of chemical bonds between atoms and dictate the electronic structure of molecules. In a condensed-matter system, a manifold of exchange mechanisms coexists, ultimately defining the local magnetic structure and phase stability. In this work, we use low-temperature scanning probe microscopy to investigate the exchange mechanisms and interaction energies between atoms on surfaces and magnetic tips. By controlling the atom-tip separations on a picometer scale, we can continuously tune the interaction energies and observe changes in the local magnetic structure of the tip. Furthermore, we explore the impact of the elemental composition of magnetic tips on their exchange interactions with surface-bound atoms and identify experimental strategies to adjust the sign and strength of these interactions.

O 90.5 Thu 16:00 H11

Switching Dynamics in Fe Spin Chains: Quantum vs. Classical Behavior — •Henrik Lichtl[1], Lukas Veldman[1], Johannes Schust[1], Nicolaj Betz[1,2], Laëtitia Farinacci[1,3], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany — [3]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm, Germany

That quantum spins transition to classical magnets at a certain size is well-known, but the behavior of magnets at this transition point has remained elusive. Here we develop a method to measure high speed magnetization curves in a scanning tunneling microscope (STM) that reach magnetic field sweep rates up to kT/s. This allows us to measure the magnetization reversal of antiferromagnetic few-atom spin chains, constructed of Fe atoms on a Cu2N surface. By resolving the statistics of the quantum jumps between the antiferromagnetic ground states, we can clearly distinguish between classical and quantum regimes of magnetic switching. Quantum mechanical behavior quenches rapidly with increasing size such that chains of more than five atoms in length can behave as classical magnets. The ability to modulate spin systems at high speed brings techniques that were previously reserved for bulk measurements to the atomic scale and provides deep insights into the coupling mechanisms between quantum spins and their environment.

O 90.6 Thu 16:15 H11

Many-body effects in impurity spectroscopy using ESR-STM — •Christoph Wolf[1,2], Xue Zhang[3], Jose Reina-Galvez[1,2], Jan Martinek[4], and Nicolas Lorente[5,6] — [1]Center for Quan tum Nanoscience, Institute for Basic Science (IBS), Seoul, Korea — [2]Ewha Womans University, Seoul, Korea — [3]Spin-X Institute, China University of Technology, Guangzhou, China — [4]Institute of Molecular Physics, Polish Academy of Science, Poland — [5]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Spain — [6]6Donostia International Physics Center (DIPC), Spain

Recent advances in understanding how harmonic electric fields drive coherent spin transitions in the ESR-STM have lead to a re-evaluation of experimentally observed phenomena in the ESR-STM spectra of atomic and molecular spin adsorbed on ultrathin insulating layers. In this talk, I will show the most up to date development of our transport approach, which is based on a single-orbital Anderson impurity model attached to magnetic leads. I will focus on two aspects: first, the DC bias control of the resonance frequency of the ESR transition, which can be interpreted as an exchange bias field. This allows the full physical characterization of the adsorbate spin and the junction parameters in ESR-STM. All simulations are qualitatively and quantitatively evaluated against experimental data of individual titanium atoms and Iron(II)phthalocyanine molecules which are prototypical spin-1/2 qubits. Second, I will discuss the optimization of quantum-coherent control in the low-current regime, which shows a distinct optimum for the quantum-bit figure of merit ΩT2.

O 90.7 Thu 16:30 H11

Driving nuclear spin transitions on a single atom using STM — •Cristina Mier Gonzalez, Hester Vennema, Evert Stolte, Jinwon Lee, and Sander Otte — Delft University of Technology, 2628 CJ Delft, The Netherlands

Nuclear spins are highly isolated from its electronic environment compared to electron spins. This degree of isolation makes nuclear spins a promising platform for quantum technologies [1]. The development of ESR-STM has made possible the indirect measurement of nuclear spins on single atoms through the hyperfine interaction [2]. More recently, single-shot read-out on Ti isotopes has shown a nuclear lifetime of about 5 seconds [3].

In this work we aim to controllably address nuclear spin transitions using ESR-STM. We propose a double resonance measurement scheme to controllably drive

the nuclear spin of a ^{47}Ti isotope (I = 5/2). Our study paves the way for coherent manipulation of single nuclear spins using STM.

[1] J. Pla et al. Nature 496, 334-338 (2013).
[2] P. Willke et al. Science 362, 336-339 (2018).
[3] E.W. Stolte et al. arXiv:2410.0870 (2024).

O 90.8 Thu 16:45 H11

Single-shot readout of an individual nuclear spin using a scanning tunnelling microscope — •Evert Stolte[1], Jinwon Lee[1], Hester Vennema[1], Rik Broekhoven[1], Esther Teng[1], Allard Katan[1], Lukas Veldman[2], Philip Willke[3], and Sander Otte[1] — [1]Department of Quantum Nanoscience, TU Delft — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart — [3]Physikalisches Institut, Karlsruhe Institute of Technology

Nuclear spins owe their long-lived magnetic states to their excellent isolation from the environment. At the same time, a limited degree of interaction with their surroundings is necessary for reading and writing the spin state. Therefore, detailed knowledge of and control over the atomic environment of a nuclear spin is key to optimizing conditions for quantum information applications. Scanning tunnelling microscopy (STM), combined with electron spin resonance (ESR), provides atomic-scale information of individual nuclear spins via the hyperfine interaction. However, STM has thus far only sparingly been used to investigate nuclear spins in the time domain. As such, no nuclear spin lifetimes have yet been reported. Here, we demonstrate single-shot readout of an individual ^{49}Ti nuclear spin with an STM. Employing a pulsed measurement scheme, we find its lifetime to be in the order of seconds. Furthermore, we shed light on the pumping and relaxation mechanisms of the nuclear spin by investigating its response to both ESR driving and tunnelling current. These findings give an atomic-scale insight into the nature of nuclear spin relaxation and are relevant for the development of atomically assembled qubit platforms.

O 90.9 Thu 17:00 H11

Spin Excitations of High-Spin Fe(II) in Metal-Organic Chains on Metal and Superconductor — •Jung-Ching Liu[1,2], Chao Li[2], Outhmane Chahib[2], Xing Wang[3], Simon Rothenbühler[4], Robert Häner[4], Silvio Decurtins[4], Ulrich Aschauer[5], Shi-Xia Liu[4], Ernst Meyer[2], and Rémy Pawlak[2] — [1]Department of Physics, Technical University of Munich, James-Franck-Str.1, 85748 Garching, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland — [4]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland — [5]Department of Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Strasse 2A, 5020 Salzburg, Austria

Magnetic anisotropy induced by the substrate plays an important role in many-body interactions in metal-organic frameworks at surfaces. Investigated by STM at 1K, we present the study of magnetic signature at Fe atoms with high spin-state (S=2) using PTO as ligands. On Ag(111), we found long-range Fe-Fe coupling in addition to low-energy spin-flip excitations. Despite of the identical chain structure, such long-range superexchange through PTO is not observed on tunneling spectra on Pb(111) superconductor. We ascribe this distinct spin-spin coupling behavior to the depletion of electronic states around the Fermi level on Pb(111) as compare to Ag(111). We believe our study provides a route for fundamental studies in spin-spin and spin-substrate interactions with different lattice structures.

O 90.10 Thu 17:15 H11

Control of the Landau-Zener Gap in Atomic Structures — •Piotr Kot[1,2], Yaowu Lei[1,2], Valeria Sheina[1,2], We-hyo Seo[1,2], Andreas Heinrich[1,2], and Soo-hyon Phark[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, South Korea — [2]Department of Physics, Ewha Womans University, Seoul, South Korea

Avoided crossings in quantum systems have been shown to be a useful tool for the study of qubits and the actualization of faster qubit operations. This is done by taking advantage of Landau-Zener transitions, allowing one to measure quantum interferometric effects. However, implementing these techniques in on surface atoms has not yet been demonstrated experimentally, and is a crucial next step for studying this new class of spin qubits. Here we present preliminary steps towards studying quantum interferometric effects in Ti dimers using electron spin resonance scanning tunnelling microscopy. Firstly, we have fine-tuned the Landau-Zener gap in our dimers by studying the dipole and exchange interaction between the atoms. We have found that only several dimers have the correct gap magnitude for our experimental conditions. Secondly, we have found that by using three atom structures we are able to position the avoided crossing within our range of interest. Experiments in the near future will include measuring Landau-Zener transitions, Stueckelberg oscillations and quantum interferometry maps.

O 91: Focus Session Chemical Imaging for the Elucidation of Molecular Structure I (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Thursday 15:00–17:30 Location: H24

Invited Talk O 91.1 Thu 15:00 H24

Infrared Nanoscopy and Tomography of Intracellular Structures — Joachim Heberle[1], Katerina Kanevche[1], •Emmanuel Pfitzner[1], David Burr[2], Janina Drauschke[2], Andreas Elsaesser[2], and Jacek Kozuch[1] — [1]Freie Universität Berlin, Department of Physics, Experimental Molecular Biophysics, — [2]Experimental Biophysics and Space Sciences, Arnimallee 14, 14195, Berlin, Germany

Although techniques such as fluorescence-based super-resolution imaging or confocal microscopy simultaneously gather morphological and chemical data, these techniques often rely on localized and chemically specific markers. To eliminate this flaw, we have developed a method of examining cellular cross-sections using the imaging power of scattering-type scanning near-field optical microscopy (sSNOM) and Fourier-transform infrared spectroscopy at a spatial resolution far beyond the diffraction limit (nanoFTIR). Herewith, nanoscale surface and volumetric chemical imaging are performed using the intrinsic contrast generated by the characteristic absorption of mid-infrared radiation by the covalent bonds. We employ infrared nanoscopy to study the subcellular structures of eukaryotic (C. reinhardtii) and prokaryotic (E. coli) species, revealing chemically distinct regions within each cell. Serial 100 nm-thick cellular cross-sections were compiled into a tomogram, yielding a three-dimensional infrared image of subcellular structure distribution at 20 nm spatial resolution. The presented methodology can image biological samples with less interference due to the low energy of infrared radiation and the absence of labeling.

Invited Talk O 91.2 Thu 15:30 H24

Coherent Raman Imaging — •Michael Schmitt[1] and Juergen Popp[1,2] — [1]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany — [2]Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Albert-Einstein-Straße 9, 07745 Jena, Germany

Raman-based technologies have profoundly impacted life sciences and biomedical research. Despite their unmatched molecular specificity, traditional Raman spectroscopy suffers from limited sensitivity, making it less suitable for rapid imaging. This limitation is addressed by coherent Raman scattering (CRS) microscopy, primarily through coherent anti-Stokes Raman scattering (CARS) and

stimulated Raman scattering (SRS). This talk examines the potential of CARS and SRS imaging for biological and biomedical analysis, offering detailed insights into the molecular composition of biomedical specimens, such as cells or tissue. The presentation will focus on the applications of these techniques in molecular and functional diagnostics in the fields of medicine and life sciences. Furthermore, recent developments in translating CRS into compact, clinically viable systems, such as handheld probes, will be presented, focusing on intraoperative tumour diagnostics for early detection and improved improved therapeutic outcomes.

Acknowledgement: Financial support of the EU, the *Thüringer Ministerium für Wirtschaft, Wissenschaft und Digitale Gesellschaft*, the *Thüringer Aufbaubank*, the BMBF, the DFG, and the Carl Zeiss Stiftung is acknowledged.

Invited Talk O 91.3 Thu 16:00 H24

Sum Frequency Generation Microscopy of Electrochemical Interfaces — •Steven Baldelli — University of Houston, Houston, Texas

Sum frequency generation spectroscopy (SFG) is a valuable technique to study the molecular properties of surfaces. As a second-order technique, it is uniquely sensitive to the average organization of molecules at the surface. However, as most surfaces are spatially heterogeneous, it isn't easy to interpret the spectrum as a single domain. The development of SFG into microscopy has allowed a more detailed and accurate analysis of the spatio-spectro-temporal evolution of surface chemistry. The SFG microscope development will be presented, and compressive sensing and the application toward electrocatalysis will be used.

O 91.4 Thu 16:30 H24

Elucidating the Composition, Order, and 3D Molecular Orientation of Thin Films with Phase-Resolved Sum-Frequency Generation Microscopy — •Alexander Fellows, Ben John, Martin Wolf, and Martin Thämer — Fritz-Haber-Institute, Berlin, Germany

The vast majority of molecular interfaces have highly heterogeneous structures, ranging across all length-scales. These manifest as variations in density, composition, and molecular packing structure, all of which are critical in controlling the macroscopic properties and functional behaviour of the films. While various chemical imaging techniques can access many of these important structural details, characterising their relative order and specific packing arrangements represents a formidable challenge.

Here, we present a chemical imaging approach based on phase-resolved sum-frequency generation (SFG) microscopy. By probing molecular vibrations, this technique achieves molecular recognition and thus is sensitive to the local composition and density. Furthermore, through its symmetry selection rules, output SFG signals are dependent on absolute molecular orientations. This hence allows it to distinguish different molecular conformations and characterise the amount of orientational order in the system. Finally, with an azimuthal-scanning approach, the in-plane and out-of-plane signal contributions can be separated, allowing the 3D molecular orientations to be elucidated. By applying SFG imaging to model lipid monolayers, we gain an unprecedented overview of their hierarchical packing structures.

O 91.5 Thu 16:45 H24

Low temperature multimode atomic force microscopy using an active MEMS cantilever — Michael G. Ruppert[1], Miguel Wiche[2], André Schirmeisen[2], and •Daniel Ebeling[2] — [1]University of Technology Sydney, Australia — [2]Justus Liebig University Giessen, Germany

Low-temperature atomic force microscopy (AFM) is one of the most powerful tools in surface science. With the chemical bond imaging technique, i.e., by using CO functionalized AFM tips, it became possible to visualize the chemical structure of individual organic molecules, which is essential for studying on-surface reactions and molecular manipulation processes. Routinely, such measurements are performed with qPlus sensors. Here, we present a proof of concept for an active microelectromechanical systems (MEMS) microcantilever with integrated piezoelectric sensing and demonstrate its capability to obtain scanning tunneling microscopy as well as high-resolution non-contact atomic force microscopy images on an atomically flat Au(111) surface. Equipped with a focused ion beam deposited tungsten tip, the active MEMS cantilever is able to obtain high contrast scanning tunneling and frequency shift images at the fundamental and a higher eigenmode of the cantilever. This is interesting for the application of multifrequency AFM operation modes that could enhance the capabilities of the bond imaging technique.

O 91.6 Thu 17:00 H24

Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD) — •Lukas Eriksson[1], Tim Esser[1,2], and Stephan Rauschenbach[1] — [1]University of Oxford, Oxford, UK — [2]Thermo Fisher Scientific, Eindhoven, Netherlands

Direct imaging of (bio-)molecules with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for elucidating molecular structure. However, sample preparation can be a major challenge: either very time- and resource-intensive or incompatible with the vacuum environment required by the imaging method.

Here, we explore preparative mass spectrometry as an alternative workflow towards structural elucidation of biomolecules. A novel, custom-built deposition stage extending a commercial mass spectrometer (Thermo Fisher Scientific Orbitrap UHMR) allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules (m = 100 to 10^6 Da) onto various surfaces, including cryo-EM grids and metal crystals for SPM. Successful deposition and subsequent imaging requires extensive control over conditions such as pressure, temperature, ion trajectories, sample surfaces, and sample transfer to obtain clean, chemically pure samples of the desired species in the right (i.e. native) configuration. The sample holder also enables controlled growth of ice layers for embedding deposited molecules, allowing high-resolution reconstructions of proteins from cryo-EM.

O 91.7 Thu 17:15 H24

LFM study of copper oxide — •Sophia Schweiss, Alfred J. Weymouth, and Franz J. Giessibl — Universität Regensburg, Regensburg, Deutschland

Small-amplitude FM-AFM is a method to study surfaces and adsorbates with atomic resolution. At low temperature, the tip apex can be prepared so that it ends in a single O-atom, making the tip inert and enhancing imaging [1, 2]. With a laterally oscillating tip, i.e. lateral force microscopy (LFM), the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction can also be independently measured. Here too, inert tip apices are commonly used. One measurement of E_{diss} relies on the cocking and snapping of the tip over a single chemical bond, for which the current state of the art utilizes CO-terminated tips. In this work, a CO-terminated tip [1] is used to investigate the (2×1)O reconstruction of Cu(110) with LFM. Simulations are performed to guide interpretation. In this larger ongoing study, these LFM measurements will be repeated for a CuOx tip [2] to evaluate it as a tool for measuring E_{diss}.

[1] Gross et al., Science, **325**, 1110 (2009)
[2] Mönig et al., Nat. Nano., **13**, 371 (2018)

O 92: Electronic Structure Theory

Time: Thursday 15:00–18:15 Location: H25

O 92.1 Thu 15:00 H25

Electronic and Optical properties of K-Sb and Na-Sb binary crystals from ab initio many-body theory — •Richard Schier and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik

Alkali-based photocathode materials have come into the limelight as novel semiconducting materials for electron sources. However, challenges in sample purity and polycrystallinity hinder the direct experimental determination of their intrinsic properties. First-principles methods can effectively complement experiments in predicting favorable structures and gaining insight into their electronic and optical properties. In this work, we investigate K-Sb and Na-Sb binary crystals emerged as stable phases from high-throughput screening [1]. Using many-body perturbation theory on top of density functional theory, we find that all considered materials have optical gaps in the near-infrared region between 0.7 - 1.2 eV. The character of the excitations and electron-hole correlations therein are highly dependent on the composition and crystal structure of the compound. Excitonic effects appear more pronounced in the K-Sb crystals, where binding energies are of the order of 100 - 200 meV and the oscillator strength is sizably redistributed to lower-energy peaks. These characteristics indicate that K-Sb crystals are favorable candidates for efficient electron sources. [1] R. Schier, D. Guo, H.-D. Saßnick, and C. Cocchi, Adv. Theory Simulations (2024), https://doi.org/10.1002/adts.202400680.

O 92.2 Thu 15:15 H25

Automated Wannier functions inspired by topological quantum chemistry — •Stepan S. Tsirkin — Centro de Física de Materiales, San Sebastián, Spain

Despite Wannier functions (WFs) becoming a popular and powerful technique for studying diverse electronic properties of materials, the construction of high-quality WFs remains a non-trivial task, often requiring manual intervention and expertise, which obstructs high-throughput calculations using WF-based methods.

I present an approach for selecting initial projections for Wannier functions based on the symmetry indicators of DFT bandsstructure. The initial projections

are searched among the possible orbitals at the Wyckoff positions of the crystal, referred to as Elementary Band Representations in the terminology of Topological Quantum Chemistry [Nature 547, 298 (2017)]. Thus, the projections are by construction compatible with the symmetry of the bands, making them suitable for the construction of symmetry-adapted WFs (SAWFs) [Sakuma, PRB 87, 235109 (2013)]. This approach has been implemented in the codes WannierBerri (WB) [NPJ Comput. Mater. 7, 33 (2021)] and IrRep [CPC 272, 108226 (2022)]. Additionally, WannierBerri now implements the construction of SAWFs without several limitations found in the corresponding implementation in Wannier90. In particular, WB can handle spin-orbit coupling, a frozen window, and is compatible with multiple DFT codes (VASP, Quantum Espresso, Abinit, etc.).

This method does not require manual inspection on bands, which makes it suitable for high-throughput calculations.

O 92.3 Thu 15:30 H25

Learning conductance of aromatic and antiaromatic molecular junctions — •Mohammad Ali Mohammadi Keshtan and Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

Single-molecule junction conductance depends on molecular conformation. The standard computational method to study the conductance of a molecular junction is DFT-NEGF. However, DFT-NEGF is computationally expensive, so finding a fast and accurate method to compute the conductance of a large numbers of structures is vital.

Here, we use machine learning (ML) methods, including kernel ridge regression and Gaussian process regression, to overcome these limitations. To train the regression models, we first generate thousands of junction geometries using classical molecular dynamics at room temperature. For each geometry we then compute conductance using a computationally efficient approximation which considers a Au-molecule-Au complex [1], and build SOAP and Coulomb matrix descriptors.

We study a pair of aromatic/antiaromatic porphyrin-like molecules [2], whose large size further hampers the use of DFT-NEGF. We explore the performance of the different ML models, compare the results with DFT-NEGF, and discuss the relative importance of the different descriptors. Our work demonstrates how ML models can be efficiently trained and used to compute single molecule junction conductance.

[1] H. Vazquez, J. Phys. Chem. Lett. 2022, 13, 9326
[2] S. Fujii et al., Nat. Commun. 2017, 8, 15984

O 92.4 Thu 15:45 H25

Electronic excitations in nanostructures from the Bethe-Salpeter equation — •Maximilian Graml, Štěpán Marek, and Jan Wilhelm — Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany

Electronic structure calculations are a well-established tool for the identification of candidate materials for technological applications, e.g., in photocatalysis, photovoltaics and energy storage. For the quantitative description of optical properties, many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation (BSE) on top of GW is regarded as the state-of-the-art method.

In this contribution, we present the implementation of the BSE within the open-source package CP2K, enabling the accurate calculation of electronic excitations in molecules and nanostructures. To validate our approach, we benchmark the excitation energies against those obtained with the FHI-aims package.

We further apply our BSE implementation to study electronic excitations in graphene nanostructures, where we investigate the optical absorption spectra and the spatial extent of excited states as a function of nanostructure size. We observe that both properties converge on the scale of 5 nm nanostructure size, guiding experiments towards the rational design of nanostructures in graphene-based optical devices.

O 92.5 Thu 16:00 H25

Electronic Coupling on Surfaces from First-Principles: Chemisorped Systems — •Simiam Ghan and Jens Nørskov — Technical University of Denmark DTU

We use density-functional theory to calculate the electronic coupling matrix elements between adsorbates and surfaces, applying a recently developed diabatization method[1] to fully chemisorped systems. The scheme is demonstrated by calculating ultrafast electron transfer lifetimes within a Fermi golden rule framework, which compares favorably to core-hole-clock measurements for systems including Black Phosphorous, S/Ru(0001) and CO/Ru(0001). We thereby demonstrate the suitability of diabatization schemes for the description of coupling in chemisorped systems, enabling an advantageous interpretation of the electron transfer process. We discuss prospects for the use of first-principles coupling matrix elements to describe other surface phenomena, such as chemisorption and heterogenous catalysis, e.g. within Newns-Anderson models.

[1] S. Ghan *et al.*, J. Chem. Phys. 158, 234103 (2023).

O 92.6 Thu 16:15 H25

Enhancing structure relaxation with machine-learned interatomic potentials — Sudarshan Vijay[1,2], Martijn Marsman[1], Georg Kresse[1,3], and •Martin Schlipf[1] — [1]VASP Software GmbH, Berggasse 21, 1090 Vienna, Austria — [2]Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076 India — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

Machine learning interatomic potentials (MLIPs) offer a cost-effective way to predict ground-state properties of materials compared to density functional theory (DFT) calculations. MLIPs are often used to replace DFT due to their ability to access large length and longer time scales. In this study, we explore whether MLIPs can also enhance DFT by preconditioning commonly used optimization algorithms for structure relaxation. We demonstrate that applying this preconditioner to methods such as conjugate gradient (CG) and Broyden-Fletcher-Goldfarb-Shanno (BFGS) results in faster convergence but at the expense of stability. For this particular tasks, state-of-the-art MLIPs are not accurate enough to replace DFT; prerelaxing the structures with MLIPs tends to perform worse compared to starting the relaxation directly within DFT. Our analysis of the convergence behavior for both standard and preconditioned methods suggests that advancements in line-search techniques could enhance the effectiveness of this preconditioning approach for structure relaxation.

O 92.7 Thu 16:30 H25

Constrained Density Functional Theory with Numeric Atomic Orbitals — •Tavinder Singh[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology

Even in perfectly crystalline materials, simulation of some phenomena, such as the occurence and transport of polarons, rests on the simulation method's ability to describe localized charge carriers. This is generally hampered by both, the need to break a system's symmetry to accommodate such a localized state, and the infamous electron delocalization error of most semi-local density functionals. In this respect, constrained density functional theory (CDFT) has proven to be a viable tool addressing both. Constraining charges to pre-selected localized states naturally breaks the symmetry and mitigates DFT errors. In our contribution, we describe our implementation of CDFT in the FHI-aims package based on Numeric Atomic Orbital (NAOs) projectors. As a prototype, we consider polaron localization in the zero-strain anode material, $Li_4Ti_5O_{12}$ (LTO), and compared the computed relative energies and barriers with the literature as benchmark. Our results provide valuable insights into the applicability and accuracy of CDFT for studying localized electronic states in complex materials.

O 92.8 Thu 16:45 H25

Efficient Phonon Dispersions of 2D Films by Extension of DFPT in FLAPW Method *FLEUR* to Film Geometry. — •Thomas Bornhake[1,2], Alexander Neukirchen[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Physics Department, RWTH Aachen University, Aachen, Germany

Phonons are crucial in 2D materials, governing a range of physical properties and phenomena, *e.g.* from dynamical stability to spin-flip scattering. Thus, an efficient method for calculating phonons under arbitrary excitations is inevitable. Typically, phonons of film systems are calculated from *ab initio* using supercells that separate the film from periodic images by computationally costly empty space. Recently, we have succeeded in calculating the phonon dispersion using the state of the art density functional perturbation theory (DFPT) in the all-electron full-potential linearized augmented planewave (FLAPW) method *FLEUR* [1,2]. In this talk we present our extension to a truly 2D treatment of films embedded in semi-infinite vacuum [3]. We discuss some details of the implementation and compare results with respect to accuracy and efficiency to the repeated slab approaches.

This work was supported by CoE-MaX (EuroHPC JU, Grant No. 101093374) and DFG through CRC 1238 (Project C01).

[1] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de
[2] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).
[3] H. Krakauer *et al.*, Phys. Rev. B **19**, 1706 (1979).

O 92.9 Thu 17:00 H25

Excitations in oxides: from bits to qubits — •Vijaya Begum-Hudde[1], Yi-Ting Lee[1], Barbara Jones[2], and Andre Schleife[1] — [1]University of Illinois, Urbana-Champaign, USA. — [2]IBM

Defects in materials are ubiquitous and may adversely affect their functional properties. Often the defects are confined to a small space, and defect embedding allows us to define an active space comprising of these defect states and to incorporate screening effects of the host material, enabling access to electronic properties with a high-level theory.

In this talk I will focus on the structural and electronic properties of near-surface vacancies in α-Al_2O_3 (0001) to investigate the influence of defects and hydration on the initiation and propagation of corrosion in this material. Utilizing first-

principles calculations and quantum-defect embedding theory calculations, this study will analyse defect states and their ground- and excited-state properties. An active space is defined consisting of strongly localized states of the surface O vacany, and the remainder is treated as the environment. Next, an effective Hamiltonian is used for the active space that also includes the environment's effective screening and is solved via full configuration interaction (FCI). Simulations are performed on a quantum computer with a Unitary coupled-cluster ansatz for the determination of ground- and excited-state properties. Error mitigation techniques will be demonstrated, reducing error due to the hardware noise and showing very good concordance with the FCI results within chemical accuracy.

We acknowledge funding by the IBM-Illinois Discovery Accelerator Institute.

O 92.10 Thu 17:15 H25

Electronic band structure at finite temperature: A unifying approach that incorporates electron-electron and electron-vibration interactions — •Min-Ye Zhang[1,2], Xinguo Ren[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft — [2]Institute of Physics, Chinese Academy of Sciences, China

An accurate first-principles description of electronic band structure at finite temperature requires accounting for self-energy contributions from both electron-electron (e-e) and electron-vibration (e-vib) interactions. In the widely used electron-phonon coupling (EPC) model[1], the two types of interactions are considered separately, and the model fails for strongly anharmonic materials. In this work, we integrate the two types of interactions beyond the EPC model by extending the statistically anharmonic, higher-order vibronic coupling approach[2] with the many-body *GW* method. This is achieved by combining *ab initio* molecular dynamics and periodic G^0W^0 method in an all-electron framework employing numeric atom-centered orbitals[3]. We demonstrate the robustness and efficiency of our G^0W^0 implementation, particularly through a proper treatment of long-range dielectric responses. As a proof of concept, we present the temperature-dependent electronic band structure of Si, incorporating both e-e and e-vib interactions.

[1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
[2] M. Zacharias, M. Scheffler, and C. Carbogno, *Phys. Rev. B* **102**, 045126 (2020).
[3] X. Ren, et al, *Phys. Rev. Materials* **5**, 013807 (2021).

O 92.11 Thu 17:30 H25

Electronic and optical properties of computationally predicted Na-K-Sb crystals — •Chung Xu, Richard Schier, and Caterina Cocchi — University of Oldenburg

Due to their favorable electronic and optical properties, sodium-potassium-antimonides are an emerging class of crystals used as photocathodes in particle accelerators. Using first-principles methods based on density-functional theory and many-body perturbation theory, we investigate the electronic and optical properties of cubic NaK_2Sb and hexagonal Na_2KSb, two computationally predicted polymorphs of established photocathode materials that can emerge as metastable phases in polycrystalline samples. Our results indicate that both systems are indirect band-gap semiconductors with fundamental gaps on the order of 0.7 and 0.8 eV, respectively. Their direct gaps are very close to these values and Their optical spectra are characterized by weakly bound excitons in the near-infrared region which represent favorable characteristics for efficient photoemission. Our study suggests that the presence of cubic NaK_2Sb and hexagonal Na_2KSb in photocathode samples is not detrimental for their application as photocathodes [1].

[1] arXiv:2411.13330

O 92.12 Thu 17:45 H25

Thermal dependence of conductance in short pi-conjugated single-molecule junctions — •Václav Kubíček and Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

Conductance measurements at room temperature in single-molecule junctions are affected by the internal dynamics of the molecule, since many different internal conformations are averaged. Further temperature changes lead to different conformational sampling and may alter conductance values, opening the possibility of thermally active molecular devices.

For example, it was measured that raising the temperature from 300 K to 330 K results in a change in conductance for oligophenylenes [1]. In our work, we calculate the temperature dependence of conductance for several short pi-conjugated molecular wires. By combining classical statistical model with DFT simulations, we explore their accessible geometries and compute the resulting changes in conductance.

Our results show that by engineering chain composition, conductance increases or decreases are achievable with increasing temperature. Our results demonstrate the importance and potential applicability of thermally induced conformational changes in conductance.

[1] Lee, W.; et al., Nano Lett. 2022, 22, 4919

O 92.13 Thu 18:00 H25

Comparison of non-equilibrium Green function and wave packet methods for studying the CISS effect — •Thibaut Lacroix, Clemens Vittmann, Jaemin Lim, Susana F. Huelga, and Martin B. Plenio — Intitut für Theoretische Physik, Universität Ulm, Ulm, Deutschland

Non-equilibrium Green function (NEGF) technique has been widely employed to simulate quantum transport at the molecular scale. It is one of the main methods used to study transport properties of chiral molecules which are central to the investigation of chirality induced spin selectivity (CISS). Equivalent to the solution of a scattering problem, this approach leads to an energy resolved description of transport properties that can be used to obtained spin-dependent currents.

Alternatively, the description of electronic transport can be performed at the level of the Schrödinger equation. In that case, one considers an initial wave packet in the position basis – which therefore corresponds to a superposition of energy eigenstates – and computes its dynamics under the total Hamiltonian of the molecule and the leads. One benefit of this approach is to readily give access to the transient dynamics of the electron inside of the molecule, thus opening the possibility to study the internal mechanisms underlying CISS. We demonstrate that NEGF results can be recovered from wave packet evolution and that tailored wave packets enable to access directly specific transport properties of interest. These results show that while they rely on different formalisms wave packet evolution and NEGF do give the same information about the response of the system.

O 93: Members' Assembly

Time: Thursday 19:00–19:30 Location: H1

break

O 94: Post Deadline Session

Time: Thursday 19:30–20:30 Location: H1

O 95: Overview Talk Kai Rossnagel

Time: Friday 9:30–10:15 Location: H24

Topical Talk O 95.1 Fri 9:30 H24

A quantum sandwich world and how we can explore it with soft x-rays — •Kai Rossnagel — Kiel University, Kiel, Germany — DESY, Hamburg, Germany

Without materials, there is nothing. Without quantum materials, there is nothing interesting.

Quantum materials express our desire to find and explain new states of matter and new physical phenomena induced by the quantum mechanical interactions of electrons. Paradigmatic examples are quantum material sandwiches made by stacking and twisting single layers of layered materials, which currently represent one of the richest and most tunable discovery and engineering platforms in all of condensed matter physics.

To see and understand how these and other quantum materials work, we need spectroscopic tools that can provide direct snapshots of electron behavior in energy-momentum space. The most powerful toolbox for this is soft x-ray spectroscopy. And the single most powerful tool is angle-resolved photoelectron spectroscopy (ARPES), which has recently been transformed into a true *in operando* technique using both nanofocused and ultrashort-pulsed soft x-ray beams to directly probe nonequilibrium electronic function in materials and devices on relevant nanometer length and femtosecond time scales, respectively.

Here, we give an overview of recent innovations in quantum material sandwiches, focusing on transition-metal dichalcogenides, and in nanoscopic and femtostroboscopic imaging of their electronic structures.

O 96: Plasmonics and Nanooptics: Light-Matter Interaction, Spectroscopy II

Time: Friday 10:30–13:00 Location: H4

O 96.1 Fri 10:30 H4

Enhancing light-matter interaction through inverse design of optical devices. — •Carlos Bustamante[1], Mark Svendsen[2], Franco Bonafé[1], Burak Gurlek[1], Maxim Sukharev[3], Abraham Nitzan[4], and Angel Rubio[1] — [1]MPSD, Hamburg, Germany — [2]Niels Bohr Institute, University of Copenhagen, Denmark — [3]Department of Physics, Arizona State University, USA — [4]Department of Chemistry, University of Pennsylvania, USA

Light-matter interaction plays a crucial role in processes such as spontaneous emission, energy transfer and polaritonic formation. This interaction is sensitive to alterations in the electromagnetic environment which can be caused by the presence of optical materials. In classical optics, changes in the topology of optical materials can lead to the fabrication of optical devices tailored towards specific characteristics, using inverse design methodologies like density-based topology optimization (TO). This work presents the application of optical devices, derived from TO, that can be used to modify light-matter interaction among molecules. To achieve this, we have implemented a TO algorithm that can solve Maxwell equations in the frequency domain on a 2D grid. These tailored devices enhance locally one component of the transverse electric field obtained from classical emitters. In subsequent semiclassical simulations, Maxwell equations were classically propagated with the emitters replaced by pentacene molecules using the quantum mechanical simulation software DFTB+. The results highlight the significant potential of optical devices produced by TO to influence the above-mentioned processes.

O 96.2 Fri 10:45 H4

Squeezing few-cycle light pulses in space and time in the gap of a nanoplasmonic resonator — •Tom Jehle, Sam S. Nochowitz, Juanmei Duan, and Christoph Lienau — Universität Oldenburg, D-26129, Germany

The spatial confinement of light to (sub-)nanometer spot sizes in the gap of a nanoparticle-on-mirror resonator or in the gap of a tunnelling junction has led to dramatic advances in nanosensing [1] and tip-enhanced Raman Spectroscopy [2]. So far, the time dynamics of the fields emitted from such nanocavities have achieved little attention and only recently the time structure of a Terahertz field scattered from the junction of an STM tip could be recorded [3]. Here, we introduce a broadband interferometric scattering-type SNOM technique [4] to reconstruct amplitude and phase of light scattered from a sharp gold taper acting as a near-field probe. Direct Fourier transform gives the time structure of the electric field. We distinguish the near-field scattered from the apex and that emitted by spatially well separated scattering mode of the taper. The apex field decays within 13 fs, a decay time mainly given by the radiative damping of the apex mode. Upon approaching the tip to a gold surface, we observe a 3.5-fold reduction in the decay time to less than 4 fs: coupling to the image dipole drastically increases the radiative damping in the tip-surface junction. Our results pave the way towards linear and nonlinear ultrafast oscilloscopy with nm/fs resolution. [1] R. J. Chikkardy et al., Nature 535, 127 (2016); [2] R. Zhang et al., Nature 531, 623 (2016); [3] T. Siday et al., Nature 629 (2024); [4] J. Zhan et al., Nano Lett. 2024

O 96.3 Fri 11:00 H4

Full-wave simulations of core-shell nanoparticle investigation by tapping mode near-field optical microscopy — •Dario Siebenkotten, Dinghe Dai, Richard Ciesielski, Arne Hoehl, and Bernd Kästner — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12 10587 Berlin

Core-shell nanoparticles are important in applications such as optoelectronics, biosensing, and medicine, where their unique optical and geometric properties play a critical role in functionality. Quantifying the properties of both, the core and the shell, is crucial to understand the nanoparticle's ultimate functionality. However, optical investigation of their properties, while widely employed, is generally diffraction-limited and thus unsuitable for the investigation of individual nanoparticles, as they only provide averaged ensemble information. Scattering-type scanning near-field optical microscopy (s-SNOM) promises access to a single nanoparticle's size and optical properties through the use of an atomic force microscopy tip as an optical antenna, which confines the sampling fields to nanoscale dimensions. To explore the single nanoparticle s-SNOM response, we model different core-shell nanoparticles using Finite Element Modelling, revealing complex resonance-antiresonance behaviour in dependence of their geometrical and optical properties. We further explore the origin of the emergent antiresonance through the use of Fourier-demodulation of the probe tapping [1], closely mimicking the experiment. [1] Mooshammer et al., ACS Photonics 7, 344-351 (2020)

O 96.4 Fri 11:15 H4

Near-field microscopy of complex polaritonic excitations — •Farid Aghashirinov[1], Bettina Frank[1], Harald Giessen[1], Andrea Manchini[2], Lin Nan[2], Giacomo Venturi[2], Nicola Melchioni[2], and Antonio Ambrosio[2] — [1]4-th Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]Vectorial Nano-Imaging, Istituto Italiano di Tecnologia, Milano, Italy

We investigate directional near-infrared (NIR) plasmon polaritons (PPs) in mechanically exfoliated bulk molybdenum oxide dichloride (MoOCl2) flakes on a glass substrate with gold disk launchers positioned on top of the flakes, through experimental and theoretical methods [1]. MoOCl2, a natural van der Waals crystal, exhibits low-loss, in-plane hyperbolic PPs across the visible and NIR ranges, and displays a unique anisotropic optical response based on the polarization of the incident light. When light polarization aligns with the flake's shortest axis, MoOCl2 behaves optically metallic, while aligning with the longest axis reveals a dielectric behaviour. To experimentally study the hyperbolic PPs in MoOCl2, we use a near-field excitation and detection approach. Gold disks serve as excitation sources, scattering incident light to couple it with the material's polaritonic modes, while a reflection scattering-type scanning near-field optical microscope (s-SNOM) enables subwavelength imaging. For tunable wavelength illumination, we use a broadband laser from Stuttgart Instruments (SI), which, when combined with s-SNOM, allows us to investigate these modes across a wide wavelength range, capturing detailed insights into their behavior and propagation. [1] G. Venturi et al., Nat Commun 15, 9727 (2024)

O 96.5 Fri 11:30 H4

Discovery of phonon-polaritonic skyrmions: Transition from bubble- to Néel-type — •Florian Mangold[1], Enrico Baù[2], Lin Nan[2], Julian Schwab[1], Thorsten Gölz[2], Andrea Mancini[2], Bettina Frank[1], Andreas Tittl[2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, and IQST, University of Stuttgart, Germany — [2]Chair in Hybrid Nanosystems, Nano-Institute Munich, Ludwig-Maximilians Universität München, Germany

Optical skyrmions constitute an emerging and rapidly developing field in the domain of solid-state physics and photonics, allowing for control over topological light textures through light-matter interactions. However, until now their practical applications have been severely limited by inherent restrictions of materials with high optical losses and a lack of tunability between different topological properties. We leverage the steep dispersion of silicon carbide thin films to image surface phonon polariton skyrmion lattices via near-field microscopy and experimentally demonstrate topological tuning between Bubble- and Néel-type skyrmions, a unique advantage that polar dielectrics offer over most existing approaches. The ability to control and manipulate these skyrmion lattices through

small changes (<10%) in excitation wavelength allows for tailoring the size of individual skyrmions by a factor of 4. Tuning topological properties has been a long-standing goal in the field of optics. Our results expand the tunability of skyrmions in evanescent waves and are a starting point to investigate other topological features in phononic systems such as merons, skyrmion bags and other complex structured light fields.

O 96.6 Fri 11:45 H4

Tracking Non-Equilibrium Electron Distributions to Propel Chemical Dynamics at Surfaces — •Henry T. Snowden[1], Reinhard J. Maurer[1], Markus Uehlein[2], and Baerbel Rethfeld[2] — [1]University of Warwick, Coventry, UK — [2]RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

A mechanistic understanding of ultrafast light-matter interactions with surfaces and nanoparticles is invaluable for the study of ultrafast dynamics at surfaces. Immediately after a laser pulse, non-equilibrium electrons are generated in metals which rapidly relax to a thermal distribution that follows the two-temperature model. Here, we study the longevity of electronic non-equilibrium which depends on the electronic structure and other materials properties. We simulate the temporal evolution of non-equilibrium electron distributions with the Athermal Electron Model (AthEM), which explicitly considers electronic nonequilibrium, a laser term and electron scattering in the relaxation time approximation. Equipped with this approach, we investigate how athermal electron-hole pair distributions differ in various materials configurations such as intermetallic interphases, and nanoparticles. We will use this information to discuss the requirements to create long-lived non-equilibrium distributions from which high-energy charge carriers can be harvested.

O 96.7 Fri 12:00 H4

Collective Behavior of SiC Phonon Polariton Resonators — •Richarda Niemann[1,2], Sören Wasserroth[1], Guanyu Lu[2], Christopher R. Gubbin[3], Martin Wolf[1], Simone de Liberato[3], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]Vanderbilt University, Nashville, TN, USA — [3]University of Southampton, Southampton, UK

Structuring polar materials with microresonators enables light confinement to sub-wavelength scales and the emergence of localized phonon polaritons (PhPs). Previous studies on PhP single resonators and 2D resonator arrays investigated the coupling behavior of resonators with their surrounding [1,2]. Here, we bridge the gap between a single resonator and a 2D array by studying subdiffractional SiC microresonators on a SiC substrate in 1D arrays with sumfrequency generation (SFG) spectro-microscopy [3,4]. The high spatial resolution on the order of the lateral size of the microresonators allows us an in-depth analysis of the build-up of collective modes in 1D arrays with sizes from one to several resonators. We observe different optical responses for in-phase and out-of-phase excitation showing the importance of phase relationships for coupling between the resonators. By investigating arrays with different periods, we gain information about the coupling mechanisms.

[1] Gubbin et al., Phys. Rev. B, 95 (2017)
[2] Chen et al., ACS Photonics, 1 (2014)
[3] Niemann et al., Appl. Phys. Lett. 120, 131102 (2022)
[4] Niemann et al., Adv. Mater. 2024, 36, 2312507

O 96.8 Fri 12:15 H4

High-Throughput Phonon Polariton Materials Discovery from First Principles — •Elena Gelzinyte[1], Giulia Carini[1], Niclas S. Mueller[1], Martin Wolf[1], Karsten Reuter[1], Johannes T. Margraf[2], Alexander Paarmann[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Phonon Polaritons (PhPs), quasi-particles that arise from strong coupling between infrared photons and optical lattice vibrations, are promising in nanophotonic applications for highly directional and confined light propagation with low optical loss [1]. However, little is still known about the trends in material space that drive the emergence and characteristics of PhPs. To describe these trends, we compute the permittivity function [2] as the basis for describing PhP dispersion. We employ Kubo's linear-response theory, where the harmonic and anharmonic phonon properties as well as Born effective charges are used to model the involved couplings. This approach is validated on materials with well-characterised PhP behaviour, such as h-BN, MoO_3 and β-Ga_2O_3, and then applied to 5,000 materials from the JARVIS database [3]. By analysing the trends emerging from these data, we identify qualitative metrics that capture the material's ability to support PhPs. Finally, we highlight some examples and outliers of this high-throughput screening process.

[1] E. Galiffi *et al.*, *Nat. Rev. Mater.* **9**, 9 (2024).
[2] M. Born & K. Huang, *Dynamical Theory of Crystal Lattices* (1954).
[3] K. Choudhary *et al.*, *npj Comput. Mater.* **6**, 1 (2020).

O 96.9 Fri 12:30 H4

Electron Relaxation in Noble Metals: Microscopic Theory of Orientational Relaxation, Thermalization and Cooling — •Jonas Grumm and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The excitation of electrons in noble metals by light fields with high intensities results in non-equilibrium electron occupations. The relaxation back to thermodynamic equilibrium, proceeding on scales from a few femtoseconds to several picoseconds, depends strongly on these excitation conditions: Typically, during the first tens of femtoseconds after the excitation, momentum polarization induced by the distinct polarization direction of the light field dominates the electron gas.

To address the relaxation dynamics of this momentum polarized state, we solve a kinetic momentum-resolved Boltzmann equation with focus on electron-phonon interaction and introduce orientational relaxation as first temporal step in a sequence of relaxation processes followed by thermalization and cooling. Applying a self-consistent treatment of Maxwell's equations and material dynamics we are able to present results for the optical and thermal properties of plasmonic nanostructures after linear and non-linear optical excitations. Thereby, Pauli-blocking non-linearities in the electron-phonon interaction modify the relaxation dynamics for strong excitations and effect the optical response of the electron gas.

O 96.10 Fri 12:45 H4

Sum-Frequency Generation Spectro-Microscopy in Barium Titante — •Dorothee Mader[1], David Pesquera[2], Saptam Ganguly[2], Richarda Niemann[1,3], Martin Wolf[1], Sebastian F. Maehrlein[1], Jose Santiso[2], and Alexander Paarmann[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain — [3]Vanderbilt University, Nashville, USA

Ferroelectric Barum Titanate (BTO) can be switched by excitation of phonons in the infrared (IR), enabeling the applications in future optical technologies.[1] Here, we investigate the resonance behavior of BTO in the IR by employing infrared-visible (IR-VIS) sum-frequency generation (SFG) spectro-microscopy using the free-electron laser of the Fritz Haber Institute.[2,3] As a second-order nonlinear technique, this method is sensitive to the material's symmetry. Additionally, as it is employed resonantly, it can reveal vibrations, local structure and bonding of the material. We demonstrate resonant ferroelectric imaging using SFG spectro-microscopy for bulk BTO and 500 nm thin BTO membranes.

[1] M. Kwaaitaal et al., Nat. Photonics 82(3), 2731, (2024).
[2] R. Niemann et al., Appl. Phys. Lett. 120, 131102, (2022).
[3] D. Mader et al., J. Chem. Phys. 161, 094706 (2024).

O 97: Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties II

Time: Friday 10:30–12:30 Location: H6

O 97.1 Fri 10:30 H6

Nanostructuring of organic radicals on hybrid interfaces — •Arkaprava Das, Ewa Malgorzata Nowik-Boltyk, Tobias Junghoefer, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Organic radicals are potential candidates for groundbreaking applications like energy storage, quantum computing, and spintronics. In order to investigate the nature of the adsorption of the radical derivative molecules on hybrid surfaces based on polycrystalline Au and native SiO_2, we investigate their electronic structure and morphology. The electronic structure at the interface is investigated by using X-ray photoelectron spectroscopy (XPS) and the morphology is studied with scanning electron microscopy. The substrate-dependent interface interactions have resulted in different nanostructures crucial for device fabrication whereas changes in line shape of core level spectra confer direct evidence of changed electronic properties.

O 97.2 Fri 10:45 H6

Beyond the Koopmans' theorem: Energy-level alignment of PTCDA on BlueP-Au-network on Au(111) — •Maximilian Schaal[1], Felix Otto[1], Marco Gruenewald[1], Roman Forker[1], Keisuke Fukutani[2], Satoshi Kera[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan

Koopmans' theorem is often used to relate the observed spectroscopic features in UP spectra to the orbital energies of molecules calculated by Hartree-Fock calculations. However, this theorem neglects the self-energy (charging energy),

which can be as large as 1 eV for molecules in the gas phase [1]. Therefore, the ground state energy levels of the frontier orbitals are not sufficient to describe the energy-level alignment and the initial and final states must be considered [2].
In this study, we present a framework to investigate the energy-level alignment of a monolayer of PTCDA decoupled from the Au(111) surface by a BlueP-Au-network [3]. We have determined the electronic transport and the optical gap using differential reflectance and (low-energy inverse) photoelectron spectroscopy. From these values, we determined the exciton binding energy and the charging energy. Finally, we compared the energy levels of the adsorbed monolayer with measured and calculated quantities of molecules in the gas phase.
[1] Kirchhuebel *et al.*, J. Phys. Chem. C **124** (2020).
[2] Kirchhuebel *et al.*, Phys. Chem. Chem. Phys. **21** (2019).
[3] Gruenewald *et al.*, Phys. Rev. Materials **6** (2022)

O 97.3 Fri 11:00 H6

Disentangling the components of a multireference excited state in an isolated chromophore — Rodrigo Ferreira[1,2], Tomáš Neuman[1], Amandeep Sagwal[1], Jiří Doležal[2], Petr Kahan[1], and •Martin Švec[1,2] — [1]Institute of Physics, Czech Academy of Sciences — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

Excited states of open-shell chromophores are commonly multireference in their nature. Distinguishing the components of these superposition states in a single chromophore by experimental means is a challenging task as it would essentially require capturing their orbital occupancies in the excited state. We demonstrate this can be achieved by atomically precise mapping of photon-induced tunneling current under a varying electric field, on a model case of a PTCDA anionic excited state coupled to a plasmonic nanocavity. To simulate the cascade of energy conversions and charge transfer events occurring within the molecule, a set of rate equations is derived from a many-body state scheme using an input from TD-DFT. The resulting bias-dependent tunneling current maps reach a very good agreement with the experimental data, corroborating the validity of the theoretical understanding.

O 97.4 Fri 11:15 H6

Second harmonic spectroscopy of Fe-porphyrin/Cu(001) interfaces — •Newsha Vesalimahmoud, Mahendra Kabbinahithlu, Ping Zhou, Uwe Bovensiepen, and Andrea Eschenlohr — University of Duisburg-Essen, Faculty of Physics and CENIDE, Lotharstr. 1, 47057 Duisburg, Germany

When a molecule interacts with a metal surface, metal-molecule interaction induces a rearrangement of their electronic densities, shifting the molecular orbitals relative to the metal's Fermi level. This study focuses on the FeOEP/Cu(001) interface, using interface-sensitive SHG spectroscopy. We analyze polarization- and wavelength-dependent SHG for varying molecular adsorbate thicknesses on Cu(001) using a fundamental beam in the 500-600 nm range. Polarization-dependent measurements show a higher SHG yield for p-P polarization than s-P SHG, as the intrinsic value of $\left|\chi^{(2)}_{zzz}\right|$ is much larger than $\left|\chi^{(2)}_{zxx}\right|$. As the number of monolayers increases, P-polarized SHG intensity decreases due to reduced nonlinear susceptibility from less polarizable free electrons, while S-polarized SHG shifts from 4-fold to 2-fold symmetry. The SHG spectra show an intensity peak at 2.17 eV due to a one ω resonance in Cu(001). After adsorption of 2, 5, and 8 monolayers (ML) of FeOEP on Cu(001), the spectral dependence remains similar to the Cu(001) surface, except for an enhancement at 2.21 eV for 5ML and 8ML. This enhancement is attributed to the energetic position of the lowest unoccupied molecular orbital (LUMO) at the FeOEP/Cu(001) interface.

O 97.5 Fri 11:30 H6

Probing the Roles of the Substrate Material, Spin Scattering, Temperature and Cooperative Effects in CISS — •Paul V. Möllers[1], Adrian J. Urban[2,3], Bianca C. Baciu[4], Rafael Rodriguez[5], Albert Guijarro[4], Jeanne Crassous[5], Steven De Feyter[3], Hiroshi M. Yamamoto[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience (SoN), University of Münster, Busso-Peus-Str. 10, 48149 Münster, Germany — [2]Institute for Molecular Science, Research Center of Integrative Molecular Systems, Division of Functional Molecular Systems, 38 Nishigonaka, Myodaiji Okazaki, Aichi prefecture, 444-8585 Japan — [3]Division of Molecular Imaging and Photonics, Department of Chemistry, KU Leuven, Celestijnenlaan 200 F, 3001 Leuven, Belgium — [4]Departamento de Química Orgánica, Instituto Universitario de Síntesis Orgánica, Unidad asociada al CSIC, Universidad de Alicante, E-03080, Alicante, Spain — [5]University of Rennes, CNRS, Institut des Sciences Chimiques de Rennes (ISCR), UMR 6226, Rennes, France

Monolayers of heptahelicene ([7]H) and helical tetrapyrrole (TPBT) complexes were adsorbed onto different single-crystalline metal substrates, and the spin polarization of photoelectrons emitted from these surfaces was measured. The substrate material, the temperature and the surface coverage were systematically varied to investigate the roles of the substrate spin–orbit coupling, molecular vibrations, and intermolecular interactions in the generation of the spin polarization. Furthermore, thiolized (chemisorbed) [7]H and all-carbon (physisorbed) [7]H layers were compared.

O 97.6 Fri 11:45 H6

Electrons don't wear bowties: The mechanism of Fermi-level pinning and charge for mixed donor-acceptor layers — •Richard Berger1 and Oliver T. Hofmann — TU Graz, Institute of Solid State Physics

Controlling the work function of metal substrates is critical when optimizing the performance of organic electronic devices. A particular powerful method to obtain such control is by employing a monolayer of strong electron donors or electron acceptors, i.e. so-called Fermi-level pinned systems which form charge-transfer-induced dipoles with the underlying substrate However, while the major advantage of this Fermi-level pinned systems is that the effective work function of the interface is (essentially) independent of the underlying substrate, there are only limited ways to fine-tune it. A more flexible way could be to employ a mixture of electron donors and acceptors. However, for such complex systems the underlying charge-transfer mechanism is less clear. In this work, we elucidate this mechanism using machine-learning augmented density functional theory calculations to predict both the atomistic and the electronic structure of the interface using a mixture of F4TCNQ and paraquat as an example. Counterintuitively, we find that the nominally weaker donor overpowers the stronger acceptor, resulting in a dependence of the work function that is effectively determined by the nominal coverage of the donor. At the same time, we find that multiple geometries are energetically very similar, but result in different work function, affecting the reproducibility of different experimental realizations.

O 97.7 Fri 12:00 H6

Magnetic Coupling in Triangulene Dimers: Impact of Number and Dihedral Angles of para-Biphenyl Linkers — •Marco Lozano[1], Elena Perez-Elvira[2], Qiang Huang[3], Ji Ma[3], Aurelio Gallardo[2], Ana Barragan[2], Alba Garcia-Frutos[2], Koen Lauwaet[2], Jose Gallego[4], Pavel Jelinek[1], David Ecija[2], Diego Soler-Polo[1], and Jose Urgel[2] — [1]Institute of Physics of the Czech Academy of Science, CZ-16253 Praha, Czech Republic — [2]IMDEA Nanoscience, C/ Faraday 9, Campus de Cantoblanco, 28049 Madrid, Spain — [3]Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01069 Dresden, Germany — [4]Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Cantoblanco, 28049 Madrid, Spain

Triangulene and its homologues are promising building blocks for high-spin low-dimensional networks with long-range magnetic order. Despite the recent progress in the synthesis and characterization of coupled triangulenes, key parameters such as the number or the dihedral angles of organic linking units remain scarce, making further studies crucial for an essential understanding of their implications. Here, we investigate the synthesis of two triangulene dimers linked by two or one para-biphenyl units on a metal surface in an UHV environment. First-principles calculations and model Hamiltonians reveal how the spin excitation and radicalism depend on the rotation of the para-biphenyl units.

O 97.8 Fri 12:15 H6

Insights into Nonlinear CD-ee Dependence in Tryptophan Thin Films — •Charitini Panagiotopoulou, Changseop Jeong, Ueli Heiz, and Aras Kartouzian — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chiral analysis is essential, especially for enantio-separation and -enrichment, with Circular Dichroism (CD) spectroscopy being a fast and straightforward method for studying enantiomeric excess (ee) and its dependence on circular dichroism (CD-ee dependence). While most systems show linear CD-ee dependence, studies reporting non-linear CD-ee behaviour are relatively rare and, thus, more attractive for research. Building on our earliest findings of negative nonlinear CD-ee dependence in polycrystalline BINOL thin films (Liang et al. 2023), we extend this study to a different system: the well-known amino acid responsible for synthesizing important proteins in humans, Tryptophan. We prove our hypothesis that the non-linear CD-ee dependence is not limited to BINOL films and can be applied to biomolecules, and we outline this non-linear dependence with different methods, such as CD spectroscopy, SHG-CD spectroscopy and FTIR study. This behaviour is linked to the structural characteristics of Tryptophan when a series of different enantiomeric excesses are deposited onto thin films via molecular evaporation. This approach paves the way for extensive exploration in the field of biomolecular chirality.

O 98: Metal and Semiconductor Substrates: Adsorption and Reactions of Small Molecules

Time: Friday 10:30–12:30 Location: H8

O 98.1 Fri 10:30 H8

Bonding properties of a CO molecule with metallic adatoms — •Fabian Stilp, Marco Weiss, Maximilian Krüger, and Franz J. Giessibl — Department of Physics, University of Regensburg

CO terminated AFM tips are often used to investigate molecules on surfaces as they are a powerful tool to make the internal structure of such molecules visible. Their chemical inertness results in high resolution of the single atoms and bonds in such molecule via Pauli repulsion. However, it was shown by Huber et al. [1] that CO terminated tips can form weak bonds to some species of adatoms on a Cu (111) sample such as Fe and Cu as evident by an attractive center within a repulsive ring in constant height AFM measurement. In contrast, Si adatoms only interact via van der Waals attraction and Pauli repulsion.

Can one predict the strength of the bond between the CO molecule and an arbitrary atom just from its electron configuration? To set the rules for this prediction we expand our collection of AFM measurements on various adatoms by adding Ni and Ag.

Ni has a partially filled d-shell and thus forms a chemical bond of similar strength as Fe. Surprisingly, Ag with its similar electron configuration as Cu, immediately goes to Pauli repulsion while Cu first forms a weak bond.

[1] Huber et al., Science 366, 235-238 (2019).

O 98.2 Fri 10:45 H8

Adsorption sites of merocyanines on the Ag(100) surface determined by NIXSW — •Anna Juliana Kny[1], Anja Haags[2], Sergey Subach[2], and Moritz Sokolowski[1] — [1]Clausius Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany — [2]Forschungszentrum Jülich, Germany

The growth of thin organic layers is strongly influenced by the interactions between the molecule and the substrate surface. We report about the adsorption sites of a series of merocyanine (MC) molecules on the Ag(100) surface. MCs are prochiral donor-acceptor molecules which are in focus for applications due to high transition dipole moments. [1] Remarkably, SPA-LEED data reveal commensurate structures for all of our investigated MCs, although the size of the unit cells depends on the length of the alkyl side chains.[2] In order to answer the question of what is behind the commensurate growth of these complex molecules, we performed an XPS and an NIXSW investigation. We find a strong binding of the two sulfur heteroatoms, located in the thiophene and the thiazole rings, to the Ag surface. This can be seen in charge transfer and an adsorption of the S-atoms close to on-top sites. This is found for all investigated structures. Furthermore, compatible with the symmetry of the unit cell, the results reveal that the four molecules per unit cell sit on two different adsorption sites.

We acknowledge experimental support from D.A. Duncan (DLS). Supported by the DFG through the research training group 2591 and the Diamond Light Source, UK.

[1] JACS 137 (2015) 13524. [2] Nanoscale 15 (2023) 10319.

O 98.3 Fri 11:00 H8

Electron-Induced Dehydrogenation of Acetylene and Ethylene on Si(100) — Rafik Addou, Damian Allis, Ryan Groome, Si Yue Guo, Aru Hill, Hadiya Ma, Cameron Mackie, •Oliver MacLean, Marc Savoie, Marco Taucer, Alexander Therien, Finley van Barr, and Ryan Yamachika — CBN Nanotechnologies Inc.

Low-Temperature Scanning Tunneling Microscopy (STM) is a powerful tool for manipulating individual atoms and molecules on surfaces. The Si(100) surface is a technologically relevant substrate; however, its high reactivity and structural complexity has led to limited examples of molecular manipulation. Here, we demonstrate the electron-induced dehydrogenation of two simple hydrocarbons on Si(100) at 4 K. Excitation by tunneling electrons at or above +3.2 V led to rotation, migration, or desorption of acetylene, consistent with previous observations on ethylene. At similar biases, dehydrogenation to C2 was also observed, which bound in on-dimer, inter-dimer, and inter-row configurations, as supported by STM simulations. At +4.2 V and above, excitation induced rotation of C2 between configurations, but conversion back to the starting adsorbates was never observed. Tunneling-electron excitation of ethylene yielded the same C2 products. Dehydrogenation of acetylene by field emission was also observed, with an effect ranging from a single to thousands of molecules, depending on the parameters chosen. This exploration of electron-induced dehydrogenation and rotation points to new possibilities in molecular manipulation on semiconductors.

O 98.4 Fri 11:15 H8

Selectivity on and off: adsorption of allyl ethers on Si(001) — •Sophie Göbel[1], Timo Glaser[1], Alexa Adamkiewicz[2], Jannick Peters[1], Julian Heep[1], Ulrich Höfer[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany

Adsorption of organic molecules with more than one functional group on solid surfaces is of importance in the field of molecular electronics as they can be the starting point for multilayer systems [1]. To obtain well-organized monolayers of such bifunctional molecules, the understanding of their adsorption behavior, in particular in terms of their selectivity, is mandatory.

For allyl methyl ether (AME) and allyl ethyl ether (AEE), which combine an ether group with a C=C double bond, we show by means of XPS and STM that the adsorption of these molecules on Si(001) proceeds selectively via ether cleavage up to room temperature. The results are surprising as both functional groups involved show in general high reactivity on Si(001) and the ether group is less reactive when the isolated functional groups are compared. In contrast to AME and AEE, no such selectivity was observed for methoxy butene, where both functional groups are separated by an additional CH_2 unit. The results are discussed in terms of the interplay of electronic and geometric structure and its influence on the adsorption process.

[1] T. Glaser, et al., Chem. Mater. 36, 561 (2024).

O 98.5 Fri 11:30 H8

The Effect of Doping in Inelastic H Atom Scattering from Silicon — •Malte Opfermann, Sophia Tödter, Kerstin Krüger, and Oliver Bünermann — Institut für physikalische Chemie, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Recent inelastic H atom scattering experiments from the semiconducting Ge(111)c(2x8) have shown a bimodal energy loss distribution. One of the components was narrow with a small energy loss. The other component has shown a broad and large energy loss with an onset equal to the surface band gap.[1] While the low energy loss channel is explained by an adiabatic molecular dynamics simulation, the high energy loss component is not described theoretically yet.

To gain a better understanding of the underlying mechanism, we extended our studies to the Si(100)2x1 surface which is semiconducting as well. Despite its electronic structure being similar to the Ge(111)c(2x8) surface, it shows a different H atom energy-loss distribution. The first component is much broader and the second component does not show a clear onset at the surface band gap, both indicators of electronic effects. To further investigate, we carried out scattering experiments from samples with various doping levels.

[1] Krüger et al., Nat. Chem., DOI:10.1038/s,41557-022-01085-x (2022)

O 98.6 Fri 11:45 H8

Adsorption and bowl inversion of sumenene adsorbed on Au(111): a density functional theory — •Ikutaro Hamada[1], Ranmaru Kuno[1], Kota Iwata[2], Yoshiaki Sugimoto[2], and Hidehiro Sakurai[3] — [1]Department of Precision Engineering, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan — [2]Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Chiba 277-8561, Japan — [3]Division of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan

Sumanene, a bowl-shaped π-conjugated compound, has been shown to form an ordered overlayer on noble metal surfaces. It has also been shown to exhibit conformation change, namely, bowl inversion, depending on its environment [1,2]. Experimentally, we have found that on Au(111), sumanene forms an ordered overlayer that differs from the previously reported structure for Au(111), but resembles the one observed on Ag(111). Moreover, we have demonstrated that bowl inversion can be induced using an atomic force microscopy tip. In this work, we employ van der Waals density functional to investigate the geometric and electronic structure of sumanene on Au(111). We also investigate the detailed mechanism of the bowl inversion of sumanene within the overlayer on the surface.

[1] R. Jaafar et al., J. Am. Chem. Soc. 136, 13666 (2014). [2] S. Fujii et al., J. Am. Chem. Soc. 138, 12142 (2016).

O 98.7 Fri 12:00 H8

Enhancing the electronic-coupling and conductivity of monolayer film of ferrocenyl molecules by Pd and Cu doping — •Sunny M P Gautam, Himani Malik, Vikash Meghwal, Sruthi Manoharan, Vinithra Gurunarayanan, Ramesh Ramapanicker, and Thiruvancheril G Gopakumar — Department of Chemistry, Indian Institute of Technology Kanpur, India

Enhancing the conductivity and tuning the electronic structure of molecular films is crucial for their application in electronics. In this study, we explore the impact of metal doping (Pd and Cu) on the electronic structure and conductivity of two custom-designed ferrocenyl molecules, 3-ferrocenyl propanoic acid (FcC3) and 5-ferrocenyl pentadienoic acid (FcC5), on a graphite surface. Although the microscopic arrangement of the molecules within the film remains largely unchanged after doping, the incorporation of Pd and Cu at the 4-coordinated carboxyl dimer site of FcC3/FcC5 leads to a significant increase in conductivity. Electronic structure calculations of the FcC3/FcC5 dimers with metal show a substantial reduction in the HOMO-LUMO gap compared to

their hydrogen-bonded counterparts, indicating stronger intermolecular electronic coupling through the Pd and Cu atoms, which lowers the barrier for electron/hole transport.

O 98.8 Fri 12:15 H8

Ge(CH2I)4 on Si(100) - Matching the Molecule to the Surface — •Brandon Blue, Rafik Addou, Damian G. Allis, Eduardo Barrera-Ramirez, Jeremy Barton, Adam Bottomley, Nina Culum, Michael Drew, Tyler Enright, Alan Godfrey, Ryan Groome, Aru Hill, Taleana Huff, Robert J. Kirby, Samuel Lilak, Cameron J. Mackie, Oliver MacLean, Terry McCallum, Mathieu Morin, Matthew Moses, Jonathan Myall, Ryan Plumadore, Adam Powell, Henry Rodriguez, Marc Savoie, Benjamin Scheffel, Marco Taucer, Denis Alexander Therien, Dusan Vobornik, and Janice Wong — CBN Nanotechnologies Inc.

We present an on-surface, multi-technique analysis of a synthetic, custom molecule for Si(100): tetrakis(iodomethyl)germane - Ge(CH2I)4, or TIMe-Ge. TIMe-Ge consists of four iodomethyl (CH2I) legs bound to a Ge atom core in a tetrahedral geometry. TIMe-Ge was selected based on its expected reactivity and surface behavior with Si(100)-2x1 as part of a set of design criteria which we'll present and discuss. The suitability of TIMe-Ge with respect to these criteria were supported by simulations and literature precedent. TIMe-Ge was found to covalently bond with Si(100)-2x1 in a limited number of configurations via C-I dissociative addition by STM, DFT, and XPS. The fourth CH2I is oriented away from the surface and towards the SPM for interaction, including controlled generation of C-centered radicals via bias pulses and UV photochemistry. We anticipate that TIMe-Ge and its congeners will aid in the development of molecular nanotechnologies and the study of requisite intermediates.

O 99: Ultrafast Electron Dynamics IV

Time: Friday 10:30–13:00 Location: H11

O 99.1 Fri 10:30 H11

Large-amplitude coherent phonon dynamics in a van der Waals ferroelectric — •Jan Gerrit Horstmann[1], Quintin Meier[2], Thomas Lottermoser[1], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Institut Néel, CNRS UPR2940, Grenoble, France

We explore the all-optical control of coherent phonon dynamics in the van der Waals ferroelectric WTe_2. Double-pulse optical excitation is harnessed to enhance the amplitude of the prominent interlayer shear mode beyond the limit of single-pulse excitation, with the resulting structural dynamics monitored via time-resolved second harmonic generation. A strong correlation between shear phonon amplitude and damping suggests higher-order coupling to lower-lying modes. At largest initial phonon amplitudes, Fourier transforms of the delay-dependent SHG traces reveal a frequency contribution at twice the shear-mode frequency. We discuss second-harmonic phonon generation and ultrafast phononic modulation of the nonlinear susceptibility as potential underlying mechanisms. Coherent vibrational control over relaxation pathways and electronic properties of ferroic van der Waals materials could enable novel types of devices for energy-efficient electronics.

O 99.2 Fri 10:45 H11

Giant acceleration of polaron transport by ultrafast laser-induced coherent phonon — •Huimin Wang[1,2], Xinbao Liu[1,2], Shiqi Hu[1,2], Daqiang Chen[1,2], Qing Chen[1,2], Cui Zhang[1,3], Mengxue Guan[1,2], and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China. — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China. — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

Polaron formation is ubiquitous in polarized materials, but severely hampers carrier transport for which effective controlling methods are urgently needed. Here, we show that laser-controlled coherent phonon excitation enables orders of magnitude enhancement of carrier mobility via accelerating polaron transport in a prototypical material, lithium peroxide (Li2O2). The selective excitation of specific phonon modes, whose vibrational pattern directly overlap with the polaronic lattice deformation, can remarkably reduce the energy barrier for polaron hopping. The strong nonadiabatic couplings between the electronic and ionic subsystem play a key role in triggering the migration of polarons, via promoting phonon-phonon scattering within sub-picoseconds. These results extend our understanding of polaron transport dynamics to the non-equilibrium regime and allow for optoelectronic devices with ultrahigh on-off ratio and ultrafast responsibility, competitive with those of state-of-the-art devices fabricated based on free electron transport. H.M.Wang et al. Sci.Adv.9,eadg3833(2023).

O 99.3 Fri 11:00 H11

Ultrafast charge density wave, Van Hove singularity and flat-band dynamics in the Kagome metal CsV_3Sb_5 — •Mohamed Amine Wahada[1], Chris Nicholson[1], Andrea Capa Salinas[2], Brenden R. Ortiz[2], Lawson Lloyd[3], Tommaso Pincelli[3], Tulio de Castro[1], Martin Wolf[1], Ralph Ernstorfer[3], Stephen D. Wilson[2], and Laurenz Rettig[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Materials Department and California Nanosystems Institute, University of California Santa Barbara, Santa Barbara, California 93106, USA — [3]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623 Berlin, Germany

The Kagome metal family AV3Sb5 (A=K, Rb, Cs) features an unconventional superconducting phase, coexisting with a parent charge density wave (CDW) phase. The origin of the CDW is still under debate. Moreover, this family exhibits a number of Van Hove Singularities (VHS) and a flat-band (FB) below the Fermi level, offering a unique platform for high electronic correlation. In order to gain insight into these properties, we study the ultrafast dynamics in CsV3Sb by using time and angle-resolved photoemission spectroscopy (trARPES). We discuss the ultrafast melting of CDW order, concomitant with a shift and a broadening for both the FB and the VHS, all being modulated by coherent phonon modes.

O 99.4 Fri 11:15 H11

Ultrafast Nonequilibrium Dynamics of Room Temperature Charge Density Wave Fluctuations in 1T-$TiSe_2$ — •Hibiki Orio[1], Samuel Beaulieu[2], Sarath Sasi[2], Akib Jabed[2], Muthu P.T. Masilamani[1], Maximilian Ünzelmann[1], Jan Minar[3], Friedrich Reinert[1], Kai Rossnagel[4], Sotirios Fragkos[2], and Jakub Schusser[1,3] — [1]Universität Würzburg, Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence, Würzburg, Germany — [2]Université de Bordeaux - CNRS - CEA, CELIA, Talence, France — [3]New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic — [4]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

$TiSe_2$ exhibits a 2×2×2 charge density wave (CDW) phase below 200 K, driven by the interplay between electron-hole and electron-lattice interactions. Nanoscale CDW domains, referred to as CDW fluctuations, persist even above the transition temperature. This exotic phase provides an intriguing platform for exploring the robustness of electron-hole interactions and electron-phonon coupling at elevated temperatures. Using time- and polarization-resolved XUV momentum microscopy, we investigate CDW fluctuations in $TiSe_2$ and their ultrafast light-induced dynamics. Our band structure mapping reveals that the backfolded Se 4p band associated with the CDW phase remains detectable even at room temperature. Furthermore, we demonstrate the ultrafast melting of these CDW fluctuations on an electronic timescale, followed by rapid recovery modulated by coherent amplitude phonon modes.

O 99.5 Fri 11:30 H11

Coherent phonons and quasiparticle renormalization in semimetals from first principles — •Christoph Emeis, Stephan Jauernik, Sunil Dahiya, Yiming Pan, Carl E. Jensen, Petra Hein, Michael Bauer, and Fabio Caruso — Kiel University, Germany

Coherent phonons offer a powerful means to manipulate structural and electronic properties of materials on ultrafast timescales, making them a key tool for exploring light-induced phase transitions and non-equilibrium dynamical phenomena.

We present an *ab initio* theory for the displacive excitation of coherent phonons in semimetals. We formulate a computational workflow for modelling light-induced structural changes and the resulting transient band-structure renormalization following excitation with a femtosecond laser. This framework is based on first-principles simulations of ultrafast electron and coherent phonon dynamics in the presence of electron-phonon interactions. We validate our approach through a combined theoretical and experimental study of coherent phonons in the semimetal antimony. The robust agreement between photoemission experiments and simulations corroborates our approach and paves the way for new opportunities to control structural and electronic degrees of freedom in semimetals via coherent phonon excitation.

C. Emeis *et al.* arXiv:2407.17118

O 99.6 Fri 11:45 H11

Ultrafast energy flow among electrons and phonons in a Pb/Si nanoscale heterosystem — •Christian Brand[1], Mohammad Tajik[1], Tobias Witte[1], Laurenz Rettig[2], Birk Finke[1], Björn Sothmann[1,3], Uwe Bovensiepen[1,3], and Michael Horn-von Hoegen[1,3] — [1]Department of Physics, University of Duisburg-Essen, Germany — [2]Department of Physical Chemistry, Fritz Haber Institute, Germany — [3]Center for Nanointegration Duisburg-Essen, Germany

In condensed matter, microscopic excitations interact on ultrafast time scales. The combination of suitable time domain experiments allows the analysis of processes such as the energy transfer from electrons to the nuclei subsequent to femtosecond laser pulse excitation. In this study, we used time-resolved photoelectron spectroscopy and ultrafast electron diffraction to probe the spatially confined dynamics of electrons and phonons in ultrathin epitaxial Pb films on Si(111). While the electrons lose their excess energy within 400 fs, the lattice vibrational displacements gradually increase over 3-8 ps. Within the time gap, the energy is transiently stored in high-frequency phonon modes as simulated in a three-temperature model. Their temperature is experimentally accessible by the transient electron temperature after equilibration with such hot phonons. The excitation of low-frequency phonons and the subsequent thermalization and equilibration of the lattice are facilitated by anharmonic phonon-phonon coupling within the Pb film.

O 99.7 Fri 12:00 H11

Resolving ultrafast atomic motion in WTe_2 — •Hanqian Lu[1,2], Victoria C. A. Taylor[2], Hyein Jung[1,2], Jannik Malter[1,2], Ralph Ernstorfer[1,2], and Yoav W. Windsor[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

WTe_2 is a layered transition metal dichalcogenide with a distorted layered structure leading to distinct material properties. Here we study its lattice dynamics following ultrafast photoexcitation, using femtosecond electron diffraction (FED). We observe a strong coherent lattice response as well as growth of incoherent atomic vibrations, which we qualitatively describe as previously done. With the goal of describing such motions microscopically, we develop a quantitative model that extracts both the coherent and the incoherent atomic motions of each W and Te atom in the unit cell.

O 99.8 Fri 12:15 H11

Structural dynamics of the silicon (111)-(7×7) surface upon optical excitation studied by ultrafast reflection high-energy electron diffraction — •Jonas Darius Fortmann[1], Birk Finke[1], Christian Brand[1], and Michael Horn-von Hoegen[1,2] — [1]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

We present first results on the ultrafast structural dynamics of the Si(111)-(7×7) surface subsequent to an optical excitation. The surface is excited by an 800 nm fs-laser pulse at various fluences. The structural dynamics is followed through ultrafast reflection high-energy electron diffraction (URHEED) at a sample temperature of 80 K by means of the Debye-Waller effect. The surface has been excited for incident fluences > 1.6 mJ/cm^2 at a drop of RHEED intensity by only 0.8%. For the highest fluence of 5.4 mJ/cm^2 the intensity drop was 2% which is equivalent to a rise of surface temperature by 7 K. The fluence dependence is explained by linear absorption through the metallic surface state of the 7×7 reconstruction. For higher fluences we observe an additional three photon absorption due to bulk excitation in order to overcome the direct bandgap. The recovery to the groundstate occur via several processes at different time constants. The system has not fully recovered the groundstate after 200 μs, which indicates the population of a long-lived electronic state.

O 99.9 Fri 12:30 H11

Ultrafast imaging ellipsometry or interferometry - Which one is more suitable to measure the dielectric function of laser-excited materials? — •Markus Olbrich, Theo Pflug, Andy Engel, and Alexander Horn — Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany

Changes of the dielectric function of materials due to excitation by ultrafast laser radiation are crucial for understanding fundamental processes such as absorption of electromagnetic radiation or the relaxation of the excited electrons resulting in changes in the density of state of the material. The transient dielectric function can either be measured by ultrafast ellipsometry or interferometry. This study evaluates the advantages and disadvantages of each method exemplarily for an excited thin gold film induced by ultrafast laser radiation ($\lambda = 800$ nm, $\tau_H = 40$ fs) at fluences below and above the ablation threshold. The focus of the presentation is on characterizing the methodology including the experimental effort, the obtained signal-to-noise ratio, the data evaluation particularly in the limits of the applied optical model, as well as the physical interpretation of the measured data.

O 99.10 Fri 12:45 H11

Anisotropic electronic response in hexagonal boron nitride to laser excitations from real-time time-dependent density functional theory — •Cheng Wang, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Hexagonal boron nitride (h-BN) has a graphite-derived structure where nitrogen (N) and boron (B) atoms occupy alternating sites. In the framework of real-time time-dependent density functional theory (RT-TDDFT), as implemented in the Elk code, we systematically study the response of bulk and single layer h-BN to laser pulses with in- and out-of-plane polarization, different photon energies, duration and fluences. Our analysis focuses on transient charge redistribution and changes in occupation numbers, revealing a marked dependence on both polarization and frequency in bulk and monolayer h-BN. For a photon energy of 4.8 eV, slightly above the DFT band gap, we find a notable charge transfer from N to B p_z-orbitals in both bulk and monolayer for in-plane polarization. At 9.5 eV, excitations occur primarily between occupied and unoccupied N p_x-orbitals with a small charge transfer to B. In the monolayer, these excitations are suppressed for out-of-plane polarization. Finally, we compare our findings for monolayer h-BN with analogous calculations for graphene.

We gratefully acknowledge the funding provided by the DFG through CRC 1242, project C02. We acknowledge computation time at the MagnitUDE and AmplitUDE HPC systems at the University of Duisburg-Essen.

O 100: Focus Session Chemical Imaging for the Elucidation of Molecular Structure II (joint session O/BP)

Unravelling the multiscale molecular heterogeneity at interfaces is one of the main challenges in modern biophysics and surface science due to the major role specific structural properties play in determining their macroscopic function and behavior. In the last few decades, several specialized chemical imaging techniques have been developed that can reveal many of these crucial structural details, representing an enormous advance in our elucidative capabilities. Clear examples of this range from super-resolution and 3D tomography to tag-free characterization down to the single-molecule level. This focus session will explore the vast range of methods and possibilities for characterizing the different structural aspects in heterogeneous molecular systems and specifically highlight the potential complementarity of the different techniques through multi-modal approaches. Overall, by bringing together different communities, this session aims to foster scientific exchanges that could spark the next major developments in chemical imaging.

Organized by Martin Thämer (FHI Berlin), Alexander Fellows (FHI Berlin), and Kerstin Blank (University Linz)

Time: Friday 10:30–12:45 Location: H24

Invited Talk O 100.1 Fri 10:30 H24

Multidimensional Super-resolution Imaging: Wasting Light to Learn New Things — •Steven Lee — University of Cambridge

The talk will outline two single-molecule fluorescence approaches that can be used to determine orthogonal metrics about a single emitter.

The first half introduces "POLCAM," a simplified single-molecule orientation localization microscopy (SMOLM) method based on polarised detection using a polarisation camera. POLCAM's fast algorithm operates over 1000 times faster than the current state-of-the-art, allowing near-instant determination of molecular anisotropy. To aid adoption, open-source image analysis software and visualization tools were developed. POLCAM's potential was demonstrated in studying alpha-synuclein fibrils and the actin cytoskeleton of mammalian cells. (Nature Methods 2024). The second approach focuses on "Single-Molecule Light Field Microscopy" (SMLFM), encoding 3D positions into 2D images for volumetric super-resolution microscopy. SMLFM shows an order-of-magnitude speed improvement over other 3D PSFs, resolving overlapping emitters through parallax. Experimental results reveal high accuracy and sensitivity in point detection, enabling whole-cell imaging of single membrane proteins in live primary B cells and high-density volumetric imaging in dense cytosolic tubulin datasets. (Nature Comms 2024)

Invited Talk O 100.2 Fri 11:00 H24

MALDI mass spectrometry imaging: application examples ranging from food analysis to pharmaceutical research — •Andreas Römpp — Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany

Mass spectrometry imaging is an analytical technique that provides spatially-resolved molecular information for a wide range of compound classes. In contrast to many histological methods, it does not require labeling. The capabilities and limitations of MS imaging will be discussed on the basis of several application areas with a focus on food analysis and pharmaceutical research. In our study 'MALDI mass spectrometry imaging: from constituents in fresh food to ingredients, contaminants and additives in processed food' (https://doi.org/10.1016/j.foodchem.2022.132529) we analyzed a range of plant-based and meat-based food. The analysis of natamycin in cheese and acrylamide in gingerbread constitute the first mass spectrometry imaging measurements of a food additive and a food contaminant, respectively. MS imaging is the only method that can analyze the distribution of drug compounds in animal models or human tissue (without labeling). This is exemplified on the detection of anti-tuberculosis drugs in mouse model tissue including our most recent study on the clinical stage antibiotic BTZ-043 which has just been accepted for publication in Nature Communications (https://doi.org/10.1038/s41467-025-56146-9).

O 100.3 Fri 11:30 H24

On-Surface Synthesis and Characterization of a Nitrogen-Containing Heterocycle — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Matthias Zeilerbauer[1], Shadi Fatayer[2], and Laerte Patera[1] — [1]University of Innsbruck, Austria — [2]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Nitrogen-containing heterocycles are fundamental building blocks in nature, forming the core of essential biomolecules and pharmaceuticals. This study demonstrates the on-surface formation of an N-heterocyclic organic compound via thermal activation of a tailored precursor. High-resolution non-contact atomic force microscopy (nc-AFM) provides bond-level resolution of the synthesized structures. Complementary scanning tunneling spectroscopy visualizes changes in the electronic structure resulting from the formation of the heterocycle. Density functional theory calculations (DFT) reveal the most probable reaction mechanism, highlighting the critical role of hydrogen release as the driving force of the reaction. These findings emphasize the versatility of on-surface synthesis as a powerful tool for creating complex organic compounds.

O 100.4 Fri 11:45 H24

Elasticity Mapping of Nonahelicene with Submolecular Resolution by NC-AFM — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 NishigoNaka, Myo-daiji, Okazaki 444-8585, Japan

Controlled modification of atomic configurations of molecules and materials is an exciting goal for non-contact atomic force microscopy (NC-AFM). Certain changes like shifts of the electronic energy gaps may be expected, but are not well explored and not established on the molecular scale. Here we report quantitative measurement of atomic-scale deformation in single molecules with NC-AFM. Individual molecules of nonahelicene ([9]H) and coronene (Cor) were studied on a Ag(110) surface under ultrahigh vacuum and cryogenic conditions by the measurement of frequency-shift distance curves for this. The molecular responses can be replicated with an empirical Lennard-Jones model, but for [9]H an elastic contribution is required to account for its elastic nature. Furthermore, a 3D-force mapping technique, termed molecular deformation mapping (MDM), allows to study the lateral position dependence of the elastic response. The MDM of [9]H reveals a spatially strongly anisotropic behaviour for the elasticity, interaction forces, elongation and binding energy of the tip to the molecule. The result is rationalized in terms of an aromaticity model.

O 100.5 Fri 12:00 H24

Detection and control of quantum proton ordering in hydrogen bonds at the atomic scale — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Directly probing the spatial arrangements and quantum nature of protons in hydrogen-bonded (H-bonded) materials and biosystems is the key to understand their macroscopic properties and functions. Here, exploiting bond-resolved atomic force spectroscopy (BR-AFS) combined with path-integral molecular dynamics method, we demonstrate for the first time that BR-AFS measurements along the apparent H-bond between proton donor and acceptor atoms allows the identification of both classical H-bonds with inherent directionality and non-classical H-bonds with quantum proton delocalization in self-assembled imidazole derivatives on surfaces. Unlike the conventional unidirectional H-bonding in linear chains, chiral cyclic hexamers exhibit unique quantum proton ordering in their ground states, which contain a mix of classical and non-classical H-bonds, breaking rotational symmetry. Furthermore, we show the capability to switch the quantum-proton-ordering state on and off by altering the adsorption registry coupled with a collective transfer of six protons within the cyclic H-bonds. These findings open new pathways for detecting and controlling complex proton orders and for engineering proton-based quantum states with atomic-level precision.

O 100.6 Fri 12:15 H24

Imaging of the conformations of individual β-cyclodextrins with non-contact AFM — Marko Grabarics[1], •Benjamin Mallada[1,2,3], Shayan Edalatmanesh[2,3], Stephan Rauschenbach[1], Pavel Jelinek[2,3], and Bruno de la Torre[2] — [1]Kavli Institute for Nanoscience Discovery, University of Oxford, UK — [2]CATRIN, Palacký University Olomouc, CZ — [3]Institute of Physics, Czech Academy of Sciences, CZ

Glycans, biopolymers essential to biology and materials science, are highly complex due to their structural diversity, conformational flexibility, and numerous possible isomers. Conventional methods often struggle to resolve these structures with atomic precision, especially under solvent-free conditions. We employ nc-AFM under UHV to determine the atomic structure of β-cyclodextrin (β-CD), a cyclic glucose molecule.

Our results reveal the adsorption geometries, hydroxy group positions, and stabilizing hydrogen bonds on a Au(111) surface. The primary face forms a closed hydrogen-bond network, while the secondary face exhibits pairwise interactions between OH groups of the same glucose monomer. DFT calculations validate these findings, enabling precise structural assignment and capturing subtle conformational differences.

This work highlights nc-AFM's capability to overcome the limitations of conventional sequencing techniques and represents the first application of nc-AFM to glycans. Future integration with ion deposition techniques could extend its utility to more complex glycans.

O 100.7 Fri 12:30 H24

Domain size effects in the spectra of micro-heterogeneous samples — •Thomas Mayerhöfer[1,2] and Jürgen Popp[1,2] — [1]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Helmholtzweg 4, 07743 Jena, Germany

Samples are often not composed of a single pure compound but are instead mixtures of different substances. Under the Bouguer-Beer-Lambert approximation, the absorbance spectra of such mixtures can be simply derived by summing the spectra of the individual components, with each spectrum weighted by the molar fraction of the corresponding compound.

In the context of wave optics, the resolving power of light at a given wavelength becomes crucial. If a microscope using light at this wavelength can distinguish structural details within the sample, the sample is classified as micro-heterogeneous. In this case, spatial averaging occurs at the intensity level, involving reflectance and transmittance rather than absorbance.

The shift from micro-heterogeneity to macro-heterogeneity is gradual and cannot be described by an analytical formula due to the wave nature of light. This has significant implications for spectrum interpretation, as it can lead to substantial variations in peak shapes, positions, and intensities, e.g., during mitosis.

O 101: Topology and Symmetry-protected Materials (joint session O/TT)

Time: Friday 10:30–12:15 Location: H25

O 101.1 Fri 10:30 H25

Topological material in the III–V family: heteroepitaxial InBi on InAs — •L. Nicolaï[1], J. Minár[1], M.C. Richter[2,3], O. Heckmann[2,3], J.-M. Mariot[4], U. Djukic[2], J. Adell[5], M. Leandersson[5], J. Sadowski[6], J. Braun[7], H. Ebert[7], J.D. Denlinger[8], I. Vobornik[9], J. Fujii[9], P. Šutta[1], G.R. Bell[10], M. Gmitra[11,12], and K. Hricovini[2,3] — [1]Univiversity of West Bohemia — [2]CY Cergy-Paris Université — [3]Université Paris-Saclay — [4]Sorbonne Université — [5]Lund University — [6]Polish Academy of Sciences — [7]LMU München — [8]ALS — [9]Istituto Officina dei Materiali, CNR — [10]University of Warwick — [11]Pavol Jozef Šafárik University in Košice — [12]Slovak Academy of Sciences

InBi(001) is formed epitaxially on InAs(111)-A by depositing Bi on to an In-rich surface. ARPES measurements reveal topological electronic surface states, close to the $\overline{M}$ high symmetry point. InBi surprisingly shows coexistence of Bi and In surface terminations. For the Bi termination, the study gives a consistent physi-

cal picture of the topological surface electronic structure of InBi(001) terminated by a Bi bilayer rather than a surface formed by splitting to a Bi monolayer termination. Theoretical calculations based on relativistic DFT and the one-step model of photoemission clarify the relationship between the InBi(001) surface termination and the topological surface states, supporting a predominant role of the Bi bilayer termination. Furthermore, a tight-binding model based on this Bi bilayer termination with only Bi–Bi hopping terms gives a deeper insight into the spin texture[1]. [1] Nicolaï *et al.* Phys. Rev. Research 6.4 (2024): 043116.

O 101.2 Fri 10:45 H25

Hidden spin-texture in an inversion-symmetric Dirac crystal — Kenta Hagiwara[1,2], Peter C. Schmitz[1], Philipp Rüssmann[1], Xin Liang Tan[1,2], Ying-Jiun Chen[3], Kui-Hon Ou Yang[4], Raman Sankar[5], Chien Jing[4], Yi-Hsin Shen[4], Mahmoud Zeer[1], Dongwook Go[6], Iulia Cojocariu[1], Daniel Baranowski[1], Vitaliy Feyer[1], Minn-Tsong Lin[1,6], Stefan Blügel[1], Claus M. Schneider[1,2], Yuriy Mokrousov[1,5], and •Christian Tusche[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, — [2]Faculty of Physics, University of Duisburg-Essen — [3]Ernst Ruska-Centre, Forschungszentrum Jülich — [4]Department of Physics, National Taiwan University, Taipei, Taiwan — [5]Academia Sinica, Taipei, Taiwan — [6]Johannes-Gutenberg University Mainz

A hidden spin polarization refers to a local spin polarization caused by apparent symmetry breaking and offers new perspectives for spintronics applications. Transition metal dichalcogenides can host various topological phases depending on the symmetry of their crystal structure. Here, by means of spin-resolving momentum microscopy, we reveal the spin texture of both topologically and symmetrically distinct surface and bulk Dirac cones in the inversion symmetric Dirac semimetal $NiTe_2$. We discovered a "hidden" spin polarization the bulk Dirac cone, localized at the different Te layers of the inversion symmetric bulk unit cell, such that the overlap of the two states results in a topologically trivial Dirac cone enforced by the global crystal symmetry. This work establishes a link between topology, spin-texture, and symmetry, enabling control by external perturbations.

O 101.3 Fri 11:00 H25

Edge spectroscopy of the quantum spin Hall insulator indenene — •Jonas Erhardt[1,2], Mattia Ianetti[3], Gianni Profeta[3], Domenico Di Sante[4], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Department of Physical and Chemical Sciences, University of L'Aquila — [4]Department of Physics and Astronomy, University of Bologna — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The non-trivial topology of the quantum spin Hall insulator indenene was recently demonstrated through bulk probes that reveal its topological band ordering [1,2]. According to the bulk-boundary correspondence, this ensures the existence of robust metallic states confined to the edge of this triangular indium monolayer. In this study, we employ scanning tunneling spectroscopy to investigate all three edge types of indenene for this correspondence. Our results demonstrate metallic edge density of states with suppressed backscattering near the bulk band gap, providing strong evidence for the existence of topologically protected edge states in indenene.
[1] M. Bauernfeind, J. Erhardt, and P. Eck *et al.*, Nat. Commun. **12**, 5396 (2021)
[2] J. Erhardt *et al.*, Phys. Rev. Lett. **132**, 196401 (2024)

O 101.4 Fri 11:15 H25

Bismuthene at the Graphene/SiC Interface: A Protected Quantum Spin Hall Insulator — •Niclas Tilgner[1], Susanne Wolff[1], Serguei Soubatch[2], Andres D. P. Unigarro[1], Sibylle Gemming[1], F. Stefan Tautz[2], Christian Kumpf[2], Thomas Seyller[1], Fabian Göhler[1], and Philip Schädlich[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Quantum spin Hall insulators (QSHIs) hold the potential to revolutionize next-generation technologies. Kane and Mele identified 2D honeycomb structures of heavy atoms with strong spin-orbit coupling as promising candidates for these materials. To realize this potential, however, the QSHI must be shielded from environmental influences. Previous research has demonstrated the intercalation of 2D Bi layers beneath graphene on SiC, resulting in the formation of two distinct phases. Among those, the β-phase exhibits a $(\sqrt{3}\times\sqrt{3})R30^\circ$ periodicity relative to the substrate. We identify the Bi adsorption site using x-ray standing wave imaging, a method which deterimes the element specific, 3D atomic distribution with respect to the bulk unit cell. After subsequent hydrogen intercalation, the Bi position changes significantly from hollow to top site adsorption. Further measurements with angle-resolved photoelectron spectroscopy reveal the band structure of the QSHI bismuthene with a pronounced Rashba splitting and slight p-type doping. We propose that the initial β-phase has to be considered as an electronically inactive layer of bismuthene, whose electronic structure can be established by subsequent hydrogen intercalation.

O 101.5 Fri 11:30 H25

Probing the Electronic Structure at the Boundary of Topological Insulators in the Bi2Se3 Family by Combined STM and AFM — •Christoph S. Setescak[1], Irene Aguilera[2], Adrian Weindl[1], Matthias Kronseder[1], Andrea Donarini[1], and Franz J. Giessibl[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Amsterdam and European Theoretical Spectroscopy Facility (ETSF), Amsterdam, The Netherlands

We develop a numerical scheme for the calculation of tunneling current I and differential conductance dI/dV of metal and CO terminated STM tips on the topological insulators Bi2Se3, Bi2Te2Se and Bi2Te3 and find excellent agreement with experiment. The calculation is an application of Chen's derivative rule, whereby the Bloch functions are obtained from Wannier interpolated tightbinding Hamiltonians and maximally localized Wannier functions from first-principle DFT+GW calculations. We observe signatures of the topological boundary modes, their hybridization with bulk bands, Van Hove singularities of the bulk bands and characterize the orbital character of these electronic modes using the high spatial resolution of STM and AFM. Bare DFT calculations are insufficient to explain the experimental data, which are instead accurately reproduced by many-body corrected GW calculations.

O 101.6 Fri 11:45 H25

Revealing higher-order topological bulk-boundary correspondence in Bi crystals with spin-helical hinge state loop and proximity superconductivity — •Dongming Zhao[1], Yang Zhong[1], Tian Yuan[1], Haitao Wang[1], Tianxing Jiang[1], Yang Qi[1], Hongjun Xiang[1,2,3], Xingao Gong[1,2,3], Donglai Feng[2,3,4], and Tong Zhang[1,2,3,4] — [1]Fudan University, Shanghai, China — [2]Collaborative Innovation Center for Advanced Microstructures, Nanjing, China — [3]Shanghai Research Center for Quantum Sciences, Shanghai, China — [4]Hefei National Laboratory, Hefei, China

Topological materials are typically characterized by gapless boundary states, known as bulk-boundary correspondence. Recently, this concept has been generalized in higher-order topological insulators (HOTIs). E.g., a 2nd-order 3D TI hosts 1D topological hinge states winding around the crystal. A complete verification of HOTI will require probing all crystal boundaries. Here we studied a promising candidate of 2nd-order TI, Bi, in the form of mesoscopic crystals grown on superconducting V3Si. Using low-temperature STM, we directly observed dispersive 1D states on various hinges. Upon introducing magnetic scatterers, new scattering channels emerged selectively on certain hinges, revealing their spin-helical nature. Combining first-principle calculation and global symmetry analysis, we find these hinge states topological and formed a closed loop encircling the crystal. This provides direct evidence on the HOTI in Bi. Moreover, proximity superconductivity is observed in the topological hinge states serving as a promising platform for realizing topological superconductivity.

O 101.7 Fri 12:00 H25

Simultaneous Atomic-Scale Imaging and Electronic Characterization of Wet-Chemically Prepared Bi_2Se_3 Nanoplatelets — •Auke Vlasblom, Victor Wesselingh, Jara Vliem, Daniel Vanmaekelbergh, and Ingmar Swart — Utrecht University, Utrecht, The Netherlands

Colloidal semiconductor nanoparticles are of great interest for various optoelectronic applications, such as integration in displays, solar cells and electronics. For applications, the surface of nanoparticles is of critical importance. However, until now, no technique exists to simultaneously investigate the atomic structure (e.g. the presence of defects) and the electronic properties of a nanoparticle, foremost limited by the presence of ligands that prevent direct access to the surface with a local probe. Here, we present a new and widely applicable procedure that allows investigation of the surface of a nanoparticle with a local probe. Using this method, nanoparticles are transferred to an atomically clean substrate under ultra-high vacuum conditions. We demonstrate the procedure for topological two-dimensional Bi_2Se_3 nanoplatelets deposited on Au(111). We reveal the atomic and electronic structure of the surface of colloidally synthesised Bi_2Se_3 nanoplatelets with scanning tunneling microscopy and spectroscopy measurements. In this talk, I will highlight the various types of defects that occur at the (sub-)surface of Bi_2Se_3 nanoplatelets and I will show their influence on the electronic structure.

O 102: Closing Talk Andreas Heinrich

Time: Friday 13:15–14:00 Location: H1

Topical Talk O 102.1 Fri 13:15 H1

Quantum sensing with atomic-scale spatial resolution — •Andreas Heinrich — IBS Center for Quantum Nanoscience, Seoul, Korea

There is a strong international research effort in the area of quantum nanoscience, where the concepts of quantum coherence, superposition and entanglement of quantum states are exploited in solid state and molecular systems. One of the very prominent applications in this realm is Quantum Sensing, where a quantum system is used to measure some external fields with high energy and high spatial resolution. In this talk we will focus on quantum-coherent experiments in Scanning Tunneling Microscopy (STM). STM enables the study of surfaces with atomic-scale spatial resolution and offers the ability to study individual atoms and molecules on surfaces. To make a movable quantum sensor with atomic-scale spatial resolution, we attached a single molecule of PTCDA to the spin-polarized apex of an STM tip. In contrast to all other known molecules, its coupling to the tip is so weak that this molecule performs as an excellent electron spin resonance (ESR) sensor on a bare metallic surface. We show how this sensor can be used to measure atomic-scale magnetic and electric fields emanating from single atoms on a surface and compare its performance to the well-established NV center in diamond.

Taner Esat, Dmitriy Borodin, et al., A quantum sensor for atomic-scale electric and magnetic fields, Nature Nanotechnology (2024).

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Overview of Invited Talks and Sessions

(Lecture hall H45; Poster P4)

Invited Talks

SOE 1.1	Mon	15:00–15:30	H45	**Interplay between multiscaling and rough volatility** — •Tiziana Di Matteo
SOE 4.1	Tue	9:30–10:00	H45	**Urban scaling and conflicting goals** — •Diego Rybski
SOE 6.1	Tue	14:00–14:30	H45	**Analyzing Political Regime Stability Through the Diffusion Equation: Insights from V-Dem Data (1900-2021)** — •Karoline Wiesner
SOE 7.1	Wed	9:30–10:00	H45	**When networks can think: The meaning of self-regulation in the presence of humans** — •Alina Herderich
SOE 10.1	Thu	15:00–15:30	H45	**Emergent Behaviors in LLMs-Populated Societies** — •Giordano De Marzo, Claudio Castellano, Luciano Pietronero, David Garcia

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

See SYQS for the full program of the symposium.

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — Reyhaneh Khasseh, Sascha Wald, Roderich Moessner, Christoph Weber, •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg, Greta Villa, Kilian Seibold, Vincent Dumont, Gianluca Rastelli, Mateusz Michałek, Alexander Eichler, Javier del Pino
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Sessions

SOE 1.1–1.3	Mon	15:00–16:00	H45	**Econophysics**
SOE 2.1–2.1	Mon	16:15–17:30	H45	**Award Session: Young Scientist Award for Socio- and Econophysics (YSA)**
SOE 3.1–3.10	Mon	17:30–19:30	P4	**Poster**

SOE 4.1–4.8	Tue	9:30–12:00	H45	**Urban systems, Scaling, and Social Systems**
SOE 5.1–5.3	Tue	12:15–13:00	H45	**Agent-Based Modeling**
SOE 6.1–6.3	Tue	14:00–15:00	H45	**Political Systems and Conflicts**
SOE 7.1–7.10	Wed	9:30–12:45	H45	**Focus Session: Self-Regulating and Learning Systems: from Neural to Social Networks**
SOE 8.1–8.9	Wed	15:00–17:30	H45	**Networks, From Topology to Dynamics (joint session SOE/BP/DY)**
SOE 9	Wed	18:00–19:30	H45	**Members' Assembly**
SOE 10.1–10.11	Thu	15:00–18:15	H45	**Focus Session: Large Language Models, Social Dynamics, and Assessment of Complex Systems**

Members' Assembly of the Physics of Socio-economic Systems Division

Wednesday 18:00–19:30 H45

- SOE poster award
- Report
- Election
- All other business

Sessions

– Invited Talks, Prize Talks, Topical Talks, Contributed Talks, and Posters –

SOE 1: Econophysics

Time: Monday 15:00–16:00 Location: H45

Invited Talk SOE 1.1 Mon 15:00 H45

Interplay between multiscaling and rough volatility — •Tiziana Di Matteo — King's College London, London, UK

The multiscaling behaviour of financial time-series is one of the acknowledged stylized facts in the literature [1]. Its source in financial markets has been long debated [2,3]. In this talk I will discuss the origin of multiscaling in financial time-series, investigate how to best quantify it [4] and I will introduce a new methodology that provides a robust estimation and tests the multi- scaling property in a statistically significant way [5]. I will show results on the application of the Generalized Hurst exponent tool to different financial time-series, and I will show the powerfulness of such tool to detect changes in markets' behaviours, to differentiate markets accordingly to their degree of development, to asses risk and to provide a new tool for forecasting [6]. I will also show results to assess the interplay between price multiscaling and volatility roughness, defined as the (low) Hurst exponent of the volatility process [7] and finally I will discuss some new results on the origin of the multiscaling in rough volatility models [8]. [1] T. Di Matteo, Quantitative Finance 7(1) (2007) 21. [2] J. W Kantelhardt et al., Physica A 316 (2002) 87. [3] J. Barunik et al. Physica A 391 (2012) 4234. [4] R. J. Buonocore et al., Chaos, Solitons and Fractals 88 (2016) 38 and Phys.Rev.E, 95 (4) (2017) 042311. [5] G. Brandi, T. Di Matteo, The Eur. J. of Finance, (2021) DOI: 10.1080/1351847X.2021.1908391. [6] I. P. Antoniades et al., Physica A 565 (2021) 12556. [7] G. Brandi, T. Di Matteo, Int. Rev. Financ. Anal. 84 (2022) 102324. [8] P. Casaburi, G. Brandi, T. Di Matteo, submitted (2024).

SOE 1.2 Mon 15:30 H45

The Mechanism and Impact of Ultra Extreme Fast Events on Stock Markets — •Luca Henrichs, Anton J. Heckens, and Thomas Guhr — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Recent years have seen much discussion about the mechanism of Ultra Extreme Fast Events (UEEs), which are rapid and strong price changes. In particular, the influence of algorithmic trading or high-frequency traders (HFTs) was studied [1] [2]. HFTs are computer programs that can react faster to UEEs than humans. However, the rapid trading of HFTs would make it extremely difficult to intervene to stabilize a market. Hence, a deeper understanding of UEEs is called for.

In our study, we compare various characteristics of UEEs for the years 2007, 2008, 2014 and 2021. In comparison to the study [1], we show that various statistical properties of UEEs are robust over the years. The recovery rate after a UEE is of particular interest here and indicates that certain underlying mechanisms changed only very little. In contrast to [1], which says that human traders with large market orders generate UEEs, we concluded that liquidity plays a major role in the emergence of UEEs, independent of HFTs and human traders.

[1] Tobias Braun, Jonas A. Fiegen, Daniel C. Wagner, Sebastian M. Krause, Thomas Guhr. Impact and recovery process of mini flash crashes: An empirical study PLoS ONE 13, e0196920 (2018).

[2] Johnson N, Zhao G, Hunsader E, Qi H, Meng J, et al. Abrupt rise of new machine ecology beyond human response time. Scientific reports. 2013; 3:2627. PMID: 24022120

SOE 1.3 Mon 15:45 H45

A New Traders' Game? — Cedric Schuhmann, •Anton J. Heckens, and Thomas Guhr — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Traders on financial markets generate non–Markovian dynamics through their competition with each other. This competition can be interpreted as a game between different types of traders. We study the non–stationarity of this game and show that it has changed significantly since the global crisis of 2008.

To reveal the market mechanism, we analyze self–response functions for individual stocks as well as cross–response functions for pairs of different stocks. While the non–Markovian dynamics in the former is liquidity–driven it is only expectation–driven in the latter which might be interpreted as emergence of correlations. Averages greatly improve the statistics, we work out averaged response functions for different years. We thus considerably extend the analysis of Ref. [1,2] in which only the crisis year 2008 was studied.

[1] S. Wang, R. Schäfer and T. Guhr. Cross–Response in Correlated Financial Markets: Individual Stocks Eur. Phys. J. B 89, 105 (2016).

[2] S. Wang, R. Schäfer and T. Guhr. Average Cross–Responses in Correlated Financial Market Eur. Phys. J. B 89, 207 (2016).

SOE 2: Award Session: Young Scientist Award for Socio- and Econophysics (YSA)

Time: Monday 16:15–17:30 Location: H45

Presentation of the Award to the Awardee

Prize Talk SOE 2.1 Mon 16:30 H45

Higher-order network science — •Federico Battiston — Department of Network & Data Science, Central European University, Vienna, Austria

The complexity of many biological, social and technological systems stems from the richness of the interactions among their units. Over the past decades, a variety of complex systems has been successfully described as networks whose interacting pairs of nodes are connected by links. Yet, from human communications to ecological systems, interactions can often occur in groups of three or more nodes and cannot be described simply in terms of dyads. Until recently little attention has been devoted to the higher-order architecture of real complex systems. However, a mounting body of evidence is showing that taking the higher-order structure of these systems into account can enhance our modeling capacities and help us understand and predict their emergent dynamical behavior. Here I will present an overview of network science beyond pairwise interactions. I will discuss the higher-order organization of real-world complex systems, and characterize new emergent phenomena in dynamical processes beyond pairwise interactions, with a focus on social systems.

After the Award Session, there will be an informal get-together with beer and pretzels at the Poster Session

SOE 3: Poster

Time: Monday 17:30–19:30 Location: P4

SOE 3.1 Mon 17:30 P4

Causal Hierarchy in the Financial Market Network - Uncovered by the Helmholtz-Hodge-Kodaira Decomposition — •Tobias Wand[1,2,3], Oliver Kamps[1], and Hiroshi Iyetomi[3,4] — [1]CeNoS Münster — [2]Institut für Theoretische Physik, Universität Münster — [3]Faculty for Data Science, Rissho University, Kumagaya, Japan — [4]Canon Institute for Global Studies, Tokyo, Japan

Granger causality can uncover the cause-and-effect relationships in financial networks. However, such networks can be convoluted and difficult to interpret, but the Helmholtz-Hodge-Kodaira decomposition can split them into rotational and gradient components which reveal the hierarchy of the Granger causality flow. Using Kenneth French's business sector return time series, it is revealed that during the COVID crisis, precious metals and pharmaceutical products were causal drivers of the financial network. Moreover, the estimated Granger causality network shows a high connectivity during the crisis, which means that the research presented here can be especially useful for understanding crises in the market better by revealing the dominant drivers of crisis dynamics.

This contribution is based on the publication Wand et al., Entropy 2024, 26(10), 858 and was supported by the JSPS Summer Program.

SOE 3.2 Mon 17:30 P4

A Game-Theoretic Approach to Misinformation on Social Media — •Grace Galanthay and Eckehard Olbrich — Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

Misinformation and disinformation are considered a significant problem with the rise of social media. While much research concentrates on the spread of information, our work focuses on the strategic actions of individual actors. Using a game-theoretic signaling framework, we study interactions where a sender communicates a noisy signal about the state of the world to a receiver, whose response determines payoffs for both actors. Existing "cheap talk" models explore strategic communication between two actors with misaligned preferences. We extend this framework to multiple senders and adapt the theoretical model to social media, where the traditional roles of sender and receiver merge. Our extension to a multi-actor signaling game in social media contexts represents a distinct approach to modeling the spread and strategic use of mis- and disinformation on digital platforms.

SOE 3.3 Mon 17:30 P4

Unraveling 20th-century political regime dynamics using the physics of diffusion — •Paula Pirker-Díaz[1], Sönke Beier[1], Matthew Wilson[2], and Karoline Wiesner[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Department of Political Science, University of South Carolina, Columbia, USA

Uncertainty remains regarding why some countries democratize while others do not, and why some remain democratic while others backslide into autocracy. Also the nature and changes of intermediate regimes is particularly unclear. By applying the Diffusion Map, a spectral dimensionality-reduction technique, on V-Dem political data (1900-2021), we identify a low-dimensional manifold describing electoral regimes. Using the diffusion equation from statistical physics, we measure the time scale on which countries change their degree of electoral quality, freedom of association, and freedom of expression depending on their position on the manifold. Democracies show sub-diffusive dynamics, while collapsing autocracies exhibit super-diffusive dynamics. Intermediate regimes display distinct and more unstable diffusion behaviors, linked to a higher risk of civil conflict. This research bridges statistical physics and political science, offering a quantitative framework for understanding regime transformation and risk-of-conflict assessment. [arXiv:2411.11484]

SOE 3.4 Mon 17:30 P4

Analysis of (Mis)information Spread across Telegram Communities — Roman Ventzke[1,2], Anastasia Golovin[1,2], Sebastian Mohr[1,2], Andreas Schneider[1,2], and •Viola Priesemann[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Georg-August-Universität Göttingen

Statistically, do lies spread better than the truth? To effectively combat the proliferation of misinformation in online social media, it is important to understand how content spreads in social networks. We investigate the dynamics of (mis)information diffusion on the Telegram messaging platform to understand if (and how) the spread of both true information and misinformation differs.

As a basis for this study, we employ a novel large dataset of messages from Telegram group chats and channels. This dataset comprises more than 2.3 billion messages from more than 150,000 different chats and focuses on COVID-19-related content since the start of the pandemic.

Tracking information propagation, we show that information spread can be modeled by a Random Field Ising Model. Our results show that on Telegram misinformation spreads further than reliable information and is linked to "super spreaders". We also investigate whether factors like emotional engagement can drive misinformation spread.

SOE 3.5 Mon 17:30 P4

Interplay between algorithms, cognition and social interactions — •Beniamin Sereda and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, PL-00-662 Warsaw, Poland

Modern societies are increasingly facing the issue of opinion polarisation, amplified by recommendation systems and their role in forming information cocoons. To understand how the evolution of user preferences and the topology of social networks influence opinion dynamics, the integrative agent-based model DAISY was developed. This model assumes three distinct levels of interactions: algorithmic, social, and cognitive. Algorithmic interactions are governed by recommendation algorithms, the social level reflects user preferences regarding whom to contact in the context of recommended items, and the cognitive level describes how individuals process information.The dynamics of preferences are driven by the algorithmic level, while opinion dynamics occur on the social and cognitive levels. Co-evolutional perspective on dynamics allows observation of how changes in network topology, triggered by recommendation systems, shape opinion evolution. Simulations show that increased personalisation accelerates the formation of informational cocoons, though in a non-linear and complex manner. Analysing social network evolution also revealed a deeper understanding of the irreversibility of processes within the system.

SOE 3.6 Mon 17:30 P4

Phase transition in maximally robust networks — •Thilo Gross[1,2,3] and Laura Barth[1,2,3] — [1]Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Oldenburg — [2]Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven — [3]Carl-von-Ossietzky Universität Oldenburg

Here is a puzzle: You are building a network, but you know already that a certain proportion of nodes will fail, which will remove them and their links from your network. You don't know which nodes will fail, but you want your network to retain a connected component of functioning nodes that is as large as possible, after the failures have occured. Given a certain number of nodes and links, how do you connect the nodes? What kind of structure do you build?

Here we study a closely related though slightly simpler question: Instead of a fixed number of nodes and links, we consider an infinite network with a given mean degree. And, instead of allowing control over each individual link, we assume that the network is constructed as a configuration model. Hence the challenge becomes to pick the network's degree distribution such that after a certain proportion of nodes has failed the expectation value for the size of the giant component is still as large as possible.

We show this question can be solved using an analytical calculation, which reveals an infinite sequence of phase transitions between different configuration model structures.

SOE 3.7 Mon 17:30 P4

Game-theoretic model of group work contributions, neurodiverse versus neurotypical — •Lilliana Etheridge and Jens Christian Claussen — University of Birmingham, Edgbaston, UK

Evolution of cooperation and contribution to public goods have been long standing themes in game theory. Group work in the educational context, as well as teams in industry often have formalized workflows where individuals can decide to contribute different amounts. For this context, we formulate a game-theoretic model and analyze it via agent-based simulations, both for neurotypical and neurodiverse contributors, modeled by differing decision behaviour.

SOE 3.8 Mon 17:30 P4

Weakly coupled FitzHugh-Nagumo oscillators and the influence of noise — •Max Contreras[1,2] and Philipp Hövel[2] — [1]Technische Universität Berlin, Germany — [2]Saarland University, Saarbrücken, Germany

We investigate neural oscillators modeled by FitzHugh-Nagumo systems that are weakly and diffusively coupled on a one-dimensional ring with finite coupling range. Operated in the oscillatory regime, we observe a simultaneous presence of robust collective oscillations and neuronal avalanches. The mechanism behind these avalanches is based on an inhibitory effect of interactions, which may quench the otherwise spiking of units due to an interplay with the maximal canard. The result are subthreshold oscillations close to an unstable fixed point. Furthermore, we explore the response of the networked system to noise, and find that for weak coupling, the network-mediated inhibition is weakened and that for intermediate coupling strength, noise can promote synchronized spiking.

SOE 3.9 Mon 17:30 P4

Characterizing similarities and differences in people's views based on open-ended expressions with LLMs and network science — •Ezequiel Lopez-Lopez and Stefan Herzog — Max Planck Institute for Human Development, Berlin

Citizens have diverse views on critical issues like pandemic management and climate change. Current methods to gather these views are limited: polls and surveys lack nuance, while qualitative approaches do not scale. We developed a computational framework that combines Large Language Models with network science to rapidly analyze citizens' evolving views without oversimplifying them. This novel approach extracts concepts from unstructured text and represents them in networks, offering deeper insights and faster analysis than traditional qualitative methods. We applied this framework to UK citizens' ideas on five UN Sustainable Development Goal-related policy problems. Our results demonstrate the framework's ability to capture nuanced differences across political, demographic, and cognitive variables. This approach has the potential to significantly enhance evidence-based policymaking and citizen engagement in complex societal issues.

SOE 3.10 Mon 17:30 P4

Multisensory processing in superior colliculus and primary sensory cortex — •Daniel Gerber[1], Peter Severin Graff[1,2], Björn Kampa[2], and Simon Musall[1,2,3] — [1]Institute of Biological Information Processing (IBI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Department of Systems Neurophysiology, Institute for Zoology, RWTH Aachen University, Aachen, Germany — [3]Institute of Experimental Epileptology and Cognition Research, University of Bonn Medical Center, Bonn, Germany

The superior colliculus (SC) plays a crucial role in integrating multisensory stimuli and is associated with various cognitive functions, such as decision-making. It receives inputs from different sensory modalities, either directly from sensory

organs or from primary sensory regions in the cortex. However, the distinctions between multisensory integration in the SC and the cortex remain unclear. To study the physiological underpinning of multisensory integration in these areas, awake mice were exposed to visual, tactile, and multisensory stimuli, while neural activity was recorded in primary visual cortex (V1), primary somatosensory cortex (S1) and the SC simultaneously using high-density Neuropixels electrodes. To investigate the influence of the cortical projection to the SC, in some trials V1 and/or S1 were optogenetically inhibited. A generalized linear model is used to analyse the spiking activity. We present that SC is modulated by cortical input but does not strongly rely on it. We also present the change in neural activity over the course of repeated stimulus.

SOE 4: Urban systems, Scaling, and Social Systems

Time: Tuesday 9:30–12:00 Location: H45

Invited Talk SOE 4.1 Tue 9:30 H45

Urban scaling and conflicting goals — •Diego Rybski — Institute of Ecological Urban and Regional Development (IOER) — Complexity Science Hub (CSH)

Urban scaling, the power-law correlations between an urban indicator and city population, represents the most famous theme of contemporary urban science. The vast majority of publications on the topic empirically quantify the scaling properties for given indicators and countries. Other work is dedicated to mathematically explaining the non-linear scaling based on few but plausible assumptions. In this contribution, two approaches to urban scaling are discussed in the context of conflicting goals. First, we compare cities in terms of emitted carbon emissions vs. heat island intensity. We derive a theoretical solution, but we find that empirical parameters do not allow for any optimal size. Instead, the fundamental allometry between area and population should represent an optimum. Thus, second, we propose a simple model that leads to an optimum in the form of the fundamental allometry. Although many cities are challenged, it makes sense that some sort of optimization takes place, which should also be reflected in observed scaling.

SOE 4.2 Tue 10:00 H45

Dynamics of Cities — Airton Deepman[1], •Renan Lucas Fagundes[2], Eugenio Megias[3], Roman Pasechnik[4], Fabiano Lemes Ribeiro[5], and Constantino Tsallis[6,7,8] — [1]USP, Sao Paulo, Brazil — [2]IOER, Dresden, Germany — [3]UGR, Granada, Spain — [4]Lund University, Lund, Sweden — [5]UFLA, Lavras, Brazil — [6]CBPF, Rio de Janeiro, Brazil — [7]SFI, Santa Fe, USA — [8]CSHV, Vienna, Austria

In recent years, the challenge has been to understand urban phenomena and their impact on the lives of people in cities in order to achieve the sustainable development goals. One of the most intriguing urban phenomena to emerge since the 1940s is fundamental allometry, which elucidates the manner in which urban areas evolve in tandem with their population size. However, most of the models in the literature investigate urban phenomena while employing the static properties of cities. In this study, we demonstrate that the combination of nonextensive statistics with fractal geometry provides a powerful tool for investigating the dynamic evolution of cities. We conducted a case study on Brazilian cities. Our findings indicate that cities evolve near the critical point of percolation, which facilitates connectivity and efficiency in space occupation. Additionally, we observed a correlation between the fractal dimension and the allometric exponent, which is associated with fundamental geometric and diffusion aspects. This research has implications for the design of infrastructure in urban areas and the promotion of economic growth. Early version of the respective manuscript: https://doi.org/10.48550/arXiv.2407.12681

SOE 4.3 Tue 10:15 H45

Scale-dependent Power Law Properties in Social Activities — •Kenta Yamada[1], Jiwei Jiang[2], Hideki Takayasu[2], and Misako Takayasu[2] — [1]Univ. of the Ryukyus, Okinawa, Japan — [2]Science Tokyo, Tokyo, Japan

This presentation explores the power-law characteristics of hashtag usage on Weibo, a Chinese social media platform. The study investigates the heavy-tailed distribution of daily hashtag frequencies and proposes a generalized random multiplicative model to understand the formation of these distributions[1].

Data containing approximately 20 million Weibo posts from July to August 2021 were analyzed. The analysis confirmed that hashtag frequency distributions follow a fat-tailed pattern, consistent with previous research[2]. A key finding was that the growth rate of hashtag usage depends on its frequency.

To model this, a generalized random multiplicative process incorporating size dependency was introduced. Simulations demonstrated that increasing granularity in dividing the hashtag frequency range improved the model's accuracy in replicating real distributions. The power-law exponents estimated through theoretical methods aligned closely with observed data.

[1] J. J. Jiang, K. Yamada, H. Takayasu, and M. Takayasu, Sci Rep 13, 1 (2023).

[2] Chen, H. H., Alexander, T. J., Oliveira, D. F., & Altmann, E. G. . Chaos, 30(6), 063112 (2020).

SOE 4.4 Tue 10:30 H45

Dynamical Power Laws in a Multiplicative Growth Model with Resets — •Alexander Jochim and Stefan Bornholdt — Institute for Theoretical Physics, University of Bremen

The observation that wealth distributions follow power laws – dating back to Pareto's 1897 work – has long intrigued physicists, offering a glimpse of universal principles in complex systems. Models based on multiplicative growth with resets are well-known for generating these heavy-tailed distributions, where the power-law exponent depends on the underlying parameters. Yet, such models often treat societal influences as static, ignoring the dynamic feedback between wealth and social behavior.

In this work, we introduce a minimal model where multiplicative growth with resets produces a wealth distribution that evolves dynamically through coupling to social mechanisms. This adaptive feedback leads to time-dependent power-law exponents, reflecting the interplay between wealth inequality and shifting societal behaviors. Our approach captures emergent phenomena in a non-equilibrium toy model for how collective social behaviors influence – and are influenced by – the statistical properties of wealth.

By framing wealth distributions as part of a coupled dynamical system, this work connects statistical physics with the study of adaptive social systems, offering fresh perspectives on the evolving patterns of inequality.

15 min. break

SOE 4.5 Tue 11:00 H45

Statistical mechanics of a voter model with an evolving number of opinion states — Jeehye Choi[1], Byungjoon Min[1,2], and •Tobias Galla[3] — [1]Department of Physics, Chungbuk National University, Cheongju, Chungbuk, Korea — [2]Department of Medicine, University of Florida, Gainesville FL, USA — [3]Institute for Cross-Disciplinary Physics and Complex Systems IFISC, Palma de Mallorca, Spain

The voter model (VM) describes population of interacting individuals. At each step a randomly chosen individual copies the state ("the opinion") of a neighbour.

Here, we introduce and study a VM in which new opinion states can be introduced spontaneously. Opinions can also go extinct via the voter dynamics. This leads to stationary states with a variable number of opinions in the population or network.

We use statistical physics methods to characterise these stationary states, drawing parallels to the evolution of "mating types" in biological populations. Mating types are forms of the sperm-egg system. Unlike for true sexes, there can be more than two mating types (some fungi have thousands). We transfer methods from number theory, previously used to characterise the evolution of mating types [1], to compute how many opinions will ultimately be present in a VM with a dynamic number of states.

[1] E. Berríos-Caro, T. Galla, G. W.A. Constable, Switching environments, synchronous sex, and the evolution of mating types, Theor. Pop. Biol. 138, 28 (2021)

SOE 4.6 Tue 11:15 H45

The noisy voter model with complete and partial aging — •Raul Toral — Institute for Cross-Disciplinary Physics and Complex Systems IFISC (CSIC-UIB), Campus UIB, 07122 Palma de Mallorca, Spain

Many agent-based models of social interaction use the Markovian assumption, namely that the transition rates from one to another state depend only on the current state of the system and not on its previous history. This, being obviously wrong in many situations, it is widely used because of its mathematical simplicity. In this work, I will consider the effect that a particular non-Markovian effect, known in the literature as "aging" or "inertia" has on the paradigmatic noisy voter model. This is a widely used model in social and economics situations to describe transitions to consensus or synchronized behavior. While the standard version of the model displays a discontinuous change of behavior from unsynchronized to consensus as a function of a parameter which depends on the free-will, or tendency to act independently on the neighbors, this transition is size-dependent and disappears in the thermodynamic limit. I will show that a genuine -second order- phase transition can appear as a consequence of aging,

modeled as a reluctance to change state as a function of the length of time that has been spent in the current state. We investigate the situation where aging acts on both socially influenced and random opinion changes (complete aging), and compare it with previous results where aging acts only on pairwise interactions (partial aging).

SOE 4.7 Tue 11:30 H45

Emergence of polarization in an opinion dynamics framework with bimodal random external field — •Jan Korbel[1], Remah Dahdoul[1], Rudolf Hanel[1,2], and Stefan Thurner[1,2,3] — [1]Complexity Science Hub Vienna, Austria — [2]Medical University of Vienna, Austria — [3]Santa Fe Institute, NM, US

We present the opinion dynamics model with an external field, where the individual opinions are coupled as in a standard Ising spin-spin interaction. Furthermore, we consider that the spins are coupled with the random field. Contrary to the common random-field Ising model, the random field is considered to be binary, either +h or -h. The interpretation of this model is that the particles represent the individuals influenced both by their neighborhood as well as external sources, e.g., election campaigns. With increasing field coupling, we observe that the transition from the ferromagnetic to paramagnetic phase becomes the first order. Furthermore, it can be shown that for a high enough field, the system becomes polarized, i.e., the external field is dominating in comparison with the spin-spin interactions. Finally, we show that for low enough temperatures, the system always gets polarized above the threshold external field, no matter whether the magnitude of the positive field is much larger or smaller than the magnitude of the negative field.

SOE 4.8 Tue 11:45 H45

Phase Transitions in Socially Balanced Systems: Why More Interactions Drive Polarization — •Markus Hofer[1,2], Jan Korbel[1,2], Rudolf Hanel[1,2], and Stefan Thurner[1,2,3] — [1]Medical University of Vienna, Center for Medical Data Science, Institute of the Science of Complex Systems, Spitalgasse 23, 1090, Vienna, Austria — [2]Complexity Science Hub Vienna, Metternichgasse 8, 1030, Vienna, Austria — [3]Santa Fe Institute, 1399 Hyde Park Rd, Santa Fe, NM 87501, USA

Survey data show massive evidence that the average number of close social connections has increased over the past two decades. At the same time opinions in societies are becoming increasingly divided. To understand if these phenomena are related, we use a multidimensional spin model [1] that has been experimentally shown [2] to be realistic both in terms of homophily and social balance. Within the model individuals interact dyadically yet realistic triad statistics as expected from social balance theory emerges naturally. We find a phase transition where at a critical connectivity of the underlying social network a rapid transition from practically no to strong polarization occurs. By understanding how increased social connectivity necessarily leads to polarization we discuss strategies to mitigate polarization in highly connected societies.

[1] T. M. Pham, J. Korbel, R. Hanel, and S. Thurner, Proceedings of the National Academy of Sciences 119, e2121103119 (2022).

[2] M. Galesic, H. Olsson, T. Pham, J. Sorger, and S. Thurner, OSF Preprints 10.31219/osf.io/3bmg7 (2023).

SOE 5: Agent-Based Modeling

Time: Tuesday 12:15–13:00 Location: H45

SOE 5.1 Tue 12:15 H45

Co-evolving networks for opinion and social dynamics in agent-based models — •Soeren Nagel[2], Quang Nuh Vu[1], and Nataša Djurdjevac Conrad[1] — [1]Zuse Institue Berlin — [2]Department of Mathematics and Computer Science, Institute of Computer Science, Freie Universität Berlin

The coevolution of public opinions and social interactions is a fundamental aspect of social systems, yet existing models often fail to include this feedback loop. While many studies explore how opinions influence social ties, The reversed influence is however often overlooked. To bridge this gap, we introduce a novel stochastic agent-based model (ABM) that integrates opinion dynamics and social mobility within a shared "social space."

The feedback loop between opinion and social dynamics generates emergent phenomena such as consensus and echo chambers, whose dynamics we analyze through a network-based order parameter. The model exhibits critical transitions for both noise intensity and relative size of opinion and social network.

Our findings demonstrate the potential of coevolutionary models to capture the transient dynamics of social clustering and opinion polarization.

Applying the model to empirical data from the General Social Survey, we investigate opinion distributions on politically charged issues, and demonstrate, that the model is capable of capturing real-world dynamics.

SOE 5.2 Tue 12:30 H45

An Agent-Based Model to Investigate Geder Bias in Peer Review — •Sophie Lake and Jens Christian Claussen — University of Birmingham, Edgbaston, UK

Fairness in the refereeing process is a challenging goal but essential to ensure the quality of the scientific publication landscape. Selfishness, various biases, friendship networks as well as time efficiency influence the behaviour of researchers when making decisions on refereeing manuscripts. A longstanding challenge is the under-representation of women in many scientific disciplines and therefore in editorial boards and referee pools. We build on a model by Thurner and Hanel (2011, EPJB 84:707) that introduced different referee strategies. Here we extend the model by gender-specific strategies, and use agent-based simulations to analyze the impact of evaluation bias, homophilic editors and friendship networks.

SOE 5.3 Tue 12:45 H45

Do weekends matter in agent-based models for epidemiology? — •Aleksandr Bryzgalov — Institut für Medizinische Epidemiologie, Biometrie und Informatik (IMEBI) Medizinische Fakultät der Martin-Luther-Universität Halle-Wittenberg, Deutschland

German Epidemic Micro-Simulation System (GEMS) is an agent-based framework that was recently developed to study and analyse the consequences of the COVID-19 pandemic.

Using GEMS we focused on a study of weekend impact on developing the infection spread throughout the population. We compared the dynamics in two cases: considering only regular days (people have constant contact rates) and considering workdays-weekends(contact rates are specific for workdays and weekends). The total number of contacts was the same in both cases. We used the transmission parameters related to the Omicron (B.1.1.529) pathogen. In our simulations, we varied the distribution of workplace sizes, but the household structure was fixed.

The results show the dependence of total attack rate of workplace size distribution: smaller workplaces in combination with workdays-weekend periodicity produce more infections than the same with only regular days. On the opposite, bigger workplaces in combination with workdays-weekend periodicity produce fewer infections than the same with only regular days.

[1] J. Ponge et al 2023 Winter Simulation Conference (WSC), San Antonio, TX, USA, 2023, pp. 1088-1099, doi: 10.1109/WSC60868.2023.10407633.

SOE 6: Political Systems and Conflicts

Time: Tuesday 14:00–15:00 Location: H45

Invited Talk SOE 6.1 Tue 14:00 H45

Analyzing Political Regime Stability Through the Diffusion Equation: Insights from V-Dem Data (1900-2021) — •Karoline Wiesner — University of Potsdam, Potsdam, Germany

Democratic stagnation and autocratic resurgence have marked the 21st century, raising questions about the stability of democracies and their implications for peace and prosperity. Utilizing the diffusion equation from statistical physics we provide firm evidence that democracy is the most stable regime type across the 20th and 21st centuries on average, surpassing the average life time of electoral autocracies. The latter also exhibit heightened susceptibility to sudden collapse. We explore these dynamics using the Diffusion Map dimensionality-reduction technique applied to V-Dem data (1900-2021). In this context, we will discuss some less explored mathematical aspects of the diffusion-map method, including its probabilistic interpretation and sensitivity to parameters and to the structure of the data. These recent results will be of interest, not least, to those wanting to apply the method to socio-economic data.

Wiesner, K., Bien, S., & Wilson, M. C. (2024). The principal components of electoral regimes: separating autocracies from pseudo-democracies. Royal Society Open Science, 11(10), 240262.

Pirker-Díaz, P., Wilson, M. C., Beier, S., & Wiesner, K. (2024). Unraveling 20th-century political regime dynamics using the physics of diffusion. arXiv preprint arXiv:2411.11484.

SOE 6.2 Tue 14:30 H45

Knowing armed conflict type hurts prediction — •Niraj Kushwaha[1], Edward D. Lee[1], and Woi Sok Oh[2] — [1]Complexity Science Hub, Austria — [2]Princeton University, USA

Moving beyond heuristic classifications of armed conflicts such as local, civil, interstate wars etc. to systematic categorization is useful but challenging. Using information-theoretic techniques we generate chains of related conflict events from the high-resolution Armed Conflict & Location Event Dataset and integrate them with other datasets spanning climate, geography, infrastructure, economics, raw demographics, and composite demographics. Using an unsupervised clustering algorithm based on multinomial mixture, we discover that three conflict archetypes exist; "major unrest," "local conflict," and "sporadic & spillover events." Major unrest predominantly occurs in densely populated areas with good infrastructure and flat, riparian geography. Local conflicts arise in mid-populated regions with diverse socio-economic and geographical features. Sporadic and spillover conflicts are small, occurring in sparsely populated areas with poor infrastructure and economic conditions. The three types stratify into a hierarchy of factors, revealing a quantitative taxonomy that highlights population, infrastructure, and economics as the most discriminative variables. Surprisingly, we find that knowing the type negatively impacts predictability of conflict intensity such as fatalities, conflict duration, and other measures of size. Hence, we develop an empirical and bottom-up approach that identifies conflict types but also cautions us about the limited utility of public data sets for conflict prediction.

SOE 6.3 Tue 14:45 H45

On the coincidence of weather extremes and geopolitical conflicts: Risk analysis in regional food markets — •Nkongho Ayuketang Arreyndip — Economic analysis of Climate Impacts and Policy Division, Euro-Mediterranean Center on Climate Change(CMCC), Via della Libertà, 12- 30175 Venice (VE), Italy.

Under increasing geopolitical tensions between important breadbaskets and climate extremes, the co-existence of weather and geopolitical extreme events can lead to devastating agricultural production losses. These losses can affect the entire food supply chain and lead to food shortages and price increases in regional markets. This work models these events' impacts taking the Russian-Ukrainian war and the extreme heat waves of Summer 2022 as a case study. Four(4) war scenarios are considered such as the invasion phase, the peak of the war, Ukraine's resistance, sanctions against Russia, and refugee crises in Europe. Using data from the US Department of Agriculture (USDA), Statista, WITS, and Acclimate production value losses. Results show that the agricultural sectors of southern European countries such as France, Italy, and Spain were most affected by the extreme events, although the direct impact of refugees was lower compared to their northern counterparts. Strict sanctions against Russia coupled with Ukraine's resistance will benefit EU food markets, but at the same time the agricultural sectors of smaller nations and weaker economies, particularly those of Russia's allies, will be highly vulnerable. We suggest that their impact on weak economies should not be overlooked when developing and adopting conflict resolution measures.

SOE 7: Focus Session: Self-Regulating and Learning Systems: from Neural to Social Networks

Living systems have a remarkable ability to self-stabilize. How do such systems, made up of small, active units, achieve meaningful goals without global control? This focus session will explore recent advances in self-regulating networks, demonstrating how these systems transition between states, adapt to perturbations and learn to navigate new environments.

Organized by Anastasia Golovin, Johannes Zierenberg, and Viola Priesemann

Time: Wednesday 9:30–12:45 Location: H45

Invited Talk SOE 7.1 Wed 9:30 H45

When networks can think: The meaning of self-regulation in the presence of humans — •Alina Herderich — IDea_Lab, University of Graz, Austria

Feedback, global states, adaptation - given their many parallels modeling societies as self-regulating physical systems is tempting. How do the dynamics of a system change in which each of the agents has attitudes, desires, intellect? This talk explores communalities and differences between self-regulation in psychology and physics. First, I will define and illustrate the meaning of self-regulation in psychology. Second, I will explain how regulation can differ when humans regulate themselves versus others. Third, I will showcase challenges that arise when modeling groups of humans as self-regulating systems. For example, how do humans monitor the state of their group? What are the quantities that are regulated in groups of humans? And how do we differentiate between desired and undesired states especially if the targets are not morally neutral? Finally, I will close the talk with highlighting what psychology can learn from physics and vice versa in the context of self-regulating systems.

SOE 7.2 Wed 10:00 H45

Societal self-regulation induces complex infection dynamics and chaos — Joel Wagner[1,2], •Simon Bauer[1], Sebastian Contreras[1,2], Luk Fleddermann[1,2], Ulrich Parlitz[1,2], and Viola Priesemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Classically, endemic infectious diseases are expected to display relatively stable, predictable infection dynamics, like recurrent seasonal waves. However, if the human population reacts to high infection numbers by mitigating the spread of the disease, this delayed behavioural feedback loop can generate infection waves itself, driven by periodic mitigation and subsequent relaxation. We show that such behavioural reactions, together with a seasonal effect of comparable impact, can cause complex and unpredictable infection dynamics, including Arnold tongues, co-existing attractors, and chaos [1]. Importantly, these arise in epidemiologically relevant parameter regions where the costs associated to infections and mitigation are jointly minimised. By comparing our model to data, we find signs that COVID-19 was mitigated in a way that favoured complex infection dynamics.Our results challenge the intuition that endemic disease dynamics necessarily implies predictability and seasonal waves, and show the emergence of complex infection dynamics when humans optimise their reaction to increasing infection numbers.

[1] Wagner, J., et al. arXiv:2305.15427

SOE 7.3 Wed 10:15 H45

Dynamical theory for adaptive biological systems — •Tuan Pham[1] and Kunihiko Kaneko[2] — [1]Institute of Physics, University of Amsterdam, Science Park 904, Amsterdam, The Netherlands — [2]Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, Copenhagen, 2100-DK, Denmark

Biological, social and neural networks are adaptive - their connections slowly change in response to the state of their constituting elements–the nodes, such as genes, individuals or neurons so as to make the collective states functionally robust under environmental stochasticity. To explain this kind of robust behavior, we develop an exact analytical theory for non-equilibrium phase transitions in multi-timescale and multi-agent dynamical systems, where there exists a correspondence between global adaptation and local learning. As an illustration of our general theory, we apply it to biological evolution, where phenotypes are shaped by gene-expression fast dynamics that are subjected to an external noise while genotypes are encoded by the configurations of a network of gene regulations. This network slowly evolves under natural selection with a mutation rate, depending on how adapted the shaped phenotypes are. Here we show how, high reciprocity of network interactions results in a trade-off between genotype and phenotype that, in turn, gives rise to a robust phase within an intermediate level of external noise. Reference: Tuan Minh Pham and Kunihiko Kaneko J. Stat. Mech. (2024) 113501.

SOE 7.4 Wed 10:30 H45

Response functions in residual networks as a measure for signal propagation — •Kirsten Fischer[1,2], David Dahmen[1], and Moritz Helias[1,3] — [1]Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Department of Physics, Faculty 1, RWTH Aachen University, Aachen, Germany

Residual networks (ResNets) demonstrate superior trainability and performance compared to feed-forward networks, particularly at greater depths, due to the introduction of skip connections that enhance signal propagation to deeper layers. Prior studies have shown that incorporating a scaling parameter into the residual branch can further improve generalization performance. However, the underlying mechanisms behind these effects and their robustness across network hyperparameters remain unclear.

For feed-forward networks, finite-size theories have proven valuable in understanding signal propagation and optimizing hyperparameters. Extending this approach to ResNets, we develop a finite-size field theory to systematically analyze signal propagation and its dependence on the residual branch's scaling parameter. Through this framework, we derive analytical expressions for the re-

sponse function, which measures the network's sensitivity to varying inputs. We obtain a formula for the optimal scaling parameter, revealing that it depends minimally on other hyperparameters, such as weight variance, thereby explaining its universality across hyperparameter configurations.

SOE 7.5 Wed 10:45 H45

Feature learning in deep neural networks close to criticality — Kirsten Fischer[1,2], •Javed Lindner[1,3,4], David Dahmen[1], Zohar Ringel[5], Michael Krämer[4], and Moritz Helias[1,3] — [1]Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Jülich Research Centre, Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Department of Physics, RWTH Aachen University, Aachen, Germany — [4]Institute for Theoretical Particle Physics and Cosmology, RWTH Aachen University, Aachen, Germany — [5]The Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel

Neural networks excel due to their ability to learn features, yet its theoretical understanding continues to be a field of ongoing research. We develop a finite-width theory for deep non-linear networks, showing that their Bayesian prior is a superposition of Gaussian processes with kernel variances inversely proportional to the network width. In the proportional limit where both network width and training samples scale as $N, P \to \infty$ with P/N fixed, we derive forward-backward equations for the maximum a posteriori kernels, demonstrating how layer representations align with targets across network layers. A field-theoretic approach links finite-width corrections of the network kernels to fluctuations of the prior, bridging classical edge-of-chaos theory with feature learning and revealing key interactions between criticality, response, and network scales.

15 min. break

Topical Talk SOE 7.6 Wed 11:15 H45

Self-organization in neural systems — •Philipp Hövel — Saarland University, Saarbrücken, Germany

Key feature of networked neural systems is the emergence of self-organized, collective dynamics giving rise to various forms of synchronization: The network is more that the sum of its parts. The nodes equiped with a neural model exhibit rich dynamical scenarious depending on the topology and type of coupling, which might also involve transmission delays due to finite signal propagation speed. In my talk, I will review a number of studies on coupled neural systems, where the considered examples include empirical, artificial, and adaptive networks. I will finish with recent results on network-induced inhibition giving rise to avalanches of neural activity interspersed by with long periods of quiescence.

SOE 7.7 Wed 11:45 H45

Critical drift in a neuro-inspired network — •Thilo Gross — Helmholtz Institute for Functional Marine Biodiversity (HIFMB) Im Technologiepark 5, 26129 Oldenburg, Germany — Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven, Germany — Carl-von-Ossietzky University, Oldenburg, Germany

It has been postulated that the brain operates in a self-organized critical state that brings multiple benefits, such as optimal sensitivity to input. Thus far, self-organized criticality has typically been depicted as a one-dimensional process, where one parameter is tuned to a critical value. However, the number of adjustable parameters in the brain is vast, and hence critical states can be expected to occupy a high-dimensional manifold inside a high-dimensional parameter space. Here, we show that adaptation rules inspired by homeostatic plasticity drive a neuro-inspired network to drift on a critical manifold, where the system is poised between inactivity and persistent activity. During the drift, global network parameters continue to change while the system remains at criticality.

SOE 7.8 Wed 12:00 H45

Transient Recurrent Dynamics Shapes Representations in Mice — •Lars Schutzeichel[1,2,3], Jan Bauer[1,4], Peter Bouss[1,2], Simon Musall[3], David Dahmen[1], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Germany — [2]Department of Physics, Faculty 1, RWTH Aachen University, Germany — [3]Institute of Biological Information Processing (IBI-3), Jülich Research Centre, Germany — [4]The Edmond and Lily Safra Center for Brain Sciences, The Hebrew University of Jerusalem, Israel

Different stimuli evoke transient neural responses, but how is stimulus information represented and reshaped by local recurrent circuits? We address this question using Neuropixels recordings from awake mice and recurrent network models, inferring stimulus classes (e.g., visual or tactile) from activity. A two-replica mean-field theory reduces complex network dynamics to three key quantities: the mean population activity (R) and overlaps ($Q^{=}$, $Q^{\neq}$), reflecting response variability within and across stimulus classes. The theory predicts the time evolution of R, $Q^{=}$, and $Q^{\neq}$. Validated in experiments, it reveals how inhibitory balancing governs the dynamics of R, while chaotic dynamics shape overlaps, providing insights into the mechanisms underlying transient stimulus separation. The analysis of mutual information of an optimally trained population activity readout reveals that sparse coding (small R) allows the optimal information representation of multiple stimuli.

SOE 7.9 Wed 12:15 H45

Employing normalizing flows to examine neural manifold characteristics and curvatures — •Peter Bouss[1,2], Sandra Nestler[3], Kirsten Fischer[1,2], Claudia Merger[4], Alexandre René[2,5], and Moritz Helias[1,2] — [1]IAS-6, Forschungszentrum Jülich, Germany — [2]RWTH Aachen University, Germany — [3]Technion, Haifa, Israel — [4]SISSA, Trieste, Italy — [5]University of Ottawa, Canada

Despite the vast number of active neurons, neuronal population activity supposedly lies on low-dimensional manifolds (Gallego et al., 2017). To learn the statistics of neural activity, we use Normalizing Flows (NFs) (Dinh et al., 2014). These neural networks are trained to estimate the probability distribution by learning an invertible map to a latent distribution.

We adjust NF's training objectives to distinguish between relevant and noise dimensions, by using a nested dropout procedure in the latent space (Bekasov & Murray, 2020). An approximation of the network for each mixture component as a quadratic mapping enables us to calculate the Riemannian curvature tensors of the neural manifold. We focus mainly on the directions in the tangent space, in which the sectional curvature shows local extrema.

Finally, we apply the method to electrophysiological recordings of the visual cortex in macaques (Chen et al., 2022). We show that manifolds deviate significantly from being flat. Analyzing the curvature of the manifolds yields insights into the regimes where neuron groups interact in a non-linear manner.

SOE 7.10 Wed 12:30 H45

Neural self-organization of muscle-driven robots via force-mediated networks — •Claudius Gros[1] and Bulcsu Sandor[2] — [1]Institute for Theoretical Physics, Goethe University Frankfurt — [2]Department of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

We present self-organizing control principles for simulated robots actuated by synthetic muscles. Muscles correspond to linear motors exerting force only when contracting, but not when expanding, with joints being actuated by pairs of antagonistic muscles. Individually, muscles are connected to a controller composed of a single neuron with a dynamical threshold that generates target positions for the respective muscle. A stable limit cycle is generated when the embodied feedback loop is closed, giving rise to regular locomotive patterns. In the absence of direct couplings between neurons, we show that the network generated by force-mediated intra- and inter-leg couplings between muscles suffice to generate stable gaits.

[1] Sándor, Bulcsú, and Claudius Gros. "Self-organized attractoring in locomoting animals and robots: an emerging field." International Conference on Artificial Neural Networks. Springer, 2024.

SOE 8: Networks, From Topology to Dynamics (joint session SOE/BP/DY)

Time: Wednesday 15:00–17:30 Location: H45

SOE 8.1 Wed 15:00 H45

Self-organized transport in noisy dynamic networks — •Frederic Folz[1], Joshua Rainer Ganz[1], Kurt Mehlhorn[2], and Giovanna Morigi[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Algorithms and Complexity Group, Max-Planck-Institut für Informatik, Saarland Informatics Campus, 66123 Saarbrücken, Germany

We present a numerical study of multicommodity transport in a noisy, nonlinear network. The nonlinearity determines the dynamics of the edge capacities, which can be amplified or suppressed depending on the local current flowing across an edge. We consider network self-organization for three different nonlinear functions: For all three we identify parameter regimes where noise leads to self-organization into more robust topologies, that are not found by the sole noiseless dynamics. Moreover, the interplay between noise and specific functional behavior of the nonlinearity gives rise to different features, such as (i) continuous or discontinuous responses to the demand strength and (ii) either single or multistable solutions. Our study shows the crucial role of the activation function on noise-assisted phenomena.

SOE 8.2 Wed 15:15 H45

Critical properties of Heider balance on multiplex networks — •Krishnadas Mohandas, Krzysztof Suchecki, and Janusz Hołyst — Faculty of Physics, Warsaw University of Technology, Koszykowa 75, PL-00-662 Warsaw, Poland

Heider's structural balance theory has proven invaluable in comprehending the dynamics of social groups characterized by both friendly and hostile relationships. Extending this understanding to multiplex networks, we investigate Heider balance dynamics in systems where agents exhibit correlated relations across multiple layers. In our model, intralayer interactions adhere to Heider dynamics, while interlayer correlations are governed by Ising interactions, using heat bath dynamics for link signs. This framework reveals a multifaceted equilibrium landscape, with distinct phases coexisting across layers. Starting from a paradise state with positive links in all layers, increasing temperature induces a discontinuous transition to disorder, similar to single-layer scenarios but with a higher critical temperature, as verified through extended mean-field analysis and agent-based simulations.

We extend this analysis to Erdös-Rényi random graphs in noisy environments. We predict a first-order transition with a critical temperature scaling as p^2 for monolayers and follow a more complex behavior for bilayers. To replicate dynamics observed in complete graphs, intralayer Heider interaction strengths must scale as p^{-2}, while interlayer interaction strengths scale as p^{-1} in random graphs. Numerical simulations confirm these analytical predictions for dense graphs.

SOE 8.3 Wed 15:30 H45

Functional Motifs in Food Webs and Networks — •Melanie Habermann[1,2,3], Ashkaan Fahimipour[4], Justin Yeakel[5,6], and Thilo Gross[1,2,3] — [1]Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Oldenburg, GER — [2]Alfred-Wegener Institute (AWI), Helmholtz Center for Polar and Marine Research, Bremerhaven, GER — [3]Carl-von-Ossietzky University, Institute for Chemistry and Biology of the Marine Environment (ICBM), Oldenburg, GER — [4]Florida Atlantic University, Boca Raton, FL, USA — [5]University of California Merced, Merced, CA, USA — [6]The Santa Fe Institute, Santa Fe, NM, USA

It is interesting to ask when the presence of a small subgraph in a complex network is sufficient to impose constraints on system dynamics that are independent of the broader network structure. We refer to these subgraphs as functional motifs. A classic example can be found in ecology with the competitive exclusion motif in food webs, where two species compete for the same resource without regulation. The presence of this motif precludes any stable equilibrium for the entire system. However, examples of other motifs with similarly definitive implications for system stability are rare. But our usual notion of asymptotic stability is just one among many different concepts of stability. Another one, reactivity, captures a system's immediate response to small perturbations. In this talk, we explain why functional stability motifs are rare and show that every subgraph is a functional reactivity motif. This highlights reactivity as a promising concept for exploring a vast range of networked phenomena.

SOE 8.4 Wed 15:45 H45

Infecting Apex Predators Could Lead to Their Extinction — •Fakhteh Ghanbarnejad[1] and Hooman Saveh[2] — [1]SRH University of Applied Sciences, Leipzig, Germany — [2]Sharif University of Technology, Tehran, Iran

Food webs have been extensively studied from both ecological and mathematical aspects. However, most of the models studied in this area do not capture the effects of infectious diseases simultaneously. Recently, the idea of including an infectious disease in a food web model has been investigated. We study and simulate a small food chain consisting of only prey, predators, and apex predators governed by the generalized Lotka-Volterra equations and we implement the Susceptible-Infected-Recovered (SIR) model on only one of the species at a time in the food chain. To study the effects of an infectious disease on the food chain, we introduce a new parameter that increases predation rate by a factor of w and decreases hunting rate by a factor of $1/w$ for infected species. When the infectious disease is in our predators we observe that predators do not extinct under any set of parameters, however, an oscillation in its population size occurs under some circumstances which we do not observe in ordinary SIR or the generalized Lotka-Volterra equations alone. When an infectious disease is present in apex predators, oscillations in the population size do not happen; but if the set of parameters is in a specific range the apex predators may extinct. Furthermore, the chance of survival of the community, known as community persistence, increases for the predators and decreases for the apex predators.

15 min. break

SOE 8.5 Wed 16:15 H45

Behavioral Heterogeneity in Disease Spread: Contrasting Effects of Prevention Strategies and Social Mixing — •Fabio Sartori[1,2] and Michael Maes[1] — [1]Chair of Sociology and Computational Social Science, Karlsruhe Institute of Technology, Karlsruhe — [2]Max Planck Institute for Dynamics and Self Organisation, Göttingen, Germany

Despite mounting evidence of behavioral heterogeneity in response to disease threats, the majority of epidemiological models assume uniform behavior across populations for mathematical tractability. We analyze three distinct mechanisms of behavioral response to disease threat: susceptibility reduction (e.g., mask-wearing), active testing, and vaccination propensity. Through extensive numerical analysis, we demonstrate that the impact of behavioral heterogeneity strongly depends on the specific mechanism involved. While heterogeneous susceptibility-reducing behaviors generally decrease disease spread, heterogeneity in testing rates and vaccination propensity typically amplifies epidemic severity. Furthermore, we show that non-homogeneous mixing patterns, particularly when correlated with behavioral traits, exacerbate disease spread across all three mechanisms. These findings reveal fundamental principles about the interplay between behavioral heterogeneity and epidemic dynamics, challenging the conventional homogeneous assumption and providing important implications for public health interventions and policy design.

SOE 8.6 Wed 16:30 H45

Modelling retweet cascades using multivariate Hawkes processes on sparse networks — Alexander Kreiss[1] and •Eckehard Olbrich[2] — [1]Leipzig University, Germany — [2]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

We apply a model that considers vertices in a network who are able to cast events, e.g. users of the online social media platform Twitter. Furthermore, there is a directed edge from vertex A to vertex B if A takes note of the events cast by B and changes its own behavior accordingly. More precisely, the model assumes that the activity of B increases the activity of A and likewise its other neighbors. This is called peer effects. However, there might also be other information, which also influences the activity of the vertices, e.g. the time of the day for social media posts. This is called global effects. We use a Hawkes model that incorporates, both, peer and global effects. This allows for the estimation of the network, that is, the influence structure while controlling for network effects or the estimation of the global effects while controlling for peer effects. The estimation is based on a LASSO strategy, which respects sparsity in the network. We apply this model to retweets on Twitter in order to reconstruct potential retweet cascades and identify accounts that are influential in sharing information.

SOE 8.7 Wed 16:45 H45

Influence, Incidence, Imitators and Individualists: Comparing social influence models of protective behavior in an epidemic — •Andreas Reitenbach — Karlsruhe Institute of Technology, Karlsruhe, Germany

To manage a pandemic, it is critical that citizens voluntarily engage in protective behavior (e.g. masking or vaccinating). Voluntary behavior is subject to complex dynamics of social influence, however. While various models couple social influence dynamics with disease spreading, assumptions about how individuals influence each other differ markedly. Models assuming herding implement that agents imitate their peers. On the contrary, rational agents (individualists) engage in protective behavior when their peers are not and vice versa, potentially free-riding on others' contributions to herd immunity.

Here, I study whether and why these competing behavior models translate into different disease dynamics. Following a recent call to abstract from psychological mechanisms underlying social influence, I translate the behavior theories into influence-response functions.

I find that individualists self-coordinate on a moderate level of protection and experience long-lasting but flat incidence curves. Herding, in contrast can result in rapid cycling through waves of high incidence and strong collective efforts to mitigate. Whether herders or individualists navigate an epidemic better can depend on the population's hospital capacity and disease parameters.

SOE 8.8 Wed 17:00 H45

Formalism and Physical Principles of Human Mobility and Routine — •Marlli Zambrano[1], Ashish Thampi[2], Alejandra Rincon[2], Andrzej Jarynowski[1], Steven Schulz[2], and Vitaly Belik[1] — [1]FU Berlin, Germany — [2]Machine Learning Unit, NET CHECK GmbH, Berlin, Germany

The physical principles underlying human mobility have been extensively studied in recent years, enabled by the availability of large-scale mobile phone data. While significant progress has been made in understanding general mobility patterns, capturing the dynamics of individual trajectories, specifically how mobility varies from person to person and day to day, remains challenging due to the need for highly detailed and persistent data. This study addresses this challenge by examining sequences of individual daily mobility motifs, as defined by Schneider et al., from a stochastic process perspective. The analysis uses a persistent mobile phone user panel in Berlin, with high-frequency GPS data collected over four years. Twenty motifs were identified, covering 96% of all observations. The extent of inter- and intra individual variability is explored, focusing on how motifs change within individuals over time and differ between individuals in various contexts (e.g., weekends, seasons). Additionally, sequences of motifs are modeled as a stochastic process, and properties such as transition probabilities are analyzed. These findings provide deeper insights into the variability and structure of human mobility, contributing to a better understanding of individual mobility dynamics.

SOE 8.9 Wed 17:15 H45

The world air transportation network: import risk of diseases, pandemic potentials and passenger routes — •Pascal Klamser[1,2], Adrian Zachariae[1,2], Benjamin Maier[3], Olga Baranov[4], and Dirk Brockmann[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Robert Koch-Institute, Berlin, Germany — [3]University of Copenhagen, Copenhagen, Denmark — [4]LMU München, München, Germany

Disease propagation between countries strongly depends on their effective distance, a measure derived from the world air transportation network. It reduces the complex spreading patterns of a pandemic to a wave-like propagation from the outbreak country, establishing a linear relationship to the arrival time of the unmitigated spread of a disease. However, in the early stages of an outbreak, what concerns decision-makers in countries is understanding the relative risk of active cases arriving in their country*essentially, the likelihood that an active case boarding an airplane at the outbreak location will reach them. While there are data-fitted models available to estimate these risks, accurate mechanistic, parameter-free models are still lacking.

We (i) introduce the "import risk" model, which defines import probabilities using the effective-distance framework, (ii) show its application to estimate the pandemic potential of emerging variants of COVID-19 and (iii) show that the effective distance shortest path tree, on which the "import risk" model is based on, is an extremely accurate representation of true passenger routes.

SOE 9: Members' Assembly

Time: Wednesday 18:00–19:30 Location: H45

All members of the Physics of Socio-economic Systems Division are invited to participate.

SOE 10: Focus Session: Large Language Models, Social Dynamics, and Assessment of Complex Systems

Recent Large Language Models (LLMs) learn the statistics of human communication, and hence they present a promising way of simulating societal interactions and opinion formation. Moreover, their flexible architecture makes them versatile to also learn the statistics of other complex systems. - We will discuss how to make best use of these advancements to model social interactions and dynamics across different scales and settings, how to use them to assess sentiments, narratives and opinions, and also how one can use LLMs to also understand other complex systems. Our aim is to offer an evaluative perspective on both the potential and challenges that are intrinsic to this rapidly evolving research area.

Organized by Vincent Brockers, Johannes Zierenberg, and Viola Priesemann

Time: Thursday 15:00–18:15 Location: H45

Invited Talk SOE 10.1 Thu 15:00 H45

Emergent Behaviors in LLMs-Populated Societies — •Giordano De Marzo[1,2,3], Claudio Castellano[4,2], Luciano Pietronero[2], and David Garcia[1,3] — [1]Konstanz University — [2]CREF Enrico Fermi Research Center — [3]CSH Vienna — [4]CNR-ISC Institute for Complex Systems

Applications of Large Language Models (LLMs) increasingly involve collaborative tasks where multiple agents interact, forming "LLM societies." In this context, we explore whether large groups of LLMs exhibit emergent group behaviors similar to those in human societies. First, by simulating social network formation, we observe that LLMs spontaneously form scale-free networks. Agents connect through linear preferential attachment, mirroring the Barabasi-Albert model and real-world social networks. Second, we investigate the ability of LLMs to reach consensus on arbitrary norms without external preferences, thereby self-regulating their behavior. In human societies, consensus without institutions is limited by cognitive capacities. Similarly, we find that LLMs can reach consensus, with the opinion dynamics described by a majority force coefficient that determines the likelihood of consensus. This majority force strengthens with higher language understanding but decreases with larger group sizes, resulting in a critical group size beyond which consensus becomes unattainable. For more advanced LLMs, this critical size grows exponentially with language capabilities, exceeding the typical size of informal human groups.

SOE 10.2 Thu 15:30 H45

A Framework for Multi-Step Discussions of LLM-Based Agents — •Vincent Brockers[1,2], David Ehrlich[2,3], and Viola Priesemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]University of Göttingen — [3]Göttingen Campus Institute for Dynamics of Biological Networks

Recent studies have demonstrated the utility of Large Language Models (LLMs) across various settings and domains, particularly in their ability to approximate human behavior for simulating and studying societal phenomena. A critical component of this capability is their proficiency in generating realistic dialogues. We are interested in the collective dynamics that arise from their dialogues, in particular in the context of understanding collective opinion dynamics.

We developed a framework for simulating multi-step discussions among LLM-based agents, which is crucial for these studies. We conduct an in-depth analysis of the components of such simulations, highlighting the challenges and specifically investigating potential biases.

We find that these opinion dynamics are primarily influenced by model-inherent topic biases, which exhibit attractors in the opinion space. Additionally, the framing of opinion evaluation plays a crucial role in analyzing these dynamics. Our findings offer valuable insights for future research aimed at optimizing the design of LLM agent-based simulations and enhancing our modeling capabilities of complex systems, such as human networks.

SOE 10.3 Thu 15:45 H45

Collective Turing Tests on LLMs — •Azza Bouleimen[1,2], Giordano de Marzo[3], Taehee Kim[3], Silvia Giordano[2], and David Garcia[3] — [1]University of Zurich, Zurich, Switzerland — [2]SUPSI, Lugano, Switzerland — [3]University of Konstanz, Konstanz, Germany

In this project, we investigate whether social media conversations generated by independent LLMs are indistinguishable from those of humans, i.e., whether LLMs used to generate social media content can pass the Turing test. Formally, we conduct an experiment in which we prepare a series of English Reddit submissions to which we attach two conversations. One of the conversations is an authentic human conversation ,while the other is generated artificially using an LLM. We generate conversations using GPT-4o and llama 3 70B. We vary the temperatures of the models used and the length of the conversations. We recruit participants from Prolific. These subjects are asked to select the conversation they believe is generated by AI. Our preliminary results suggest that, overall, participants are fooled by LLM 40% of the time. Llama 3 70B conversations appear to fool users more often than GPT-4o ones. Through this study, we investigate to what extent and with which configurations LLM could be best used to simulate user conversations on social media. To the best of our knowledge, this is the first attempt to evaluate the performance of LLMs in mimicking a social media conversation between a group of individuals.

SOE 10.4 Thu 16:00 H45

Dialogue React: Enhancing Conversation Synthesis for Social Science Simulations — •Ruggero Marino Lazzaroni — RWTH Aachen

Recent advancements in Large Language Models (LLMs) have spurred significant progress in conversation synthesis and social dynamics modeling. However, existing approaches often fall short in generating human-like dialogues suitable for complex social science simulations and opinion formation studies. This research introduces DialogueReact, a novel framework that builds upon previous work in conversation synthesis by incorporating react prompting, dialogue acts and agentic behaviour across different scales. By leveraging LLMs' ability to learn communication statistics, DialogueReact generates qualitatively better conversations compared to previous state-of-the-art methods. Our findings demonstrate the potential of DialogueReact to improve social science research by providing an extra tool for simulating complex social interactions and understanding collective behavior in social systems.

SOE 10.5 Thu 16:15 H45

Computational modeling of LLM powered personalized recommendations — •Alessandro Bellina[1,2,4], Giordano De Marzo[1,3,4], David Garcia[3], and Vittorio Loreto[1,2,4] — [1]Centro Ricerche Enrico Fermi, Piazza del Viminale, 1, I-00184 Rome, Italy — [2]Sony Computer Science Laboratories Rome, Joint Initiative CREF-SONY, Piazza del Viminale, 1, 00184, Rome, Italy — [3]University of Konstanz, Universitaetstrasse 10, 78457 Konstanz, Germany — [4]Dipartimento di Fisica Università La Sapienza, P.le A. Moro, 2, I-00185 Rome, Italy

Large language models (LLMs) are transforming recommendation systems by tailoring content to user preferences, but they also risk reinforcing filter bubbles and driving polarization. This study investigates the dual impact of LLM-based recommendations, analyzing their inherent biases and exploring how prompt engineering can mitigate these effects. By combining synthetic simulations with real-world Twitter data, we assess how LLMs influence user behavior and the extent to which recommendations amplify or reduce polarization. Preliminary results suggest that prompt engineering enables greater control over recommendations, fostering diversity and creativity. This research provides insights into the risks and opportunities of LLM-powered systems, offering a framework for designing more inclusive and balanced recommendation algorithms.

SOE 10.6 Thu 16:30 H45

Statistical Modelling of Physics Classroom Interactions — •Niklas Stausberg, Karina Avila, Steffen Steinert, Jochen Kuhn, and Stefan Küchemann — Lehrstuhl für Didaktik der Physik, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München

Teacher-student and student-student dialogues are one of the central means to mediate learning in classroom settings, as they foster active participation, promote cognitive engagement, scaffold conceptual understanding, and enhance metacognitive skills. However, strategies for effective classroom dialogues have primarily been studied at an organizational level, and the nuanced mechanisms through which real-time teacher-student and student-student interactions influence individual learning outcomes within the classroom remain largely unexplored.

New advances in analysis of verbal interactions now offer opportunities to perform granular analyses of classroom dialogues. Using a combination of response times and speed, voice emotion recognition, and self-regulation state detection enables clustering of patterns in students' cognitive, emotional, and self-regulatory states and map them to specific types of teacher and student responses to gain insights into the dynamics of effective classroom interactions. In this talk, we discuss how statistical modeling of classroom interactions, e.g. via percolation theory, can be used to provide additional perspectives in the understanding of social learning processes.

15 min. break

SOE 10.7 Thu 17:00 H45

Disentangling individual vs. collective contributions to polarization in political voting — Gavin Rees and •Edward Lee — Complexity Science Hub, Vienna, Austria

Politics around the world exhibit increasing polarization, most visibly demonstrated by rigid voting configurations in legislatures. This impacts their ability to seek effective compromise and pass impactful legislation. The crux of polarization is the emergence of a unidimensional ideological axis that primarily determines voting. Yet, legislative bills often negotiate multiple issues, whose effects may add up or compete for any individual vote. We develop a model inspired from statistical physics that accounts for voters with multi-dimensional preferences that can be linearly combined to generate coalitions. This allows us to capture higher-order correlations beyond those captured in direct spin-spin interaction models. As a result, the model is dramatically simpler, fits the data better, and is more interpretable than canonical maximum entropy or utility-based models from political science for large voting bodies. We study roll-call voting in US Congress, and we find coexistence of non-polarized with polarized modes. We show how increased partisan polarization is the contribution of two terms: increased party-line voting by the individual plus depletion of votes that would elicit complex, bipartisan response. Both decrease over time, but the latter falls much faster. Thus, we propose a more principled way of tracking the emergence of polarization at the level of the voter and the collective issues the many vote on.

SOE 10.8 Thu 17:15 H45

Understanding Information Spread in Social Networks through the Lense of Self-Organized Criticality: A Study on Telegram — •Roman Ventzke[1,2], Anastasia Golovin[1,2], Sebastian Bernd Mohr[1,2], Andreas Schneider[1,2], and Viola Priesemann[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Georg-August-Universität Göttingen

To effectively address the proliferation of misinformation in social media, one fundamentally needs to understand how information spreads in online social networks. We investigate the dynamics of information spread using a large dataset from the messenger platform Telegram, showing that information spread in the networks happens in bursty avalanches with scale-free statistics that resembles critical behavior of physical systems.

We find that the critcal exponents of the system can be well described by a mean-field Random Field Ising Model (RFIM), alluding to an important role of complex contagion and peer-pressure effects in the propagation of information. By coarse-graining dynamics in the topic space we show additional evidence that the process indeed belongs to the RFIM class. We demonstrate through simulations that the spreading process on the network can be well-described by mean-field models and discuss how self-regulation of the network gives rise to criticality.

SOE 10.9 Thu 17:30 H45

Dynamics of information spread: the phase space of topics on Telegram — •Anastasia Golovin[1,2], Simon Bauer[1], Sebastian Mohr[1], and Viola Priesemann[1,2] — [1]Max Planck for Dynamics and Self-Organisation, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The information that is spread on digital platforms shapes public discourse and influences decision-making. In this talk, we explore the dynamics of topics discussed on Telegram, a privacy-oriented messenger that became a hub for misinformation spread during the COVID-19 pandemic. Using transformer-based topic modeling techniques, we map each Telegram channel onto a trajectory in a high-dimensional phase space of topics. Treating these trajectories as a stochastic dynamical system, we identify topic areas that act as attractors, pulling trajectories from their neighborhood, and others that emerge only transiently in response to global events. This approach bridges computational social science and dynamical systems theory, offering a novel perspective on understanding discourse dynamics in communication networks.

SOE 10.10 Thu 17:45 H45

Computational approaches to analyzing political narratives — •Armin Pournaki[1,2,3] and Tom Willaert[4] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]Laboratoire Lattice, École Normale Supérieure - PSL - CNRS, Paris, France — [3]médialab, Sciences Po, Paris, France — [4]Brussels School of Governance, Vrije Universiteit Brussel, Brussels, Belgium

Narratives are key interpretative devices by which humans make sense of political reality. As the significance of narratives for understanding current societal issues such as polarization and misinformation becomes increasingly evident, there is a growing demand for methods that support their empirical analysis. To this end, we propose a graph-based formalism and machine-guided method for extracting, representing, and analyzing selected narrative signals from digital textual corpora, based on Abstract Meaning Representation (AMR) [1]. The formalism and method introduced here specifically cater to the study of political narratives that figure in digital trace data. We demonstrate the method on corpora gathered from archived political speeches and social media posts. [1] https://arxiv.org/abs/2411.00702

SOE 10.11 Thu 18:00 H45

Optimizing pandemic mitigation in the presence of seasonality, emerging variants and vaccination — •Laura Müller[1,2], Fabio Sartori[1,3], Jonas Dehning[1,2], Maximilian F. Eggl[4], and Viola Priesemann[1,2] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Institute of Neuroscience, CSIC-UMH, Alicante, Spain

Mitigation efforts are often necessary to control the spread of infectious diseases during pandemics and epidemics. However, these measures come with societal and economic costs. We present a general optimization framework based on control theory to balance the trade-off between mitigation costs and infection rates, aiming to identify the optimal time-dependent mitigation strategies across a range of scenarios: constant reproduction number, seasonal changes, emerging variants, vaccination rollout, and delayed mitigation onset. Our results show that timely reactions and proactive, preventative measures are crucial in pandemic management to save both lives and costs.

Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Program Overview

(Lecture Halls H31, H32, H33, H36 and Poster P3 and P4)

Plenary Talks Chaired by the Low Temperature Physics Division

PLV VI	Wed	14:00–14:45	H1	**Topological spin-textures – from domain walls to Hopfions: Current innovations and future challenges** — •Stefan Blügel
PLV XI	Fri	8:30– 9:15	H1	**Exploring correlated phases and topology in van der Waals platforms** — •Roser Valenti

Symposia Coorganized by the Low Temperature Physics Division

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium Spins in Molecular Systems: Strategies and Effects of Hyperpolarization (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Wed	15:00–15:30	H1	**Exploring the Non-Perturbative Magnetic Resonance Drive Regime with spin selection rules in a π-Conjugated Polymer** — •Christoph Boehme
SYMS 1.2	Wed	15:30–16:00	H1	**The puzzle of spin and charge transport in the chirality induced spin selectivity effect** — •Bart van Wees
SYMS 1.3	Wed	16:00–16:30	H1	**Nano- and Microscale NMR spectroscopy with spin qubits in diamond** — •Nabeel Aslam
SYMS 1.4	Wed	16:45–17:15	H1	**Spin effects in adsorbed organometallic complexes** — •Richard Berndt
SYMS 1.5	Wed	17:15–17:45	H1	**Quantum Computing with Molecules** — •Mario Ruben

Invited Talks of the joint Symposium Nonequilibrium Collective Behavior in Open Classical and Quantum Systems (SYQS)

See SYQS for the full program of the symposium.

SYQS 1.1	Thu	15:00–15:30	H1	**Active quantum flocks** — •Markus Heyl
SYQS 1.2	Thu	15:30–16:00	H1	**Robust dynamics and function in stochastic topological systems** — •Evelyn Tang
SYQS 1.3	Thu	16:00–16:30	H1	**Nonequilibrium Dynamics of Disorder-Driven Ultracold Fermi Gases** — •Artur Widera
SYQS 1.4	Thu	16:45–17:15	H1	**Topological classification of driven-dissipative nonlinear systems** — •Oded Zilberberg
SYQS 1.5	Thu	17:15–17:45	H1	**Learning dynamical behaviors in physical systems** — •Vincenzo Vitelli

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Invited Talks in Focus Sessions

Invited Talks of the Focus Session "Magnetic Phenomena from Phonon Chirality and Angular Momentum" (joint session MA/TT)

TT 1.1	Mon	9:30–10:00	H20	**Driving Coherent Phonon-Phonon Angular Momentum Transfer via Lattice Anharmonicity** — •Sebastian Maehrlein
TT 1.2	Mon	10:00–10:30	H20	**Chiral phonons, phono-magnetism, and spin-rotation coupling** — •Matthias Geilhufe
TT 1.3	Mon	10:30–11:00	H20	**Geometry of temporal chiral structures and photoinduced chirality-spin coupling** — •Olga Smirnova
TT 1.4	Mon	11:15–11:45	H20	**Phonon thermal Hall effect** — •Kamran Behnia
TT 1.5	Mon	11:45–12:15	H20	**Giant effective magnetic moment of chiral phonons** — •Swati Chaudhary

Invited Talks of the Focus Session "Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond" (joint session O/TT)

TT 6.1	Mon	15:00–15:30	H24	**Kondo and Yu-Shiba-Rusinov resonances: transport and coupling** — •Laëtitia Farinacci
TT 6.2	Mon	15:30–16:00	H24	**Electron delocalization in a 2D Mott insulator** — •Amadeo L. Vazquez de Parga
TT 6.3	Mon	16:00–16:30	H24	**Kondo or no Kondo, that is the question** — •Alexander Weismann
TT 6.4	Mon	16:30–17:00	H24	**Evidence for spinarons in Co atoms on noble metal (111) surfaces** — •Artem Odobesko
TT 6.5	Mon	17:00–17:30	H24	**Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures** — •Samir Lounis

Invited Talks of the Focus Session "Strongly Correlated Quantum States in Moire Heterostructures" (joint session TT/HL/MA)

TT 18.1	Tue	9:30–10:00	H36	**The Thermoelectric Effect and Its Natural Heavy Fermion Explanation in Twisted Bilayer and Trilayer Graphene** — •Bogdan Andrei Bernevig
TT 18.2	Tue	10:00–10:30	H36	**Angle-Tuned Chiral Phase Transition in Twisted Bilayer Graphene** — •Laura Classen
TT 18.3	Tue	10:30–11:00	H36	**Quantum Optics of Semiconductor Moire Materials** — •Atac Imamoglu
TT 18.4	Tue	11:15–11:45	H36	**Probing the Band Structures of Multilayer Graphene Using the Quantum Twisting Microscope** — •Martin Lee
TT 18.5	Tue	11:45–12:15	H36	**Gate-Tunable Bose-Fermi Mixture in a Strongly Correlated Moiré Bilayer Electron System** — •Nathan Wilson

Invited Talks of the Focus Session "Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets" (joint session TT/MA)

TT 27.1	Wed	9:30–10:00	H36	**Detecting Anyons Using Nonlinear Pump-Probe Spectroscopy** — •Max McGinley
TT 27.2	Wed	10:00–10:30	H36	**Two-Dimensional Nonlinear Dynamic Response of Frustrated Magnets** — •Wolfram Brenig
TT 27.3	Wed	10:30–11:00	H36	**Imaging Magnetization Dynamics and Collective Spin Excitations in Compensated Magnets on Ultrafast Timescales** — •Benjamin Stadtmüller
TT 27.4	Wed	11:15–11:45	H36	**Revealing Dynamics of Hidden Sectors with Nonlinear Spectroscopy** — •Yoshito Watanabe
TT 27.5	Wed	11:45–12:15	H36	**Theory of Nonlinear Spectroscopy of Quantum Magnets** — •Stefan Birnkammer

Invited Talks of the Focus Session "Ising Superconductivity in Monolayer Transition Metal Dichalcogenides" (joint session TT/HL/MA)

TT 44.1	Thu	9:30–10:00	H36	**Evidence of Unconventional Superconductivity in Monolayer and Bulk van der Waals Material TaS_2** — •Somesh Chandra Ganguli
TT 44.2	Thu	10:00–10:30	H36	**Signatures of Unconventional Superconductivity in Transition Metal Dichalcogenides** — •Miguel Ugeda
TT 44.3	Thu	10:30–11:00	H36	**Friedel Oscillations and Chiral Superconductivity in Monolayer $NbSe_2$** — •Magdalena Marganska
TT 44.4	Thu	11:15–11:45	H36	**Unconventional Pairing in Ising Superconductors** — •Andreas Kreisel
TT 44.5	Thu	11:45–12:15	H36	**High-Field Study of Ising Superconductivity in TMDs** — •Oleksandr Zheliuk

Individual Invited Talks

TT 15.1	Tue	9:30–10:00	H31	**Solving Many-Body Problems on Quantum Computers** — •Benedikt Fauseweh
TT 24.1	Wed	9:30–10:00	H31	**Possible Origin of High-Field Reentrant Superconductivity in UTe_2** — •Toni Helm
TT 24.7	Wed	11:30–12:00	H31	**Unconventional Superconductivity in Epitaxial $KTaO_3$-Based Heterostructures** — •Denis Maryenko
TT 31.1	Wed	15:00–15:30	H31	**Quantum Skyrmion Hall Effect** — •Ashley Cook
TT 33.8	Wed	17:00–17:30	H33	**Emergent Dynamical Gauge Fields in Generic Kitaev Spin Liquids: From Monolayer to Multilayers** — •Aprem Joy
TT 48.1	Thu	15:00–15:30	H32	**Optical Conductivity as a Probe for Chiral Majorana Edge Modes** — •Lina Johnsen Kamra

All Sessions

TT 1.1–1.8	Mon	9:30–13:00	H20	**Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I (joint session MA/TT)**
TT 2.1–2.11	Mon	9:30–12:30	H31	**Nonequilibrium Quantum Systems (joint session TT/DY)**
TT 3.1–3.12	Mon	9:30–12:45	H32	**Correlated Magnetism – General**
TT 4.1–4.13	Mon	9:30–13:00	H33	**Topological Insulators**
TT 5.1–5.13	Mon	9:30–13:00	H36	**Superconductivity: Properties and Electronic Structure I**
TT 6.1–6.8	Mon	15:00–18:15	H24	**Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)**
TT 7.1–7.11	Mon	15:00–18:00	H31	**Correlated Electrons: Electronic Structure Calculations**
TT 8.1–8.10	Mon	15:00–17:45	H32	**Measurement Technology and Cryogenics**
TT 9.1–9.12	Mon	15:00–18:15	H33	**Correlated Magnetism – Low-Dimensional Systems**
TT 10.1–10.10	Mon	15:00–17:45	H36	**Topological Semimetals**
TT 11.1–11.67	Mon	15:00–18:00	P4	**Superconductivity: Poster**
TT 12.1–12.6	Mon	16:45–18:15	H15	**Quantum Transport and Quantum Hall Effects (joint session HL/TT)**

TT 13.1–13.12	Tue	9:30–12:45	H16	**Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II (joint session MA/TT)**
TT 14.1–14.14	Tue	9:30–13:15	H18	**Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)**
TT 15.1–15.13	Tue	9:30–13:15	H31	**Quantum Coherence and Quantum Information Systems (joint session TT/DY)**
TT 16.1–16.12	Tue	9:30–12:45	H32	**Superconductivity: Properties and Electronic Structure II**
TT 17.1–17.14	Tue	9:30–13:15	H33	**Correlated Electrons: Method Development**
TT 18.1–18.9	Tue	9:30–13:15	H36	**Focus Session: Strongly Correlated Quantum States in Moiré Heterostructures (joint session TT/HL/MA)**
TT 19.1–19.13	Tue	9:30–13:00	H37	**Many-body Quantum Dynamics I (joint session DY/TT)**
TT 20.1–20.10	Tue	10:30–13:00	H8	**2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)**
TT 21.1–21.7	Tue	11:15–13:00	H13	**Quantum Dots and Wires: Transport (joint session HL/TT)**
TT 22.1–22.6	Tue	14:00–15:30	H37	**Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)**
TT 23	Tue	14:15–15:45	H33	**Members' Assembly**
TT 24.1–24.11	Wed	9:30–13:00	H31	**Unconventional Superconductors**
TT 25.1–25.11	Wed	9:30–12:30	H32	**Superconductivity: Supercurrent Diode Effect**
TT 26.1–26.12	Wed	9:30–12:45	H33	**Correlated Magnetism – Frustrated Systems**
TT 27.1–27.7	Wed	9:30–12:45	H36	**Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets (joint session TT/MA)**
TT 28.1–28.13	Wed	9:30–13:00	H37	**Many-body Quantum Dynamics II (joint session DY/TT)**
TT 29.1–29.8	Wed	10:30–12:45	H11	**2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)**
TT 30.1–30.3	Wed	15:00–15:45	H17	**Nanomechanical systems (joint session HL/TT)**
TT 31.1–31.6	Wed	15:00–16:45	H31	**Topology: Quantum Hall Systems**
TT 32.1–32.6	Wed	15:00–16:30	H32	**Superconductivity: Yu-Shiba-Rusinov and Andreev Physics**
TT 33.1–33.11	Wed	15:00–18:15	H33	**Correlated Magnetism – Spin Liquids**
TT 34.1–34.13	Wed	15:00–18:30	H36	**Superconductivity: Theory**
TT 35.1–35.9	Wed	15:00–18:00	P3	**Topology: Poster**
TT 36.1–36.9	Wed	15:00–18:00	P3	**Nanotubes, BEC, Cryocoolers: Poster**
TT 37.1–37.62	Wed	15:00–18:00	P4	**Correlated Electrons: Poster**
TT 38.1–38.7	Wed	16:45–18:30	H32	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED I**
TT 39.1–39.6	Wed	17:00–18:30	H31	**Twisted Materials / Systems (joint session TT/HL)**
TT 40.1–40.6	Wed	17:30–19:00	H19	**Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)**
TT 41.1–41.12	Thu	9:30–12:45	H31	**Quantum-Critical Phenomena (joint session TT/DY)**
TT 42.1–42.14	Thu	9:30–13:15	H32	**Superconductivity: Tunneling and Josephson Junctions**
TT 43.1–43.13	Thu	9:30–13:00	H33	**Correlated Electrons: Other Theoretical Topics**
TT 44.1–44.7	Thu	9:30–12:45	H36	**Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)**
TT 45.1–45.8	Thu	10:30–12:30	H11	**2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)**
TT 46.1–46.8	Thu	15:00–17:15	H13	**Transport Properties (joint session HL/TT)**
TT 47.1–47.13	Thu	15:00–18:30	H31	**Fluctuations, Noise and Other Transport Topics (joint session TT/DY)**
TT 48.1–48.5	Thu	15:00–16:30	H32	**Topology: Majorana Physics**
TT 49.1–49.13	Thu	15:00–18:30	H33	**Graphene and 2D Materials (joint session TT/HL)**
TT 50.1–50.13	Thu	15:00–18:30	H36	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED II**
TT 51.1–51.6	Thu	16:45–18:15	H32	**Topological Superconductors**
TT 52.1–52.7	Fri	9:30–11:15	H31	**Nickelates and Other Complex Oxides**
TT 53.1–53.12	Fri	9:30–12:45	H32	**Topology: Other Topics**
TT 54.1–54.12	Fri	9:30–12:45	H33	**Correlated Electrons: Charge Order**
TT 55.1–55.13	Fri	9:30–13:00	H36	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED III**
TT 56.1–56.7	Fri	9:30–11:15	H37	**Quantum Dynamics, Decoherence, and Quantum Information (joint session DY/TT)**
TT 57.1–57.7	Fri	10:30–12:15	H25	**Topology and Symmetry-protected Materials (joint session O/TT)**
TT 58.1–58.6	Fri	11:30–13:00	H31	**f-Electron Systems and Heavy Fermions**
TT 59.1–59.6	Fri	11:30–13:00	H37	**Quantum Chaos (joint session DY/TT)**

Members' Assembly of the Low Temperature Physics Division

Tuesday 14:15–15:45 H33

- Report
- Outlook 2025
- Miscellaneous

Sessions

– Invited Talks, Topical Talks, Contributed Talks, and Posters –

TT 1: Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum I (joint session MA/TT)

The magnetic moment of the electron lies at the heart of magnetism and spintronics. However, recent research has unveiled the angular momentum and magnetic moment of chiral phonons as fundamental quantities in their own right. These chiral phonons give rise to a plethora of novel lattice phenomena analogous to electronic effects, such as the phonon Hall and phonon Zeeman effects. Moreover, they play a critical role in angular momentum transfer on ultrafast timescales, as seen in the Einstein-de Haas effect. Chiral phonons can also generate effective magnetic fields reaching the tesla scale, inducing magnetization in antiferromagnetic, paramagnetic, and even nonmagnetic materials - a phenomenon reminiscent of the Barnett effect. These advancements showcase phonon chirality and angular momentum as powerful emerging tools for generating and controlling magnetism. This focus session aims to highlight the latest breakthroughs in chiral-phonon magnetism and foster connections between the rapidly evolving field of chiral phononics and the broader magnetism research community.

Coordinators: Dominik M.Juraschek, Eindhoven University of Technology, d.m.juraschek@tue.nl; Martina Basini, ETH Zürich, m.basini@ethz.ch

Time: Monday 9:30–13:00 Location: H20

Invited Talk TT 1.1 Mon 9:30 H20

Driving Coherent Phonon-Phonon Angular Momentum Transfer via Lattice Anharmonicity — •Sebastian Maehrlein — Fritz Haber Institute of the Max Planck Society — Helmholtz Zentrum Dresden Rossendorf — TU Dresden

The discrete rotational symmetry of crystal structures leads to the conservation of quantized angular momentum in solids. Whereas the exchange of energy and linear momentum between lattice vibrations (phonons) via anharmonic coupling is a cornerstone of solid-state physics, conservation and transfer of angular momentum within the lattice remained a postulate, yet. Recently, phonon angular momentum, often in the form of chiral phonons, was linked to gigantic magnetic fields, dynamical ferroelectricity, ultrafast demagnetization, or magnetic switching. However, the fundamental process of phonon to phonon angular momentum transfer required for demagnetization and other spin-related relaxation phenomena remained elusive.

Here we drive coherent phonon-phonon angular momentum transfer by establishing helical nonlinear phononics. Thereby, we directly observe phonon helicity-switching dictated by (pseudo) angular momentum conservation and the discrete rotational symmetry of the lattice. Ab-initio modeling in conjunction with classical equations of motion confirm the experimentally observed anharmonic phonon-phonon coupling as the dominating lattice angular momentum transfer channel. Our results thus open the field of helical or chiral nonlinear phononics, turning lattice angular momentum into the long missing tuning knob for ultrafast material control.

Invited Talk TT 1.2 Mon 10:00 H20

Chiral phonons, phono-magnetism, and spin-rotation coupling — •Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

High-intensity THz lasers enable the coherent excitation of individual phonon modes. The ultrafast control of emergent magnetism through phonons and phonon angular momentum opens new avenues for tuning functional materials. Recent experiments suggest a substantial magnetization in various materials [1,2], presenting a challenge for theoretical modeling. I will provide an introduction to magnetization induced by phonon angular momentum via the phonon inverse Faraday effect [3]. Additionally, I will discuss a coupling mechanism based on inertial effects, which facilitates the interaction between rotational degrees of freedom and electron spin [4].

[1] Basini et al., Nature, 628, 534 (2024)
[2] Davies et al., Nature, 628, 540 (2024)
[3] Shabala, Geilhufe, Physical Review Letters, arXiv:2405.09538
[4] Geilhufe, Physical Review Research, 4, L012004 (2022)

Invited Talk TT 1.3 Mon 10:30 H20

Geometry of temporal chiral structures and photoinduced chirality-spin coupling — •Olga Smirnova[1,2,3], Philip Flores[1], Aycke Roos[1], David Ayuso[4], Piero Decleva[5], Stefanos Carlstroem[1], Serguei Patchkovskii[1], and Andres Ordonez[4] — [1]Max-Born Institute, Berlin — [2]Technische Universität Berin — [3]Technion - Israeli Institute of Technology, Haifa, Israel — [4]Imperial College London, UK — [5]CNR IOM and Dipartimento di Scienze Chimiche e Farmaceutiche, Universita degli Studi di Trieste, Italy

In non-relativistic physics the concepts of geometry and topology are usually applied to characterize spatial structures, or structures in momentum space. We introduce the concept of temporal geometry [1], which encompasses geometric and topological properties of temporal shapes, e.g. trajectories traced by a tip of a time-dependent vector on sub-cycle time scale, and apply it to light-driven ultrafast electron currents in chiral molecules. The geometric concepts: curvature and connection emerge as ubiquitous features of photoexcited chiral electron dynamics. To demonstrate the link between the geometric fields and spin, we extend the concept of curvature to spin-resolved photoionization, and show that it is responsible for enantio-sensitive locking of the cation orientation to the photoelectron spin. This translates into chirality induced spin selectivity in photoionization of oriented chiral molecules both in one photon and two-photon processes.

[1] Geometry of temporal chiral structures, A. F. Ordonez, A. Roos, P. Mayer, D.Ayuso, O. Smirnova, arXiv preprint arXiv:2409.02500, 2024

15 min. break

Invited Talk TT 1.4 Mon 11:15 H20

Phonon thermal Hall effect — •Kamran Behnia — Ecole Supérieure de Physique et de Chimie Industrielles, Paris, France

In insulating solids and liquids, heat is carried by phonons. The phonon scattering time is close to the so-called Planckian time near the melting temperature. It increases with cooling, as phonon-phonon Umklapp scattering events rarefy. A rigorous determination of thermal conductivity of insulators from first principles has been a major accomplishment of the quantum theory of solids. In contrast, our understanding of momentum and energy exchange between phonons at low temperatures is imperfect. In this context, the experimental detection of phonon thermal Hall effect in a growing number of insulators is a challenge to the condensed matter theory. The list now includes elmental insulators, such as black phosphorus, silicon and germanium, in which the spin degree of freedom is irrelevant and the atomic bonds are covalent. We will examine how magnetic field can influence anharmonicity.

Invited Talk TT 1.5 Mon 11:45 H20

Giant effective magnetic moment of chiral phonons — •Swati Chaudhary[1,3], Dominik Juraschek[2], Martin Rodriguez-Vega[3], and Gregory A Fiete[4] — [1]The Institute for Solid State Physics, The University of Tokyo, Japan — [2]Eindhoven University of Technology, Eindhoven, Netherlands — [3]The University of Texas at Austin, Austin, USA — [4]Northeastern University, Boston, USA

Chiral phonons carry angular momentum and lead to magnetic responses in applied magnetic fields or when resonantly driven with ultrashort laser pulses. On the basis of purely circular ionic motion, these phonons are expected to carry a magnetic moment of the order of a few nuclear magnetons. However, some recent experiments have demonstrated a phonon magnetic moment of the order of a few Bohr magnetons. This kind of giant magnetic response points towards the electronic contribution to the magnetic moment of phonons. Many diverse mechanisms have been discovered for this enhanced magnetic response of chiral phonons. The orbital-lattice coupling is one such mechanism where low-energy electronic excitations on a magnetic ion hybridize with phonons and endow a large magnetic moment to phonons. In this talk, I'll present a microscopic model for the effective magnetic moments of chiral phonons based on this mechanism.

We apply our model to two types of materials: rare-earth halide paramagnets and transition-metal oxide magnets. In both cases, we find that chiral phonons can carry giant effective magnetic moments of the order of a Bohr magneton, orders of magnitude larger than previous predictions.

TT 1.6 Mon 12:15 H20

Extrinsic Phonon Thermal Hall Effect — •Dimos Chatzichrysafis[1], Robin Richard Neumann[1,2], and Alexander Mook[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Germany

The thermal Hall effect is a developing tool to investigate charge-neutral excitations, exposing the quantum many-body ground state of correlated materials. Since a sense of chirality for the energy carriers is necessary for the generation of a thermal Hall effect, it is natural to expect that quasiparticles of magnetic excitations are responsible for the Hall transport. This conventional wisdom has been recently challenged in experiments [1] which revealed a universal character of the thermal Hall effect independent on the magnetic texture and the lattice structure, even in systems where magnetism is completely absent. This finding asks for the re-investigation of the role of phonons in the thermal Hall effect.

Here, we develop a theory for a phononic thermal Hall effect where the source of chirality is given by the presence of the molecular Berry phase. As a toy model we study a non-magnetic system on a Bravais square lattice. We go beyond the intrinsic mechanism [2] usually studied in literature and consider the contribution of different possible extrinsic sources of phonon Hall transport. Our results demonstrate that phonon thermal Hall effects can be native to very generic systems.

[1] Xiaobo Jin et al, arXiv:2404.02863
[2] Takuma Saito et. al, Phys. Rev. Lett. 123, 255901, December 2019

TT 1.7 Mon 12:30 H20

Signatures of chiral phonons in $MnPS_3$ — •Banhi Chatterjee and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057, Duisburg, Germany

Chiral phonons can exist in two-dimensional transition metal dichalcogenide (TMDC) monolayers without inversion symmetry. They can be observed in the non-equilibrium state triggered by optical excitations using circularly polarized light. In existing literature a detailed theoretical calculation of the circular phonons production rate has already been done for the TMDC MoS_2. We investigate the antiferromagnetic semiconductor $MnPS_3$ with a similar hexagonal crystal structure and band-structure like MoS_2 but a larger unit cell as a novel candidate material that may allow for excitation of circular phonons. In $MnPS_3$, although the total magnetic moment is zero in the ground state, exciting the system using circularly polarized light induces a net magnetic moment. The damping of the magnons observed experimentally points to the transfer of orbital angular moment to combined phonon-magnon excitations. Using DFT+U and density functional perturbation theory (DFPT) we obtain in-plane chiral phonon modes at the valley-points of a monolayer $MnPS_3$ and for these modes the S atoms make circular motions. We further study the electron-phonon coupling between these chiral phonon modes and the excited electronic states carrying orbital angular momentum, particularly the dominant d-electrons, in order to theoretically investigate the experimentally observed damping of magnons.

TT 1.8 Mon 12:45 H20

Elliptically polarized coherent phonons in a degenerate mode — Arne Ungeheuer, Mashood T. Mir, Ahmed Hassanien, Lukas Nöding, Thomas Baumert, and •Arne Senftleben — Institut für Physik, Universität Kassel

Controlled excitation of phonons in crystalline solids is an emerging way to alter the property of a material to create phenomena such as transient magnetic polarization [1,2]. Here, we want to focus on controlling the polarization properties of coherent optical phonons that can be launched by ultrashort laser pulses. we demonstrate the excitation of elliptically polarized coherent optical phonons of the E_{2g} shearing mode in graphite. This is achieved by exciting the superposition of two orthogonally polarized phonon modes using a tailored pair of time-delayed optical pulses with tilted polarization. The elliptically polarized coherent phonons are detected by ultrafast electron diffraction [3], where we determine the amount of ellipticity and the sense of rotation.

[1] D. M. Juraschek, et al. *Phys. Rev. Lett.* **118**, 054101 (2017).
[2] A. S. Disa, et al. *Nature Phys.* **16**, 937–941 (2018).
[3] C. Gerbig, et al. *New J. Phys.* **17**, 043050 (2015).

TT 2: Nonequilibrium Quantum Systems (joint session TT/DY)

Time: Monday 9:30–12:30 Location: H31

TT 2.1 Mon 9:30 H31

Solving the nonequilibrium Dyson equation with quantics tensor trains — •Ken Inayoshi[1], Maksymilian Środa[2], Anna Kauch[3], Philipp Werner[2], and Hiroshi Shinaoka[1] — [1]Department of Physics, Saitama University, Saitama, Japan — [2]Department of Physics, University of Fribourg, Fribourg, Switzerland — [3]Institute of Solid State Physics, TU Wien, Vienna, Austria

The nonequilibrium Green's function (NEGF) method is a powerful tool to investigate dynamical phenomena in quantum many-body systems. However, the time-translational symmetry breaking of Green's functions (GFs) makes the simulation of long-time dynamics computationally and memory-intensive. To overcome these, various memory compression techniques have been proposed for the NEGF method [1,2]. Among these, quantics tensor trains (QTT) have been attracting a focus for its ability to exponentially compress the data size of GFs [3]. While a prototype NEGF method with QTT has been developed [4], its benchmarks were limited to the short-time dynamics due to technical challenges such as the slow convergence of self-consistent calculations. We propose an improved implementation to reach the longer time regions, using a variational method for solving the Dyson equation and a causality-based divide-and-conquer algorithm [5,6]. In this contribution, we benchmark our method in relevant test cases [6].

[1] J. Kaye and D. Golež, SciPost Phys. **10**, 091 (2021).
[2] M. Eckstein, arXiv:2410.19707.
[3] H. Shinaoka *et al.*, Phys. Rev. X **13**, 021015 (2023).
[4] M. Murray *et al.*, Phys. Rev. B **109**, 165135 (2024).
[5] M. Środa *et al.*, in preparation
[6] K. Inayoshi *et al.*, in preparation

TT 2.2 Mon 9:45 H31

Fractionalized prethermalization in the one-dimensional Hubbard model — •Anton Romen[1,2], Johannes Knolle[1,2,3], and Michael Knap[1,2] — [1]Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Blackett Laboratory, Imperial College London, London, United Kingdom

Prethermalization phenomena in driven systems are generally understood via a local effective Floquet Hamiltonian. It turns out that this picture is insufficient for systems with fractionalized excitations. A first example is a driven Kitaev spin liquid which realizes a quasistationary state with vastly different temperatures of the matter and flux sectors, a phenomenon dubbed fractionalized prethermalization. In our work we argue that similar heating dynamics also occur in driven 1D tJ-models. In the weak doping limit of this model, the electron fractionalizes into quasiparticles carrying charge and spin. We show that the nonequilibrium heating dynamics of this model feature a quasistationary state characterized by a low spin and high charge temperature. We argue that the lifetime of this quasistationary state is determined by two competing processes depending on the specific drive chosen: A Fermi Golden Rule that describes the lifetime of the quasiparticles and the exponential lifetime of a Floquet prethermal plateau. Using a time dependent variant of the Schrieffer-Wolff transformation we systematically analyze the different classes of drives emerging from the respective Hubbard model. Lastly, we discuss potential ways towards an experimental realization in cold atom experiments.

TT 2.3 Mon 10:00 H31

Computing the lifetime of spin-orbital excitations in TiOCl using Lanczos techniques — •Paul Fadler[1,2], Philipp Hansmann[1], Kai Phillip Schmidt[1], Angela Montanaro[1,3], Filippo Glerean[4], Enrico Maria Rigoni[1,3], Daniele Fausti[1,3], and Martin Eckstein[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Universität Hamburg — [3]University of Trieste — [4]Harvard University, Cambridge

TiOCl is a spin-Peierls compound with optically active d-d-transitions at 0.7 eV and 1.5 eV. A pump-push-probe spectroscopy experiment on this system revealed a nonlinear signal asymmetric with respect to the order in which these transitions are pumped. This asymmetry could arise from differing lifetimes of the excitations due to multi-magnon and orbital-fission decay processes. To test this hypothesis we derive a spin-orbital Hamiltonian from ab-initio calculation. Within this description the pumped excitations are orbitons, i.e., hybrid spin-orbital quasiparticles, that can be understood as orbital excitations surrounded by a magnon cloud. We evaluate their lifetimes using Fermi's golden rule for all spin-orbital decay channels, which we compute on a large cluster using Lanczos techniques. Comparing the theoretical prediction to the asymmetry and absolute decay times of the nonlinear signal in the experiment we conclude, that multi-magnon and orbital-fission decay processes could be the dominant decay channels for the 0.7 eV excitation. On the other hand for the 1.5 eV excitation other types of processes such as phonon-assisted decays or non-linearities in the double-pump scheme have to be taken into account.

TT 2.4 Mon 10:15 H31

Comprehensive analysis of electronic relaxation in one dimension Kondo lattice model — •Arturo Perez Romero, Mica Schwarm, and Fabian Heidrich-Meisner — Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Recent advancements in laser technology have made it possible to create non-equilibrium conditions on timescales that outpace energy exchange across a wide range of degrees of freedom. The above represents a challenge not only for condensed matter experimental physicist, but also for theoretical physicist who are motivated to describe a great variety of far-from-equilibrium systems. In this paper, we study the real-time dynamics of two paradigmatic models: the Kondo lattice model (KLM) and Kondo-Heisenberg model (KHM) in one dimension. We analyze the role of exchange couplings for the relaxation of a single charge carrier via the time-dependent Lanczos method. We conduct a comprehensive study of the time evolution by evaluating the z-spin component of the conduction electron, the local spin-spin correlation between localized and conduction electron, the spin-spin correlation between localized spins, and the electronic momentum distribution momentum. The study includes a comparison with statistical mechanics predictions for steady state and a research of the effect of diagonal disorder.

This work was funded by the Deutsche Forschungsgemeinschaft (DPG, German Research Foundation) via CRC 1073

TT 2.5 Mon 10:30 H31

An attempt to extend the adiabatic theorem — •Sarah Damerow[1,2] and Stefan Kehrein[1] — [1]Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg

A conjectured extension of the adiabatic theorem to quantum quenches, i.e., maximally non-adiabatic changes, is presented.The proposed extension is framed as follows: "as long as quenched states within the same magnetic phase are concerned, the overlap between the initial and final ground states is the largest possible." This conjecture is investigated analytically and is tested numerically using Exact Diagonalisation in two models: the Transverse Field Ising Model (TFIM) and the Axial Next Nearest Neighbour Ising Model (ANNNI).

TT 2.6 Mon 10:45 H31

Towards Floquet-GW: interacting electrons in time-periodic potentials — •Ayan Pal[1,2], Erik G. C. P. Van Loon[1,2], and Ferdi Aryasetiawan[1] — [1]Division of Mathematical Physics, Department of Physics, Lund University, Professorsgatan 1, 223 63, Lund, Sweden — [2]NanoLund, Lund University, Professorsgatan 1B, 223 63, Lund, Sweden

The Floquet theory of time-periodic systems provides a middle ground between equilibrium and completely non-equilibrium physics. Here, we study interacting electrons in time-periodic potentials using the combination of Floquet theory and many-body methods such as RPA and GW. We apply these techniques to the electron gas and to lattice models and study the electronic and dielectric properties, for example the appearance of side bands in the spectral functions. These methods have the potential to describe the impact of periodic laser pulses on the plasmonic and optical properties of (moderately) correlated materials.

15 min. break

TT 2.7 Mon 11:15 H31

Universal quench dynamics in Yukawa-Sachdev-Ye-Kitaev models — •Haixin Qiu and Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Understanding the non-equilibrium properties of non-Fermi liquids without quasiparticles is essential for exploring the dynamics of strongly correlated systems. Here we investigate the quantum quench of a non-Fermi liquid model, the Yukawa-Sachdev-Ye-Kitaev model with interactions involving one boson and q fermions and its lattice extensions. We compute various in and out of equilibrium quantities for general q within the large-N dynamical mean field scheme by integrating the Kadanoff-Baym equations. We find transient oscillations and relaxation dynamics are insensitive to the quench amplitudes deep inside the non-Fermi liquid phase. Notably, the relaxation dynamics involve two distinct transient temperatures and relaxation rates for bosonic and fermionic degrees of freedom, both of which show non-Fermi liquid or universal behaviors. Signatures of prethermalization are also found when quenching near the Fermi liquid phase.

This work is supported by Deutsche Forschungsgemeinschaft (DFG) SFB 1073 (217133147) and FOR 5522 (499180199).

TT 2.8 Mon 11:30 H31

Long-range induced synchronization of Higgs oscillations in topological superconductors — Andreas Alexander Buchheit[1], Benedikt Fauseweh[2,3], and •Torsten Kessler[4] — [1]Saarland University, Department of Mathematics and Computer Science, Germany — [2]TU Dortmund University, Department of Physics, Germany — [3]German Aerospace Center (DLR), Cologne, Germany — [4]Eindhoven University of Technology, Department of Mechanical Engineering, Netherlands

We investigate the impact of long-range electron-electron interactions on the non-equilibrium dynamics of unconventional superconductors. Using recently developed mathematical tools for the efficient treatment of longe-range interactions on lattices, we simulate the time evolution of a triplet superconductor with arbitrary power law interaction. Owing to the long-range interaction, a chiral phase with d+p symmetry emerges. We find that the long-range interaction stabilizes the Higgs oscillation in this phase. While the d-wave's initial mode decays rapidly, it begins to mirror the stable Higgs oscillation of the p-wave condensate part. Eventually, the two parts oscillate with a joint frequency. We demonstrate that this behavior can also be observed in the optical conductivity resulting from an external probe pulse.

TT 2.9 Mon 11:45 H31

Tuning of slow dynamics in quantum East Hamiltonians motivated by Graph theory — •Heiko Georg Menzler[1], Mari Carmen Bañuls[2,3], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schelling Strasse 4, D-80799 München

In-between fully ergodic/localized quantum system there exist many systems with atypical relaxation behaviors. One of these systems is the quantum East (QE) model. The classical East model is a central, exemplary model for glassy dynamics and kinetic constraints. Also its quantum counterpart features slow dynamics without conservation laws or disorder. However, the presence of slow dynamics has not yet been fully understood from a quantum perspective. Introducing an interpretation of constrained dynamics based on graph theory, we theoretically demonstrate control over the slow dynamics of QE models. As a general hypothesis, we propose that strong hierarchies between nodes on the Fock space graph are related to the presence of slow dynamics. To quantify hierarchical structures, we develop a measure of centrality for generic Hamiltonian matrices, reminiscent of established centrality measures from graph theory. Based on these ideas, we show how we can introduce detuning to alter the hierarchical structure in the QE model and acutely change the resulting constrained dynamics, evidenced by eigenstate structure in the detuned QE models.

Supported by DFG, German Research Foundation via FOR 5522

TT 2.10 Mon 12:00 H31

Optical signatures of dynamical excitonic condensates — •Alexander Osterkorn[1], Yuta Murakami[2], Tatsuya Kaneko[3], Zhiyuan Sun[4], Andrew J. Millis[5,6], and Denis Golež[1,7] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]RIKEN, Wako, Japan — [3]Osaka University, Toyonaka, Japan — [4]Tsinghua University, Beijing, P.R. China — [5]Columbia University, New York, USA — [6]Flatiron Institute, New York, USA — [7]University of Ljubljana, Ljubljana, Slovenia

Excitons, or bound electron-hole pairs, can condense into an excitonic insulator state, similarly to Cooper pairs in superconductors. A non-equilibrium carrier concentration, such as the one transiently induced by photo-doping or sustained by a tuneable bias voltage in bilayers, can create a dynamical excitonic insulator state, yet proving phase coherence in such setups remains challenging. We examine the condensate phase behavior theoretically and show that optical spectroscopy can distinguish between phase-trapped and phase-delocalized dynamical regimes. In the weak-bias regime, trapped phase dynamics result in an in-gap absorption peak nearly independent of bias voltage, while at higher biases its frequency increases approximately linearly. In the large bias regime, the response current grows strongly under the application of a weak electric probe leading to negative weight in the optical response, which we analyze relative to predictions from a minimal model for the phase. This work opens new avenues for experimentally probing coherence in excitonic condensates and the detection of their dynamical regimes.

TT 2.11 Mon 12:15 H31

Visualizing dynamics of charges and strings in (2+1)D lattice gauge theories — Tyler A. Cochran[1,2], •Bernhard Jobst[3,4], Eliott Rosenberg[1], Yuri D. Lensky[1], Adam Gammon-Smith[5], Michael Knap[3,4], Frank Pollmann[3,4], and Pedram Roushan[1] — [1]Google Research, CA, USA — [2]Princeton University, NJ, USA — [3]Technical University of Munich, 85748 Garching, Germany — [4]MCQST, 80799 München, Germany — [5]University of Nottingham, NG7 2RD, UK

Lattice gauge theories (LGTs) can be employed to understand a wide range of phenomena. Studying their dynamical properties can be challenging as it requires solving many-body problems that are generally beyond perturbative limits. We investigate the dynamics of local excitations in a $\mathbb{Z}_2$ LGT using a two-dimensional lattice of superconducting qubits. We first construct a simple variational circuit which prepares low-energy states that have a large overlap with the ground state; then we create particles with local gates and simulate their quan-

tum dynamics via a discretized time evolution. As the effective magnetic field is increased, our measurements show signatures of transitioning from deconfined to confined dynamics. For confined excitations, the magnetic field induces a tension in the string connecting them. Our method allows us to experimentally image string dynamics in a (2+1)D LGT from which we uncover two distinct regimes inside the confining phase: for weak confinement the string fluctuates strongly in the transverse direction, while for strong confinement transverse fluctuations are effectively frozen.

TT 3: Correlated Magnetism – General

Time: Monday 9:30–12:45 Location: H32

TT 3.1 Mon 9:30 H32

The zoo of states in the 2D Hubbard model — •Robin Scholle[1], Pietro Bonetti[1,2], Demetrio Vilardi[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Harvard University, Cambridge, USA

We use real-space Hartree-Fock theory to construct a magnetic phase diagram of the two-dimensional Hubbard model as a function of temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order without biasing the system towards one of them. For an intermediate interaction strength we predominatly find Néel order close to half-filling, stripe order for low temperatures or large doping, and an intermediate region of spiral order.

I will give a short summary of the method followed by a presentation of our current results and an outlook for possible further applications.

TT 3.2 Mon 9:45 H32

Hidden quantum correlations in the ground states of quasiclassical spin systems — •Levente Rózsa[1,2], Dennis Wuhrer[3], Sebastián A. Díaz[3], Ulrich Nowak[3], and Wolfgang Belzig[3] — [1]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]University of Konstanz, Konstanz, Germany

Entanglement is a unique property of quantum systems, which is widely studied in strongly correlated materials and in quantum information theory. Here, we investigate the entanglement between magnons, the quanta of spin waves, around a classical spin-spiral ground state stabilized by frustrated exchange interactions [1]. We find that the entanglement between pairs of sites completely vanishes in certain parameter regimes, where quantum correlations can only be observed in multi-site clusters. We analyze the magnitude and the spatial dependence of the entanglement in the vicinity of classical phase transitions, and discuss the role of the symmetries of the ground state.

[1] L. Rózsa et al., arXiv:2411.08394.

TT 3.3 Mon 10:00 H32

Measurement of magnetic anisotropy in CsV_3Sb_5 using torque magnetometry — •Tobi Gaggl[1], Toshiki Kiyosue[2], Ryo Misawa[3], Tomoya Asaba[2], Max Hirschberger[3], and Yuji Matsuda[2] — [1]Technical University of Munich, Germany — [2]Kyoto University, Japan — [3]The University of Tokyo, Japan

Materials with a kagome lattice have emerged as a fertile ground for exploring nontrivial electronic states arising from the interplay between band topology and magnetic frustration. The kagome metals AV_3Sb_5 (A=K, Cs or Rb), which exhibit charge density wave ordering (CDW), may host such exotic states. It is believed that the CDW in kagome metals is of unconventional nature, thus advanced techniques for precise measurements are required for characterization.

This study investigates the CDW phase transition in CsV_3Sb_5 using a piezoresistive cantilever rotating in a magnetic field as an angular-dependent torquemeter. This method enables precise measurements of magnetization in single crystals and a powerful setup sensitive to changes in rotational symmetry. The results show a distinct two-fold out-of-plane magnetic anisotropy, which is due to the two-dimensional nature of the kagome lattice and consistent with previous calculations. The progression of the measured temperature-dependent magnetic anisotropy shows a clear kink at 94 K, confirming previously published results for the onset of CDW. My current work focuses on the development of novel kagome materials that could exhibit CDWs.

TT 3.4 Mon 10:15 H32

Detection of skyrmion lattices by dilatometric measurements — •Mathias Doerr[1], Justus Grumbach[1], Sergey Granovsky[1], Martin Rotter[1], and Max Hirschberger[2,3] — [1]Technische Universität Dresden, Institut für Festkörper- und Materialphysik, 01062 Dresden, Germany — [2]Department of Applied Physics and Quantum-Phase Electronics Center, University of Tokyo, Tokyo 113-8656, Japan — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan

Magnetic skyrmion lattices (SkL) with a characteristic structure size smaller than 3 nm in metallic $Gd_3Ru_4Al_{12}$ with a planar breathing kagome lattice, already demonstrated by X-ray diffraction and topological Hall effect studies [1], open up new possibilities for the effective transmission of information. The interplay between helically determined skyrmion patterns and underlying crystallographic structures offers the possibility to clearly determine the stability region of skyrmions by dilatometric measurements. We report high-precision measurements of magnetostriction and thermal expansion on $Gd_3Ru_4Al_{12}$ and construct the magnetic phase diagram. Additional MonteCarlo simulations with *McPhase* confirm an asymmetric magnetic triple-$\boldsymbol{q}$ structure without symmetry breaking at the ordering temperature. The relationship between crystallographic distortion and formation of the SkL is also discussed.

[1] M. Hirschberger *et al*., Nat. Commun. 10, 5831 (2019).

TT 3.5 Mon 10:30 H32

Electronic structure of the noncentrosymmtric tetragonal antiferromagnet $EuPtSi_3$ — •Katharina Müller[1], André Deyerling[1], Andreas Bauer[1,2], Wolfgang Simeth[1,3], Christian Franz[1,4], Christian Pfleiderer[1,2,5,6], and Marc A. Wilde[1,2] — [1]Physik Department, TUM School of Natural Sciences, TUM, Germany — [2]Zentrum für Quantum Engineering (ZQE), TUM, Germany — [3]Los Alamos National Laboratory, Los Alamos, NM, USA — [4]Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Germany — [5]Munich Center for Quantum Science and Technology (MCQST), TUM, Germany — [6]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Germany

The localized Eu^{2+} moments of the rare-earth compound $EuPtSi_3$ were reported to show magnetic ordering below the Néel temperature T_N = 17 K [1]. With a magnetic field applied in the magnetically hard basal plane, four different types of noncollinear antiferromagnetic order emerge, one of which is commensurate with the lattice [2]. This coplanar canted magnetic structure breaks the crystal symmetry such that Berry curvature contributions are allowed and electronic transport phenomena may be affected. We study this link between the magnetic and the electronic structure with ab initio calculations, in particular highlighting the effect of changing the canting angle from the antiferromagnetic towards the spin-polarized state.

[1] A. Bauer et al., PRM **6**, 034406 (2022).
[2] W. Simeth et al., PRL **130**, 266701 (2023).

TT 3.6 Mon 10:45 H32

Thermal Hall transport driven by spin fluctuations — •Ignacio Salgado-Linares[1,2], Alexander Mook[3], and Johannes Knolle[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Johannes Gutenberg University Mainz, Institute of Physics, Staudingerweg 7, Mainz 55128, Germany

In recent years, the thermal Hall effect has emerged as a powerful tool for probing topological phenomena of magnetic systems. At low temperatures, the thermal Hall transport of long-range ordered magnets can be described in the framework of linear spin-wave theory (LSWT). However, how to treat regimes with increased thermal fluctuations or non-linearities beyond LSWT is an outstanding question. Therefore, within this project, we developed a numerical technique to extract the thermal Hall transport properties, which intrinsically includes nonlinear effects. In particular, we use semi-classical spin dynamics simulations to compute thermal currents due to chiral spin fluctuations in a square lattice model with Heisenberg interaction and DMI. The results are expected to shed new light on the topological thermal transport in systems where topology does not arise from static spin textures, but from spin fluctuations.

TT 3.7 Mon 11:00 H32

Pressure tuning of ferromagnetism in the Kagome metal CrNiAs — •Bin Shen[1], Franziska Breitner[1], Victoria A. Ginga[2], Philipp Gegenwart[1], and Alexander A. Tsirlin[2] — [1]EP VI, EKM, University of Augsburg, Germany — [2]Felix Bloch Institute, University of Leipzig, Germany

Ferromagnetic Kagome metals attract considerable interest as quantum materials with nontrivial topological electronic states. Here, we present our extensive study on single crystals of CrNiAs, crystallizing in a hexagonal structure with space group of $P\bar{6}2m$, featuring a distored kagome lattice of magnetic Cr. CrNiAs undergoes a ferromagnetic phase transition at T_C = 135 K, where the *c*-axis is the easy axis. At T^* = 90 K another phase transition is found, likely driven by magnetism, associated with a shrinkage of the *c*-axis while the *ab*-plane expands. Anomalous Hall effect is observed in the magnetically ordered state of CrNiAs. We also report the pressure tuning of ferromagnetism.

Supported by DFG-TRR 360-492547816 and the Alexander von Humboldt Foundation.

15 min. break

TT 3.8 Mon 11:30 H32

Electronic transport measurements in Kagome metal $Yb_{0.5}Co_3Ge_3$ — •Zhiyuan Cheng[1], Heng Wu[2], Yaojia Wang[2], Peter van Veldhuizen[1], Federica Galli[1], Mazhar Ali[2], Julia Chan[3], and Semonti Bhattacharyya[1] — [1]Leiden University, Leiden, the Netherlands — [2]Delft University of Technology, Delft, the Netherlands — [3]Baylor University, Waco, United States

Kagome lattice has a unique geometry that gives rise to interesting band structures. As a result, Kagome lattices exhibit various properties, such as superconductivity, topological surface states, and complex magnetism. However, it is still yet to be well understood how these quantum properties intertwine with each other. Electrical doping, strain, and pressure can be utilized as powerful tools to modulate and investigate the rich physics of such complex systems.

In this project, we investigate a Kagome metal $Yb_{0.5}Co_3Ge_3$ that is known to exhibit charge density wave and complex magnetism. Susceptibility measurements performed in this material demonstrate the presence of Yb^{3+} moments with anti-ferromagnetic interactions and an onset of a week magnetic transition below 25 K. Yet, this complex magnetism is not completely understood.

We carried out magnetotransport measurements on $Yb_{0.5}Co_3Ge_3$ to study the interplay of its quantum properties at both ambient pressure (0 GPa) and high pressure (up to 2.0 GPa). Our ambient-pressure measurement shows that this complex magnetism gives rise to Kondo effect. High-pressure measurements reveal a clear signature of an enhancement of the Kondo effect with respect to the pressure.

TT 3.9 Mon 11:45 H32

Altermagnetism from interaction-driven itinerant magnetism — Samuele Giuli[1], •Carlos Mejuto-Zaera[1,2], and Massimo Capone[1,3] — [1]International School for Advanced Studies (SISSA), Trieste, Italy — [2]Current: Laboratoire de Physique Théorique (LPT), Toulouse, France — [3]CNR-IOM Democritos, Trieste, Italy

Altermagnetism is a phase of collinear spin-ordering presenting anisotropic magnetic properties, leading to great interest in its potential application for spintronic and thermoelectric devices. Realizing this promise will likely hinge on the design of tunable altermagnetic platforms, in which the magnetic and electric responses can be reliably controlled. A viable path towards this goal concerns leveraging electron interactions for the stabilization of altermagnetism, a strategy which is developing increasing traction in the field. In this work, we propose a mechanism driven by the interplay between a local Hubbard repulsion and the presence of a van Hove singularity in a two-band model. Here, the itinerant magnetism caused by the van Hove singularity colludes with the exchange mechanism driven by the Hubbard repulsion to generate an altermagnetic state in a sizeable portion of the phase diagram. Importantly, this correlated altermagnetic phase exhibits a tuneable spin-current, whose sign can be changed by tuning the interaction strength and/or particle doping. We study the role of strong electronic correlations in the stabilization of this phase by leveraging on the ghost rotationally invariant slave boson embedding. Further, we comment on the stability of the phase, and potential material realizations.

TT 3.10 Mon 12:00 H32

Investigation of the magnetoelastic coupling in $CaMn_2P_2$ and $SrMn_2P_2$ — •Sven Graus, Ashiwini Balodhi, N. S. Sangeetha, Teslin R. Thomas, Maximilian van de Loo, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

Mn-based 122-compounds exhibit complex magnetic ordering in the antiferromagnetic state. In contrast to other related materials $CaMn_2P_2$ shows a strong first-order and $SrMn_2P_2$ a weak first-order antiferromagnetic phase transition [1]. Since the antiferromagnetic ordering breaks the three-fold symmetry of the lattice, one expects lattice distortions, which we investigated by high-resolution thermal expansion measurements. Thermal-expansion data of $CaMn_2P_2$ show a significant decrease of the sample length upon entering the antiferromagnetic state. Applying different uniaxial pressures along the [1 1 0] and [1 -1 0] directions alters the transition in qualitatively distinct ways. Increasing uniaxial pressure shifts the transition temperature upwards which shows magnetoelastic coupling and is consistent with the interpretation of an orthorhombic lattice distortion in the antiferromagnetic phase. In $SrMn_2P_2$, an anomaly in the thermal expansion is clearly resolvable upon entering the antiferromagnetic state. From 300 K to 6 K the linear thermal expansion coefficient α continuously decreases, reaching negative values below ~100 K.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] Sangeetha et al., PNAS **118**, e2108724118 (2021).

TT 3.11 Mon 12:15 H32

Synthesis of $CsMn_2P_2$ and study of its low temperature physical properties — •Matthias Kroll, N. S. Sangeetha, Sven Graus, Maik Golombiewski, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

The growth of $CsMn_2P_2$ single crystals is challenging due to the high vapor pressure of cesium and phosphorus and the high melting point of manganese. We optimized the growth conditions for the reproducible synthesis of $CsMn_2P_2$ single crystals by systematically studying various growth techniques. The quantity and quality of the phase of interest in the resulting samples was characterized by x-ray powder diffraction, electron microscopy and energy-dispersive x-ray analysis. We perform thermal-expansion and magnetic field-dependent resistivity measurements at low temperatures to analyze the nature of the three phase transitions at 64, 17 and 11 K that cannot be explained conclusively so far [1,2]. At 17 K, a dramatic change of the electrical-transport behavior as well as a large thermal-expansion anomaly are observed.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] F. Hummel, Magnetism and superconductivity in layered manganese and iron pnictides. Diss. LMU (2015).
[2] H. G. von Schnering et al., ZAAC 628, 2772 (2002)

TT 3.12 Mon 12:30 H32

Strain-tuning of magnetic properties of $Ca_{1-x}Sr_xCo_{2-y}As_2$ and elastoresistance measurements in different symmetry channels — •Teslin Rose Thomas, Michael Paul, N. S. Sangeetha, Sven Graus, Max Brückner, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

The $Ca_{1-x}Sr_xCo_{2-y}As_2$ system belongs to the well-studied $ThCr_2Si_2$ structural family where Sr substitution induces a crossover from a collapsed tetragonal (cT) phase to an uncollapsed tetragonal (ucT) phase, along with different magnetic anisotropies [1,2].

In this study, we investigate how the cT-ucT crossover and the associated magnetic orders respond to in-plane symmetric and asymmetric strain in different configurations. We show that large in-plane symmetric strain can effectively tune the magnetic properties of the system. We also find a significant response of the resistance to in-plane symmetric strain with a temperature dependence that varies dramatically based on the doping level. The resistance response to symmetric strain dominates the response to asymmetric strain.

We acknowledge support from the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] N. S. Sangeetha et al., Phys. Rev. Lett. 119, 257203 (2017).
[2] Bing Li et al., Phys. Rev. B 100, 024415 (2019).

TT 4: Topological Insulators

Time: Monday 9:30–13:00 Location: H33

TT 4.1 Mon 9:30 H33

Magnetotransport measurements on magnetic topological insulator nanostructures fabricated with shadow wall epitaxy — •Jan Karthein[1,2], Gion Toehgiono[1,2], Max Vassen-Carl[1,2], Taizo Kawano[3], Sosuke Otsubo[3], Makoto Kohda[3], Peter Schüffelgen[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany — [3]Department of Materials Science, Graduate School of Engineering, Tohoku University, 6-6-02 Aramaki-Aza Aoba, Aoba-ku, 980-8579 Sendai, Japan

We present a novel way to fabricate magnetic topological insulator nanostructures based on digital alloying and shadow wall epitaxy. The combination of these two techniques allows the preparation of structures in the micrometer and nanometer range without the need for lithography and etching steps on the material under investigation. The magnetotransport properties of micro and nano Hall bars fabricated in this way are investigated at cryogenic temperatures and in high magnetic fields. Different sizes of Hall bars are measured and their magnetic properties are studied. An anomalous Hall effect is observed, indicating the successful preparation of Hall bars based on magnetic topological insulator thin films. The Curie temperature of Hall bars with different widths is extracted and found to be systematically dependent on the dimensions.

TT 4.2 Mon 9:45 H33

Thermopower and resistivity of the topological insulator Bi_2Te_3 in the amorphous and crystalline phase — •Ena Osmic[1,2], Jose Barzola Quiquia[3], Stephan Winnerl[4], Winfried Böhlmann[5], Peter Häussler[3], and Joachim Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Division of Thin Film Physics, TU Chemnitz, Germany — [4]Institut für Ionenstrahlphysik und Materialforschung, HZDR, Dresden, Germany — [5]Felix-Bloch Institute for Solid-state Physics, Universität Leipzig, Germany

We investigated the temperature dependence of the thermopower $S(T)$ and resistance $R(T)$ in thin films of the topological insulator Bi_2Te_3, prepared *in situ* by sequential flash-evaporation at 4 K. In the amorphous phase, $S(T)$ is negative and significantly larger than in other amorphous materials, while in the crystalline phase, it remains negative and shows a linear temperature dependence. The resistivity $\rho(T)$ transitions from semiconducting behavior in the amorphous state to linear metallic behavior upon crystallization. For $T > 15$ K, the linear $\rho(T)$ reflects metallic surface states typical of topological insulators, while for $T < 10$ K, the conductivity shows a logarithmic temperature dependence dominated by electron-electron interactions. Raman spectroscopy confirms crystallization in the trigonal *R*3*m* space group, and energy-dispersive X-ray spectroscopy indicates high compositional homogeneity with no magnetic impurities.

TT 4.3 Mon 10:00 H33

Phonon thermal Hall effect in weakly compensated topological insulators — •Rohit Sharma[1], Yongjian Wang[1], Yoichi Ando[1], Achim Rosch[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The phonon thermal Hall effect has recently been observed in various classes of insulating materials, yet its origin remains unresolved [1-3]. In a series of well-compensated $Bi_{2-x}Sb_xTe_{3-y}Se_y$ samples, the thermal Hall conductivity $\kappa_{xy}(B)$ exhibits a linear and negative field dependence, with a thermal Hall ratio κ_{xy}/κ_{xx} on the order of 10^{-3}, consistent with observations in other insulating materials. Conversely, weakly compensated samples of $TlBi_{0.15}Sb_{0.85}Te_2$ exhibit a nonlinear dependence of $\kappa_{xy}(B)$, with κ_{xy}/κ_{xx} exceeding 2% across an extended temperature range. The electronic contribution to thermal transport, $\kappa_{xy}^{\mathrm{el}} = \sigma_{xy}L_0T$, was calculated using the Wiedemann-Franz law and compared to the measured κ_{xy}. Remarkably, the measured κ_{xy} is significantly larger than $\kappa_{xy}^{\mathrm{el}}$ throughout the temperature range investigated. Possible mechanisms driving the nonlinear $\kappa_{xy}(B)$ and the large thermal Hall ratio in $TlBi_{0.15}Sb_{0.85}Te_2$ will be discussed.

Funded by the DFG via CRC 1238 Projects A04, B01, and C02.

[1] R. Sharma *et al.*, Phys. Rev. B **109**, 104304 (2024).
[2] R. Sharma *et al.*, Phys. Rev. B **110**, L100301 (2024).
[3] X. Li *et al.*, Nat. Commun.**14**, 1027 (2023).

TT 4.4 Mon 10:15 H33

Scattering theory of chiral edge modes in topological magnon insulators — •Stefan Birnkammer[1,2], Michael Knap[1,2], Johannes Knolle[1,2], Alexander Mook[3], and Alvise Bastianello[1,2] — [1]Technical University Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Johannes Gutenberg Universtät, Mainz, Germany

Topological magnon insulators exhibit robust edge modes with chiral properties similar to quantum Hall edge states. However, due to their strong localization at the edges, interactions between these chiral edge magnons can be significant, as we show in a model of coupled magnon-conserving spin chains in an electric field gradient. The chiral edge modes remain edge-localized and do not scatter into the bulk, and we characterize their scattering phase: for strongly-localized edge modes we observe significant deviation from the bare scattering phase. This renormalization of edge scattering can be attributed to bound bulk modes resonating with the chiral edge magnons, in the spirit of Feshbach resonances in atomic physics. We argue a real-time measurement protocol using spin-polarized scanning tunneling spectroscopy to study their scattering dynamics. Our result show that interaction among magnons can be encoded in an effective edge model of reduced dimensionality, where the interactions with the bulk renormalize the effective couplings. This work paves the way to develop a many-body effective theory for chiral edge magnons.

TT 4.5 Mon 10:30 H33

Multiplicative Chern insulators — •Archi Banerjee[1,2] and Ashley M. Cook[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany

Extending on the previous work on multiplicative topological phases, here we study bulk-boundary correspondence and response signatures of multiplicative Chern insulators (MCIs). Constructing the MCI Bloch Hamiltonian as a symmetry-protected tensor product of two topologically non-trivial parent Chern insulators (CIs), we study 2D MCIs and introduce 3D MCIs, constructed by requiring the two 2D parent Hamiltonians share only one momentum component, rather than both as in the case of the 2D MCI. We study the robustness of bulk-boundary correspondence against bulk perturbations breaking the tensor product structure of the child Hamiltonian, and find the bulk-boundary correspondence remains gapless and evolves to that of a topological skyrmion phase in cases considered here. We also study the response of the 2D MCI to time reversal symmetric flux insertion through two spatially-separated locations in the lattice. We observe a 4π periodic Aharonov-Bohm (AB) effect in which unpaired Majorana zero-modes and associated spin angular momentum are transferred between these two locations. We interpret the AB effect from the perspective of the effective field theories of the quantum skyrmion Hall effect as corresponding to a generalised $\nu = 1/2$ FQHE.

TT 4.6 Mon 10:45 H33

Probing the tomographic regime by nonlinear thermoelectric and magneto-transport in topological Fermi liquids — •Habib Rostami[1] and Johannes Hofmann[2] — [1]Department of Physics, University of Bath, United Kingdom — [2]Department of Physics, Gothenburg University, Sweden

In 2D Fermi liquids, odd-parity Fermi surface deformations [PRL. 123, 116601 (2019)] exhibit anomalously slow relaxation rates, suppressed as $\tau_{\mathrm{AN}}^{-1} \sim T^4$ with temperature T, deviating from the standard Fermi-liquid scaling, $\tau_{\mathrm{FL}}^{-1} \sim T^2$. This near ballistic (tomographic) regime currently lack a precise experimental probes. We link light-induced nonlinear thermoelectric currents to prolonged relaxation times, τ_{AN} [Phys. Rev. Research 6, L042042 (2024)]. These currents, arising in topological Fermi liquids, depend on novel heat capacities, including the Berry curvature capacity $C_\Omega = \partial_T\langle\Omega^2\rangle$ and velocity-curvature capacity $C_{\mathrm{v}} = \partial_T\langle v\Omega\rangle$. Quantified in Bi_2Te_3, these effects predict non-monotonic thermoelectric responses, providing features for experimental testing. In another study [arXiv:2411.08102v1], we show that weak magnetic fields suppress tomographic transport signatures by breaking time-reversal symmetry, a prerequisite for the odd-parity collisional relaxation effect. This suppression, occurring at much lower fields than those needed to disrupt hydrodynamic transport, suggests a practical experimental method to extract the odd-parity mean free path.

TT 4.7 Mon 11:00 H33

Finite size topology in magnetic topological insulators — •Joe Winter[1,2], Michał Pacholski[1], and Ashley Cook[1] — [1]MPI PKS, Dresden, Germany — [2]University of St Andrews, St Andrews, Scotland

The antiferromagnetic topological insulator phase is a foundational realization of three-dimensional topological phases of matter with magnetic order. It is furthermore an example of an axion insulator and condensed matter platform for realizing exotic axion dynamics of high-energy physics. At systems sizes where the sample size is comparable with the correlation length of the topological surface states, it is expected for these states to hybridise. We however show the strength of this hybridisation is oscillatory with respect to system parameters and resonances occur where the surface states can reform. We then confirm the defining response signature of the underlying 3D AFM TI phase persists in this geometry, at these resonances. We then open boundary conditions in a second direction to confirm the additional bulk-boundary correspondence of the finite-size topological phases spectral flow, finding q(3-2)D topologically-protected, gapless edge modes. The co-existence of the q(3-2)D topologically non-trivial edge states with a topological response associated with the 3D bulk topological invariant, the magnetoelectric polarizability, confirms finite-size AFM topological phases occur. This further demonstrates that finite-size topology is a generic feature of topological phases and very relevant experimentally.

15 min. break

TT 4.8 Mon 11:30 H33

Genuine topological Anderson insulator from impurity induced chirality reversal — •Avedis Neehus, Frank Pollmann, and Johannes Knolle — Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany

We investigate a model of Dirac fermions with topological mass impurities which open a global topological gap even in the dilute limit. Surprisingly, we find that the chirality of this mass term, i.e., the sign of the Chern number, can be reversed by tuning the magnitude of the single-impurity scattering. Consequently, the disorder induces a phase disconnected from the clean topological phase, i.e., a genuine topological Anderson insulator. In seeming contradiction to the expectation that mass disorder is an irrelevant perturbation to the Dirac semimetal, the tri-critical point separating these two Chern insulating phases and a thermal metal phase is located at zero impurity density and connected to the appearance of a zero energy bound state in the continuum corresponding to a divergent topological mass impurity. Our conclusions based on the T-matrix expansion are substantiated by large scale Chebyshev-Polynomial-Green-Function numerics. We discuss possible experimental platforms.

TT 4.9 Mon 11:45 H33

Topological phases of arbitrary numbers of coupled Su-Schrieffer-Heeger wires — •Anas Abdelwahab — Leibniz Univesität Hannover, Institut für Theoretische Physik, Hannover

The phase diagrams of arbitrary number N_w of Su-Schrieffer-Heeger (SSH) wires have been identified, with respect to the dimerization and the single particle wire-wire coupling, where the latter is either perpendicular or diagonal between adjacent wires. Even number of perpendicularly coupled wires exhibit either gapless or trivial topological phases. Odd number of perpendicularly coupled wires can exhibit gapless, trivial or nontrivial topological phases with winding number $w = 1$. The diagonally coupled wires reveal topological phases with winding numbers in the range $0 \leq w \leq N_w$. The critical lines in their phase diagrams can reveal topological critical phases [1]. Each band of the diagonally coupled wires becomes a comletely flat band at specific lines in the phase diagram. The presence of W states [2] at the edges of coupled SSH wires with open boundary conditions will be dicussed.

[1] R.Verresen, R.Thorngren, N.G.Jones,F.Pollmann, Phys. Rev. X, 120, 057001 (2018).
[2] W.Dür, G.Vidal, J.I.Cirac, Phys. Rev. A 62, 062314 (2000).

TT 4.10 Mon 12:00 H33

Local and energy-resolved topological invariants for Floquet systems — •Arnob Kumar Ghosh, Rodrigo Arouca, and Annica M. Black-Schaffer — Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden

Periodically driven systems offer a perfect breeding ground for out-of-equilibrium engineering of topological boundary states at zero energy (0-mode), as well as finite energy (π-mode), with the latter having no static analog. The Floquet operator and the effective Floquet Hamiltonian, which encapsulate the stroboscopic features of the driven system, capture both spectral and localization properties of the 0- and π-modes but sometimes fail to provide complete topological characterization, especially when 0- and π-modes coexist. In this work [1], we utilize the spectral localizer, a powerful local probe that can provide numerically efficient, spatially local, and energy-resolved topological characterization. In particular, we apply the spectral localizer to the effective Floquet Hamiltonian for driven one- and two-dimensional topological systems with no or limited symmetries and are able to assign topological invariants, or local markers, that characterize the 0- and the π-boundary modes individually and unambiguously. Due to the spatial resolution, we also demonstrate that the extracted topological invariants are suitable for studying driven disordered systems and can even capture disorder-induced phase transitions.

[1] A.K.Ghosh, R.Arouca, A.M.Black-Schaffer, arXiv:2408.08548.

TT 4.11 Mon 12:15 H33

Characterizing exceptional topology through tropical geometry — •Ayan Banerjee[1], Rimika Jaiswal[2], Madhusudan Manjunath[3], and Awadhesh Narayan[4] — [1]Max Planck Institute for the Science of Light, Erlangen — [2]University of California Santa Barbara, USA — [3]Indian Institute of Technology Bombay, India — [4]Indian Institute of Science, Bangalore

Non-Hermitian Hamiltonians describing open quantum systems have been widely explored in platforms ranging from photonics to electric circuits [1]. A defining feature of non-Hermitian systems is exceptional points (EPs), where both eigenvalues and eigenvectors coalesce. The study of EPs has become an exciting frontier at the crossroads of optics, photonics, acoustics, and quantum physics. Tropical geometry is an emerging field of mathematics at the interface between algebraic geometry and polyhedral geometry, with diverse applications to science [2]. Here, we introduce Newton's polygon method and adopt the notion of a geometrical object known as amoeba in developing a unified tropical geometric framework to characterize different facets of non-Hermitian systems [3]. We introduce a framework linking tropical geometry to non-Hermitian physics, enabling the study of EPs, skin effects, and disorder properties.

[1] E.J.Bergholtz, J.C.Budich, F.K.Kunst, Rev.Mod.Phys.93, 015005 (2021).
[2] D.Maclagan, B.Sturmfels, Graduate Stud. Math.161, 75 (2009).
[3] A.Banerjee, R.Jaiswal, M.Manjunath, A.Narayan, Proc. Natl. Acad. Sci. U.S.A. 120, e2302572120 (2023).

TT 4.12 Mon 12:30 H33

Operator approach to quantum geometry and semi-classical dynamics — •Chen Xu[1,2], Andreas Haller[1], Suraj Hegde[3], Tobias Meng[2], and Thomas Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]TU Dresden, Department of Physics — [3]IISER-Thiruvananthapuram, India

We develop an operator-based approach for computing the quantum geometric contributions to the equations of motion of the position and momentum operators in an multiband system, without resorting to semiclassical wave-packet approximations. We identify contributions such as the Berry curvature and the quantum metric tensor induced anomalous velocity as fundamentally effective multiband effects. We show using this approach that in general higher-order operator-valued geometric quantities emerge in studying the dynamics in the presence of inhomogeneous external fields. We also demonstrate how to derive the dynamics from a generic coupling between Bloch momentum and an inhomogeneous external field, thus generalizing previous studies.

TT 4.13 Mon 12:45 H33

Exciton condensation driven by bound states of Green's function zeros — •Ivan Pasqua, Andrea Blason, and Michele Fabrizio — International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

The spectral properties of electronic systems are encoded in the single-particle Green's function, with theoretical efforts traditionally focusing on the position and nature of its poles. Only recently, Green's function zeros have been recognized as important hallmarks of non-symmetry breaking strongly correlated insulators and, possibly, of fractionalized excitations. The analysis of the zeros offers a new perspective on the increasingly studied topic of excitonic insulators (EI), typically understood as the condensation of bound states between the valence and conduction bands of poles of the Green's function. Indeed this picture appears paradoxical in Mott insulators (MI), where the large gap between the Hubbard bands seemingly precludes the formation of such bound states. Yet, a continuous transition from a MI and an EI is observed in the Bernevig-Hughes-Zhang model using the dynamical cluster approximation. We find that a non-topological EI intrudes between the QSH and MI regimes. Our analysis suggests that excitons in the MI, which soften at the transition to the EI, could be bound states between valence and conduction bands of Green's function zeros. Our work proposes a novel mechanism for exciton condensation and highlights the role of Green's function zeros in diagnosing the properties of correlated phase of matter.

TT 5: Superconductivity: Properties and Electronic Structure I

Time: Monday 9:30–13:00 Location: H36

TT 5.1 Mon 9:30 H36

Superconducting properties of $[(SnSe)_{1+\delta}]_m[NbSe_2]$ superlattices with varying $NbSe_2$ interlayer spacing — •Linus P. Grote[1], Wieland G. Stoffel[1], Tom Herter-Lehmann[1], Willi Vallant[1], Alina Dietrich[1], Olivio Chiatti[1], Danielle Hamann[2], David C. Johnson[2], and Saskia F. Fischer[1,3] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene OR 97403, USA — [3]Center for the Science of Materials Berlin, 12489 Berlin, Germany

In layered superconductors understanding and controlling the coupling of superconducting layers is crucial due to its strong impact on their properties [1]. We examine the properties of $[(SnSe)_{1+\delta}]_m[NbSe_2]$ superlattices, which allow for nearly arbitrary stacking sequences due to the growth technique [2]. Given this degree of freedom we study how coupling mechanisms enable the occurance of superconductivity. Temperature-dependent resistance measurements revealed superconductivity for $NbSe_2$ interlayer distances of 2.4 nm or smaller. This behaviour is explained by the interplay of grain boundaries, cross-plane tunneling and systematical variation of the $NbSe_2$ interlayer distances. Additionally, magnetoresistance hysteresis measurements were conducted to investigate the charge carrier states and microscopic superconducting structures. The results provide new insights into the coupling mechanisms of 2D superconductors.

[1] O. Chiatti et al., J. Phys.: Condens. Matter **35**, 215701 (2023);
[2] C. Grosse et al., Sci. Rep. **6**, 33457 (2016).

TT 5.2 Mon 9:45 H36

Atomic-scale mapping of superconductivity in the incoherent CDW mosaic phase of a transition metal dichalcogenide — •Sandra Sajan[1], Haojie Guo[1], Tarushi Agarwal[2], Irián S. Ramírez[1], Chandan Patra[2], Maia G. Vergniory[1], Fernando de Juan[1], Ravi P. Singh[2], and Miguel M. Ugeda[1] — [1]Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [2]Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhopal 462066, India

The emergence of superconductivity in the 1T phase of TaS_2 is preceded by the intriguing loss of long-range order in the charge density wave (CDW). Such decoherence, attainable by different methods, results in the formation of nm-sized coherent CDW domains bound by a two-dimensional network of domain walls (DW)-mosaic phase, which has been proposed as the spatial origin of the superconductivity. We report the atomic-scale characterization of the supercon-

ducting state of 1T-TaSSe, a model 1T compound exhibiting the CDW mosaic phase. We use high-resolution scanning tunneling spectroscopy and Andreev spectroscopy to probe the microscopic nature of the superconducting state in connection with the electronic structure of the DW network. Spatially resolved conductance maps at the Fermi level reveal a uniform landscape, independent of domain structure, indicating no link to superconductivity. This is confirmed at 340mK within the superconducting dome, where the gap's subtle inhomogeneity remains unconnected to DWs providing new insights into the fundamental interplay between SC and CDW in these relevant strongly correlated systems.

TT 5.3 Mon 10:00 H36

Ab-initio investigation of transition metal – superconductor interfaces — •Adamantia Kosma[1], Stefan Blügel[1], and Philipp Rüssmann[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

The realisation of Majorana-based topologically protected qubits requires a careful design and optimization of material interfaces for superconductor (SC)/topological insulator (TI) heterostructures. To this end, we perform ab-initio simulations to investigate the superconducting properties at the interface of transition metal overlayers (M = Os, Ir, Pt, Au) deposited on a Nb(110) film. Our density functional theory calculations are based on the full-potential Korringa-Kohn-Rostoker (KKR) Green function method and its Kohn-Sham Bogoliubov-de Gennes (KS-BdG) extension [1,2]. In our study we explore the possibility to control the work function mismatch through the overlayer, and we uncover the proximity induced superconductivity. Our findings show that some of these structures might be promising material candidates for interfacing a TI with a superconductor without unwanted band bending effects at SC/M/TI interfaces.

We thank the ML4Q (EXC 2004/1 – 390534769) for funding.

[1] JuDFTteam/JuKKR (2022). doi: 10.5281/zenodo.7284738

[2] P. Rüßmann, and S. Blügel, Phys. Rev. B **105**, 125143 (2022).

TT 5.4 Mon 10:15 H36

Local limit disorder characteristics of superconducting radio frequency cavities I. Frequency shift — •Matúš Hladký, Anastasiya Lebedeva, Marcel Polák, and František Herman — Comenius University in Bratislava

Negative resonant frequency shift abnormalities in the vicinity of the critical temperature have been observed in recent experiments on Superconducting Radio Frequency cavities.

We present a simple, straightforward approach using the Dynes superconductor theory [1] and discuss its results. In the ideal dirty limit, we analytically elaborate on the width and depth of the resulting dip. Studying the sign of the slope of the resonant frequency shift at crit. temperature in the moderately clean regime reveals the role of the pair-breaking and pair-conserving disorder. Next, we compare and also fit our results with the recent experimental data from the N-doped Nb sample presented in Ref. [2]. Our analysis remarkably complies with the experimental findings, especially concerning the dip width. We offer straightforward, homogeneous-disorder-based interpretation within the moderately clean regime.

This work has been supported by the APVV-23-0515 grant and by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 945478.

[1] A. Lebedeva, M. Hladký, M. Polák, F. Herman, arXiv:2409.04203v1.

[2] M. Zarea, H. Ueki, J. A. Sauls, Frontiers in Superconducting Materials, 3: 1-7, arXiv:2307.07905v1 (2023).

TT 5.5 Mon 10:30 H36

Local limit disorder characteristics of superconducting radio frequency cavities II. Quality factor — Anastasiya Lebedeva, Matúš Hladký, Marcel Polák, and •František Herman — Comenius University in Bratislava

Nowadays superconducting radio frequency (SRF) cavities represent fundamental tools used for (Standard Model) particle acceleration, (beyond Standard Model) particle probing, and long-lifetime photon preservation. We study their Quality factor properties mainly at low temperatures within the Dynes superconductor model [1]. We scrutinize and use the local limit response to the external electromagnetic field. Assuming the same regime at low temperatures, we address details of the high-quality plateaus. This work presents (and studies the limits of) the simple effective description of the complex problem corresponding to the electromagnetic response in the superconductors combining homogeneous conventional pairing and two different kinds of disorder scattering.

This work has been supported by the Slovak Research and Development Agency under the Contract no. APVV-23-0515, by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 945478.

[1] A. Lebedeva, M. Hladký, M. Polák, F. Herman, arXiv:2409.04203v1.

TT 5.6 Mon 10:45 H36

THz response of ultra thin NbN films grown by atomic layer deposition — •Frederik Bolle[1], Yayi Lin[1], Heidemarie Schmidt[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Leibniz IPHT, Jena

Most elementary excitations and collective modes of superconductors lie in the THz frequency range, making THz spectroscopy an ideal tool to directly measure the superconducting energy gap and superfluid density. By combining the spectral ranges from continuous, coherent backward wave oscillators and time-domain methods we can investigate a broad frequency range from 1.6 cm^{-1} (0.2 meV) up to 100 cm^{-1} (12.4 meV). We characterize the superconducting state of grown NbN films in particular concerning the behavior of its energy scales as the film becomes increasingly two dimensional approaching the superconductor insulator transition (SIT). We investigate films with thickness ranging from 4.5 nm and 20 nm and find a continuous suppression of the superconducting energy gap and superfluid density with reduced film thickness. These results enable a quantitative device design for various applications of NbN thin films such as high kinetic inductance circuitry.

TT 5.7 Mon 11:00 H36

Superfluid stiffness in strongly disordered NbN superconducting films — •Alexander Weitel Weitzel[1], Lea Pfaffinger[1], Matthias Stosiek[2], Animesh Panda[3], Ferdinand Evers[3], and Christoph Strunk[1] — [1]Inst. of Exp. a. Appl. Phys., University of Regensburg, D-93040 Regensburg, Germany — [2]TUM Sch. of Nat. Sci., Dep. of Phys. PH-I, D-85748 Garching bei München — [3]Inst. of Theoretical Phys., University of Regensburg, D-93040 Regensburg, Germany

In BCS-superconductors, the spectral gap, E_g, the pairing amplitude, Δ, and the mean-field critical temperature T_{c0} are essentially identical. At strong disorder, close to the superconductor-insulator transition (SIT), this is no longer the case. Moreover, in BCS-theory the superfluid stiffness, J_s, is determined by Δ and normal state resistance R_N. Also this relation typically no longer holds close to SIT. Recently, we have experimentally determined $J_s(T)$ in ultra-thin NbN films by measuring kinetic inductance and found a sharp Berezinski-Kosterlitz-Thouless (BKT) transition. Our latest experimental data cover $J_s(T)$ over a wide range of disorder strength, up to normal state resistance $\sim h/e^2$. We find a sharp BKT-transition right up to the SIT and independently measure the characteristic scales E_g, J_s, T_{c0} and T_{BKT} over two orders of magnitude in R_N. We present complementary numerical calculations of the superfluid stiffness, obtained from the Boguliubov-de Gennes (BdG) theory of disordered samples in a very broad range of disorder strengths. A detailed comparison of our measurements with the computational results will be presented.

15 min. break

TT 5.8 Mon 11:30 H36

Molecular hydrogen in the N-doped LuH_3 system as a possible path to superconductivity — •Cesare Tresca[1], Pietro Forcella[2], Andrea Angeletti[3], Luigi Ranalli[3], Cesare Franchini[3,4], Michele Reticcioli[3], and Gianni Profeta[1,2] — [1]CNR-SPIN L'Aquila, Italy — [2]University of L'Aquila, L'Aquila, Italy — [3]University of Vienna, Vienna, Austria — [4]University of Bologna, Bologna, Italy

The discovery of ambient superconductivity would mark an epochal breakthrough long-awaited for over a century, potentially ushering in unprecedented scientific and technological advancements. The recent findings on high-temperature superconducting phases in various hydrides under high pressure have ignited optimism, suggesting that the realization of near-ambient superconductivity might be on the horizon. However, the preparation of hydride samples tends to promote the emergence of various metastable phases, marked by a low level of experimental reproducibility. Identifying these phases through theoretical and computational methods poses a considerable challenge, often resulting in contentious outcomes. In this contribution, we consider N-doped LuH_3 as a prototypical complex hydride: By means of machine-learning-accelerated force-field molecular dynamics, we have identified the formation of H_2 molecules stabilized at ambient pressure by nitrogen impurities. Importantly, we demonstrate that this molecular phase plays a pivotal role in the emergence of a dynamically stable, low-temperature, experimental-ambient-pressure superconductivity.

TT 5.9 Mon 11:45 H36

Challenges in identifying nematic superconductivity of CsV_3Sb_5 kagome metal via transport measurements — •Yu-Chi Yao[1,2], Fei Sun[1], José Guimarães[1,2], and Haijing Zhang[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, UK

Nematicity refers to the spontaneous symmetry breaking beyond the crystal-imposed anisotropy in the electron wavefunction. On the other hand, understanding the interplay between nematicity and superconductivity could be crucial for determining the underlying pairing mechanism in various correlated systems, such as cuprates [1] and iron-based [2] unconventional superconductors.

In this study, we focus on the recently discovered kagome metal CsV_3Sb_5, which is famous for its multiple competing or coexisting orders [3,4]. By using CsV_3Sb_5 as the prototypical system, we address the challenges of identifying nematic superconductivity in transport measurements and systematically disentangle the extrinsic factors, such as imperfections in field alignment, from intrinsic nematic supercondcuting behavior.

[1] R. Daou *et al*. Nature **463**, 519-522 (2010).
[2] J. H. Chu *et al*. Science, **329**(5993), 824-826 (2010).
[3] B. R. Ortiz *et al*. Phys. Rev. Lett. **125**(24), 247002 (2020).
[4] F. Sun, H. Zhang *et al*. arXiv:2408.08117.

TT 5.10 Mon 12:00 H36

Unique electronic transport characteristics in superconducting MgB_2 films — •Clemens Schmid[1], Markus Gruber[1], Corentin Pfaff[2], Theo Courtois[2], Anton Pokusinskyi[3], Alexander Kasatkin[4], Karine Dumesnil[2], Stephane Mangin[2], Thomas Hauet[2], and Oleksandr Dobrovolskiy[3] — [1]Faculty of Physics and Vienna Doctoral School in Physics, University of Vienna, Austria — [2]Institute Jean Lamour, Université de Lorraine-CNRS, Nancy, France — [3]Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Germany — [4]G.V. Kurdyumov Institute for Metal Physics, NAS Ukraine, Kyiv, Ukraine

Maximizing the velocity of Abrikosov vortices in superconductors and characterizing the associated energy relaxation times is essential for possible applications like single photon detectors. Here, we investigate the current-voltage curves of MgB_2, a material whose thin film structures remain superconducting at temperatures up to 30 K. Furthermore, capabilities of a single photon response have been observed previously in MgB_2 films. Our experiments reveal peculiar shapes of the current-voltage curves, showing multiple steps in their transitions to the normal state. While the microscopic mechanisms underlying these steps are a topic of current debates, one explanation could imply the occurrence of composite and fractional vortices associated with the two-band nature of the superconductivity in MgB_2, a property which is in-line with the presence of two slopes in the temperature-magnetic-field phase diagram. We compare our findings across multiple layered structures and for varying thicknesses of the MgB_2.

TT 5.11 Mon 12:15 H36

Single-crystal growth and superconducting properties of $Sr_xBi_2Se_3$ — •Max Brückner[1], Jule Kirschke[1], Fatih Cetin[1], Sven Graus[1], Maik Golombiewski[1], Fotios Maragkos[2,3], Varvara Foteinou[2], Shibabrata Nandi[4,5], Haneen Abushammala[1], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum — [2]Central Unit for Ion Beams and Radionuclides, Ruhr-Universität Bochum, 44801 Bochum — [3]Department of Physics, National Technical University of Athens, 15780 Athens, Greece — [4]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science and Peter Grünberg Institut, JARA-FIT, 52425 Jülich — [5]Experimentalphysik IVc, JARA-FIT, RWTH Aachen, 52074 Aachen

Bi_2Se_3 is a topological insulator in which Sr-intercalation induces superconductivity with an unexpected two-fold anisotropy of H_{c2} in the basal plane. We examine how its properties relate to different single-crystal growth conditions, including self-flux growth of free-standing single crystals from a Bi-rich melt. The Sr-content was determined by proton-induced x-ray emission spectroscopy in our as-grown crystals with a resolution of up to 30 ppm. Transport measurements in magnetic fields showed superconductivity with $T_c \sim 2$-3 K at surprisingly low Sr-content. In addition, we identified $SrBi_2Se_4$ as a secondary phase in our growth. Its superconducting properties were found to be similar to the ones of $Sr_xBi_2Se_3$.

This work is supported by the ERC grant Distort-to-Grasp (No. 101040811).

TT 5.12 Mon 12:30 H36

Tuning superconducting properties in 3D nanoarchitectures — •Elina Zhakina[1], Luke Turnbull[1], Weijie Xu[1], Markus König[1], Paul Simon[1], Wilder Carrillo-Cabrera[1], Amalio Fernandez-Pacheco[2], Dieter Suess[3], Claas Abert[3], Vladimir M. Fomin[4], Uri Vool[1], and Claire Donnelly[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187, Dresden, Germany — [2]Institute of Applied Physics, TU Wien, Wiedner Hauptstr. 8-10/134,1040 Vienna, Austria — [3]University of Vienna, Vienna, Austria — [4]Leibniz IFW Dresden, Dresden, Germany

Introducing 3D nanoconfinement into the superconducting system can open a path for local geometrical control and the possibility of going beyond intrinsic properties. However, the fabrication of such intricate nanoarchitectures remains challenging.

In this context, we present an extended approach to creating superconducting 3D nanoarchitectures through focused electron-beam-induced deposition of tungsten. This method allows the realisation of 3D superconducting nanostructures with arbitrary geometries within a wide range of critical temperatures, providing local geometrical control of critical fields and, for example, the realisation of reconfigurable weak links. With transport measurements, we demonstrate the motion of superconducting vortices within these 3D superconducting nanostructures. Therefore, three-dimensional superconducting nanostructures offer new horizons for experimental investigations of the dynamics of vortices, anisotropy and possible applications of curvilinear 3D nanoarchitectures.

TT 5.13 Mon 12:45 H36

Vortex mass observed in far-infrared circular dichroism of high-T_c superconductors — •Roman Tesař[1], Michal Šindler[1], Pavel Lipavský[2], Jan Koláček[1], Christelle Kadlec[1], Wen-Yen Tzeng[3], Chih-Wei Luo[4], and Jiunn-Yuan Lin[4] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]National Formosa University, Yunlin, Taiwan — [4]National Yang Ming Chiao Tung University, Hsinchu, Taiwan

The effective mass of the Abrikosov vortex (fluxon) in type-II superconductors remains an open and still not fully solved problem. Only a few experimental techniques are currently known to examine the fluxon mass, while numerous theoretical models have been developed that predict inconsistent values scattered over several orders of magnitude. We present an experimental method to determine fluxon mass based on the interaction with circularly polarized FIR/THz laser radiation. A rotating electric field induces the motion of fluxons along cyclotron trajectories, which leads to magnetic circular dichroism at terahertz frequencies. The modified Kopnin-Vinokur theory with experimentally established parameters provides a sufficient framework for estimating fluxon mass at low temperatures. We demonstrate the proposed method on thin films of $YBa_2Cu_3O_{7-\delta}$ with different doping levels. We also briefly mention other applications of the experimental technique used, such as probing cyclotron resonance in semiconductors and magnon modes in magnetic materials.

[1] Sci. Rep. 11, 21708 (2021).
[2] IEEE Trans. Appl. Supercond. 34, 0601005 (2024).

TT 6: Focus Session Many-Body Phenomena in Nanomagnets: Kondo, Spinons, Spinarons and Beyond (joint session O/TT)

The electron spin, a fundamental quantum mechanical property, plays a crucial role in determining the electronic and magnetic properties as well as the dynamics of matter. Its role becomes even more important at surfaces, 2D materials and nanomagnets as the low-dimensionality increases electron correlation. A fundamental understanding of spin excitations is significant for both fundamental science and modern applications. For decades, the interpretation of experimental signatures of spin excitations were focused on the Kondo effect paradigm, with Co atoms on the (111) surface of noble metals as the prototypical example. However, recent first-principles predictions and spin-polarized scanning tunnelling spectroscopy in high magnetic fields have demonstrated the existence of many-body states, called spinarons. These states arise from the binding of electronic states to spin excitations in the presence of spin-orbit coupling. Such findings, along with other studies, challenge the Kondo interpretation. Furthermore, related non-trivial many-body states may emerge in thin-film geometries, as shown by photoemission spectroscopy and first-principles manybody investigations or in quantum spin liquids. These examples testify that many-body phenomena are not only critically important for the fundamental understanding of spin excitations, they also impact a wide range of material characteristics, including electronic, magnetic, thermodynamic, and transport properties. This focus session will provide a forum to discuss intriguing many-body states driven by spin excitations, and serve as a forum to discuss the current knowledge on their origins, unique properties, and implications.

Organized by
Matthias Bode (Würzburg University), Yujeong Bae (Swiss EMPA), and Stefan Blügel (FZ-Jülich).

Time: Monday 15:00–18:15 Location: H24

Invited Talk TT 6.1 Mon 15:00 H24

Kondo and Yu-Shiba-Rusinov resonances: transport and coupling — •Laëtitia Farinacci[1,2,3], Gelavizh Ahmadi[3], Gaël Reecht[3], Benjamin W. Heinrich[3], Contanstin Czekelius[3], Felix von Oppen[3], and Katharina J. Franke[3] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Germany

The exchange coupling between a magnetic impurity and a superconducting substrate leads to the formation of magnetic bound states, known as Yu-Shiba-Rusinov (YSR) states, inside the superconducting gap, as well as a Kondo resonance outside the gap. Studying these two many-body phenomena in parallel provides valuable insights into their characteristic properties.

We observed striking correlations between the asymmetries of the YSR state and the Kondo effect induced by FeTPyP molecules on Pb(111) in a scanning tunneling microscope (STM) [1]. We show that both asymmetries originate from interfering tunneling paths via a spin-carrying orbital and the highest occupied molecular orbital.

Additionally, we studied the formation of YSR bands in a self-assembled kagome lattice of magnetic molecules on Pb(111) and track YSR hybridization from kagome precursors to larger islands [2]. This work will motivate further studies to resolve possible spin-liquid or Kondo-lattice-type behavior.

[1] PRL 125, 256805 (2020). [2] Nat. Comm. 15, 6474 (2024).

Invited Talk TT 6.2 Mon 15:30 H24

Electron delocalization in a 2D Mott insulator — •Amadeo L. Vazquez de Parga[1,2,4,5], Cosme G. Ayani[1,2], Michele Pisarra[3], Iván M. Ibarburu[1], Clara Rebanal[1], Manuela Garnica[2,4], Fabián Calleja[2], and Fernando Martín[1,2] — [1]Universidad Autónoma de Madrid, Madrid, Spain — [2]IMDEA Nanociencia, Madrid, Spain — [3]Universitá della Calabria, Rende, Italy — [4]Instituto Nicolás Cabrera, Madrid, Spain — [5]Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We follow by means of low temperature Scanning Tunneling Microscopy and Spectroscopy, the buildup of a 2D Kondo lattice in a system composed by a 2D Mott insulator, a single 1T-TaS2 layer, stacked on the surface of a metallic crystal, 2H-TaS2. When the sample temperature is lower than 27K, the magnetic moments present in the Mott insulator experience the Kondo screening by the conduction electrons of the metal, leading to the appearance of a Kondo resonance at the Fermi level. Below 11 K, a gap opens within the Kondo resonance, which is the signature of the formation of a coherent quantum state that extends all over the sample, i.e., a Kondo lattice [1]. Quasi particles interference maps reveal the emergence of a Fermi contour in the 2D Mott insulator when the temperature drops below 11K, indicating the delocalization of the highly correlated Mott electrons [2]. The observed modifications in the LDOS are well explained by state-of-the-art Density Functional Theory calculations.

[1] Small 20, 2303275 (2024) [2] Nat. Commun. 15, 10272 (2024)

Invited Talk TT 6.3 Mon 16:00 H24

Kondo or no Kondo, that is the question — •Alexander Weismann, Neda Noei, Niklas Ide, and Richard Berndt — Institut für experimentelle und angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

The spin properties of individual atoms and molecules can produce distinctive spectral features in tunneling spectra near zero bias. Among these features, Kondo resonances and inelastic spin-flip excitations are often challenging to distinguish, despite their markedly different spectral line shapes. A Kondo resonance indicates a non-magnetic ground state, where the atomic spin is screened by conduction band electrons. In contrast, spin-flip excitations observed in zero-field tunneling spectra require magnetic anisotropy, which arises from spin-orbit coupling (SOC), to play a significant role. In this study, we demonstrate that the well-known Co/Cu(111) system, long believed to exhibit a Kondo resonance, instead adopts a magnetic ground state that is protected from Kondo screening by substantial magnetic anisotropy. The zero-bias anomaly in scanning tunneling spectra undergoes significant modification when Co atoms are attached to monoatomic Cu chains. Measurements conducted at 340 mK in a magnetic vector field reveal clear signatures of inelastic spin-flip excitations, with the anisotropy axis tilted away from the surface normal. The magnitude and orientation of this anisotropy are consistent with density functional theory (DFT) calculations. Moreover, quantum Monte Carlo many-body simulations confirm that the Kondo effect is suppressed when SOC is properly accounted for.

Invited Talk TT 6.4 Mon 16:30 H24

Evidence for spinarons in Co atoms on noble metal (111) surfaces — •Artem Odobesko — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The zero-bias anomaly in the tunnelling differential conductance of Co atoms on Au(111) [1], long attributed to the Kondo effect, has recently been reinterpreted [2] as evidence of the spinaron – a novel many-body excitation arising from the interplay between spin excitations and conduction electrons. In our study, we used spin-polarized scanning tunneling spectroscopy (STS) on Co atoms on Cu(111) and Au(111) under high magnetic fields, revealing field-induced energy shifts and spin-resolved spectral features that challenge the conventional Kondo interpretation. Instead, our findings provide the first experimental confirmation of the spinaron [3].

We also investigated the role of hybridization with the substrate in spinaron formation, focusing on the reconstructed Au(111) surface. The unique local electronic environments created by the herringbone reconstruction strongly influence the hybridization strength and spectral features of Co adatoms, revealing a clear link between adsorption site, hybridization, and spinaronic excitations. Our results shed light on the fundamental mechanisms driving spinaron formation.

[1] V. Madhavan, et al., Science 280, 567 (1998)
[2] J. Bouaziz, et al., Nat. Comm. 11, 6112 (2020)
[3] F. Friedrich, et al., Nat. Phys. (2023)

Invited Talk TT 6.5 Mon 17:00 H24

Spinarons: A new view on emerging spin-driven many-body phenomena in nanostructures — •Samir Lounis — Peter Grünberg Institut, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Many-body phenomena are crucial in physics, particularly in condensed mat-

ter, influencing electronic, magnetic, thermodynamic, and transport properties. They leave distinct spectroscopic signatures, such as Kondo, excitonic, and polaronic features, arising from specific degrees of freedom. Since more than two decades Cobalt atoms on the (111) surfaces of noble metals have been a paradigm for the Kondo effect in scanning tunnelling spectroscopy experiments [1]. However, our recent first-principles predictions [2] followed by STS experiments in high magnetic fields [3,4] challenge this notion. Our findings reveal that the observed transport anomalies stem from spin excitations of Co atoms, forming a new many-body state – the spinaron – distinct from the Kondo resonance. I will delve into the spinaron origins, their unique properties, and implications explored through the recent atomic manipulation experiments. This work opens pathways to investigate and engineer these hybrid states in nanostructures, offering new insights into fundamental many-body states.

[1] V. Madhavan et al., Science 280, 567 (1998); [2] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [3] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [4] N. Noei et al., Nanoletters 23, 8988 (2023)

TT 6.6 Mon 17:30 H24

Emergence of spinaronic states in Fe adatoms — Ilias Klepetsanis[1,2], Juba Bouaziz[4], •Philipp Rüssman[1,3], and Samir Lounis[1,2] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]University of Würzburg, Germany — [4]Research Center for Advanced Science and Technology, University of Tokyo, Japan

In recent years, spinarons, predicted from first-principles calculations [1], have been observed in Co adatoms on the Cu(111) surface, using spin-polarized scanning tunnelling spectroscopy (STS) in high magnetic fields [2]. Spinarons leave a non-trivial spectroscopic signature, for long interpreted to originate from the Kondo effect [3]. Here, we employ relativistic time-dependent density functional and many-body perturbation theory, to investigate the case of Fe adatoms on the Cu(111) surface, which carry a large magnetic moment of $3.25\mu_B$ preferring an out-of-plane orientation as dictated by a magnetic anisotropy energy of 2meV. In contrast to the Co adatom, the spinarons in Fe do not overlap with trivial spin-excitations. We discuss the spinaronic response to an out-of-plane magnetic field, the orbital character and the impact of spin-orbit coupling. [1] J. Bouaziz et al., Nat. Commun. 11, 6112 (2020); [2] F. Friedrich et al., Nat. Phys. 20, 28 (2024); [3] V. Madhavan et al., Science 280, 567 (1998)

TT 6.7 Mon 17:45 H24

Revising the Superconductivity in Iron Based Superconductors from the Perspective of Electron Phonon Coupling — •Lanlin Du[1,2] and Sheng Meng[1,2,3] — [1]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong, China

There are currently two mainstream superconducting pairing mechanisms, namely electron phonon coupling and spin fluctuation, which are believed to play a dominant role in conventional superconductors like simple metal superconductors and unconventional superconductors like Copper oxides, respectively. Iron based superconductors are believed to connect these two aspects, that is, both mechanisms are important in it. In fact, some studies have shown that electron phonon coupling is also important in cuprates, and even provide evidence for s-wave pairing symmetry in them. Therefore, it is important to consider the role of electron phonon coupling in unconventional superconductors. Here, we revise the superconductivity in Iron based superconductors using Migdal-Eliashberg formalism and electron phonon coupling strength corrected by many body method from the two perspectives of doping and pressurization. Our results are in good agreement with the experiments. Based on this, we predict a new two-dimensional high-Tc Iron based superconductor.

TT 6.8 Mon 18:00 H24

Theoretical model for multiorbital Kondo screening in strongly correlated molecules with several unpaired electrons — •Manish Kumar[1], Aitor Calvo-Fernandez[2], Diego Solar-Polo[1], Asier Eiguren[2], Maria Blanco-Rey[3], and Pavel Jelinek[1] — [1]Institute of Physics, Academy of Sciences of the Czech Republic , Cukrovarnicka 10, Prague 6, CZ 16200, Czech Republic — [2]Department of Physics, University of the Basque Country UPV-EHU, 48080 Leioa, Spain — [3]Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, University of the Basque Country UPV-EHU, 20018 Donostia-San Sebastián, Spain

The mechanism of Kondo screening in strongly correlated molecules with several unpaired electrons on a metal surface is still under debate. Here, we provide a theoretical framework that rationalizes the emergence of Kondo screening involving several extended molecular orbitals with unpaired electrons. We introduce a perturbative model, which provides simple rules to identify the presence of antiferromagnetic spin-flip channels involving charged molecular multiplets responsible for Kondo screening. The Kondo regime is confirmed by numerical renormalization group calculations. In addition, we introduce the concept of Kondo orbitals as molecular orbitals associated with the Kondo screening process, which provide a direct interpretation of experimental dI/dV maps of Kondo resonances. We demonstrate that this theoretical framework can be applied to different strongly correlated open-shell molecules on metal surfaces, obtaining good agreement with previously published experimental data.

TT 7: Correlated Electrons: Electronic Structure Calculations

Time: Monday 15:00–18:00 Location: H31

TT 7.1 Mon 15:00 H31

Wannier interpolation of reciprocal-space periodic and non-periodic matrix elements in the optimally smooth subspace — •Giulio Volpato, Stefano Mocatti, Giovanni Marini, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Maximally localized Wannier functions use the gauge freedom of Bloch wavefunctions to define the optimally smooth subspace with matrix elements that depend smoothly on crystal momentum. The associated Wannier functions are real-space localized, a feature often used to Fourier interpolate periodic observables in reciprocal space on ultradense momentum grids. However, Fourier interpolation cannot handle non-periodic quantities in reciprocal space, such as the oscillator strength matrix elements, which are crucial for the evaluation of optical properties. We show that a direct multidimensional interpolation in the optimally smooth subspace yields comparable accuracy with respect to Fourier interpolation at a similar or lower computational cost. This approach can also interpolate and extrapolate non-periodic observables, enabling the calculation of optical properties on ultradense momentum grids. Finally, we underline that direct interpolation in the optimally smooth subspace can be employed for periodic and non-periodic tensors of any order without any information on the position of the Wannier centers in real space.

Funded by the European Union (ERC, DELIGHT, 101052708).

TT 7.2 Mon 15:15 H31

LCAO fragment orbital projectors for DFT+U — •Christoph Freysoldt, Hao Chen, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

DFT+U is an efficient approach to describe correlated mixed-valence transition metal oxides such as Fe_3O_4=$Fe^{II}Fe_2^{III}O_4$. The correlated orbitals are derived from, but not identical to the metal d-orbitals. Most DFT+U implementations employ local projectors with d-orbital symmetry centered on the transition metal atoms to extract the on-site occupation matrix of the correlated orbitals. Unfortunately, such projectors pick up not only intended occupations of localized orbitals, but also contributions from the extended metal-oxygen bonding states involving the O-2p orbitals. The spurious occupations are sensitive to the projector definition and the M-O bond length, and lead to artifacts in energies and structures. To arrive at a more reliable scheme, one must account for inter-atomic orbital overlap when defining the projectors. We propose using fragment orbitals from a linear combination of atomic orbitals (LCAO) that include the orbital mixing with the first ligand shell of each transition metal ion. To obtain analytic Pulay-like forces when atoms are displaced, the projectors are constructed from a simplified tight-binding model that reflects the atomic positions, but does not rely on the self-consistent electronic structure. We present preliminary results for iron oxides that exhibit improved occupations (closer to 0 and 1) and a reduced sensitivity to bonding distances.

TT 7.3 Mon 15:30 H31

Single- and two-particle observables in the Emery model: A dynamical mean-field perspective — •Yi-Ting Tseng[1], Mario Malcolms[2], Henri Menke[1,2], Marcel Klett[2], Thomas Schäfer[2], and Philipp Hansmann[1] — [1]Friedrich-Alexander-University Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart

We investigate dynamical mean-field calculations of the three-band Emery model at the one- and two-particle level for material-realistic parameters of high-T_c superconductors[1]. Our study shows that even within dynamical mean-field theory, which accounts solely for temporal fluctuations, the intrinsic multi-orbital nature of the Emery model introduces effective non-local correlations. These correlations lead to a non-Curie-like temperature dependence of the magnetic susceptibility, consistent with nuclear magnetic resonance experiments in the pseudogap regime. By analyzing the temperature dependence of the static dynamical mean-field theory spin susceptibility, we find indications of emerging oxygen-copper singlet fluctuations, explicitly captured by the model. Despite correctly describing the hallmark of the pseudogap at the two-particle level, such

as the drop in the Knight shift of nuclear magnetic resonance, dynamical mean-field theory fails to capture the spectral properties of the pseudogap.
[1] YiTing Tseng *et al.*, arXiv:2311.09023.

TT 7.4 Mon 15:45 H31

Origin of transitions inversion in rare-earth vanadates — •Xuejing Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany

The surprising inversion of the orbital- and magnetic-order transitions in the RVO_3 series with increasing the rare-earth radius makes the series unique among orbitally-ordered materials [1]. Here, augmenting dynamical mean-field theory with order-parameter irreducible-tensor decomposition [2], we show that this anomalous behavior emerges from an unusual hierarchy of interactions. First, increasing the rare-earth radius, orbital physics comes to be controlled by *xz*-*xz* quadrupolar super-exchange rather than by lattice distortion. Next, for antiferromagnetic spin order, orbital super-exchange terms with different spin rank compete, so that the dipolar spin-spin interaction dominates. Eventually, G-type magnetic order (anti-ferro in all directions) can appear already above the orbital ordering transition and C-type order (anti-ferro in the *ab* plane) right around it. The strict constraints we found also explain why the inversion is rare, and give at the same time criteria to look for similar behavior in other materials [3].
[1] S. Miyasaka, Y. Okimoto, M. Iwama, Y. Tokura, Phys. Rev. B 68, 100406(R) (2003).
[2] X.J.Zhang, E.Koch, E.Pavarini, Phys.Rev.B 105, 115104 (2022).
[3] X. J. Zhang, E. Koch, E. Pavarini, arXiv:2411.16351 (2024).

TT 7.5 Mon 16:00 H31

Engineering correlated Dirac fermions and flat bands on SiC with transition metal adatom lattices — •Niklas Enderlein[1], Henri Menke[1,2], Yi-Ting Tseng[1], Michel Bockstedte[3], Janina Maultzsch[1], Giorgio Sangiovanni[4], and Philipp Hansmann[1] — [1]Friedrich-Alexander-University Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Johannes Kepler University Linz — [4]Julius-Maximilian-University of Würzburg

In our recent study [1] we propose three transition-metal adatom systems on 3C-SiC(111) surfaces as a versatile platform to realize massless Dirac fermions and flat bands with strong electronic correlations. Using density functional theory combined with the constrained random phase approximation and dynamical mean-field theory, we investigate the electronic properties of Ti, V, and Cr adatoms. The triangular surface lattices exhibit narrow bandwidths and effective two-band Hubbard models near the Fermi level, originating from partially filled, localized d-orbitals of the adatoms. Our study reveals a materials trend from a flat band Fermi liquid (Cr) via a paramagnetic Mott insulator with large local moments (V) to a Mott insulator on the verge to a heavy Dirac semimetal (Ti) showcasing the diverse nature of these strongly correlated systems. Specifically, the flat bands in the Cr and the well-defined Dirac cones in the strained metallic Ti lattice indicate high potential for realizing topological and correlated phases.
[1] H.Menke, N.Enderlein *et al.*, arXiv:2410.17165.

TT 7.6 Mon 16:15 H31

Antiferromagnetism in iridates revisited: Mott versus Slater physics — Francesco Cassol, Michele Casula, and •Benjamin Lenz — IMPMC, Sorbonne University - CNRS, Paris, France

Since its discovery, the antiferromagnetic low-temperature phase of the iridates Ba_2IrO_4 and Sr_2IrO_4 has been subject to numerous studies. Whereas their underlying spin-orbit entangled ground state of a half-filled $j_{\text{eff}} = 1/2$ orbital is well accepted, the origin and nature of the antiferromagnetism is still debated. Are the materials classical Mott insulators or is the antiferromagnetism rather of Slater type? In this talk, we will revisit the question based on dynamical mean-field theory (DMFT) calculations that include the $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ states within the DMFT self-consistency. Comparing to both experiment and *ab initio* simulations from literature, we will depict a complex phase diagram at the crossroads between Slater and Mott physics.

15 min. break

TT 7.7 Mon 16:45 H31

Optical conductivity of Sr_2IrO_4 and Ba_2IrO_4: beyond the traditional interpretation of the double peak structure — •Francesco Cassol, Michele Casula, and Benjamin Lenz — IMPMC, Sorbonne University - CNRS, Paris, France

Since the discovery of their exotic spin-orbital entangled insulating ground state, Sr_2IrO_4 and Ba_2IrO_4 have attracted considerable attention. Spurred by the structural similarities with cuprate high T_C superconductors, numerous studies have explored their magnetic and electronic properties. Herein, we investigate the optical transport properties, by computing the optical conductivity beyond the Peierls substitution scheme within dynamical mean-field theory (DMFT) for both compounds. By explicitly including both $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ states in the DMFT self-consistency, we characterize the nature of the double peak structure found in the optical conductivity at low energy. In contrast with the traditional interpretation, we assign a mixed j_{eff} character to both peaks. Moreover, we accurately capture their temperature dependence, further corroborating our findings.

TT 7.8 Mon 17:00 H31

Non-flat bands and chiral symmetry in magic angle twisted bilayer graphene — •Miguel Sánchez[1], José González[2], and Tobias Stauber[1] — [1]Insituto de Ciencia de Materiales de Madrid ICMM-CSIC. Madrid, Spain — [2]Insituto de Estrrcutura de la Materia IEM-CSIC. Madrid, Spain)

We find that in any effective theory of magic angle twisted bilayer graphene (MATBG) that integrates out high-energy modes, the flat bands are prone to a significant increase in bandwidth. This effect from the Coulomb interaction is comparable to and even exceeding the perturbations due to strain and electron-phonon coupling.

As a result of this band widening, we identify a pattern of explicit symmetry breaking in MATBG from the ideal $U(4) \times U(4)$ symmetry down to the chiral non-flat $U(4)$ group, in contrast to the flat $U(4)$ symmetry that prevails when the bands are very flat.

Our work builds upon and extends a previous study [1]. For instance, we employ an atomistic model of MATBG that treats the full bandwidth accurately. Moreoever, we discuss the implications of our results for the latest experimental and theoretical findings.
[1] Phys. Rev. Lett. **125**, 257602 (2020).

TT 7.9 Mon 17:15 H31

Electronic structure of CrB_2 and implications for the incommensurate antiferromagnetic order — •André Deyerling[1], Alexander Regnat[1], Schorsch Sauther[1], Christian Pfleiderer[1,2,3,4], and Marc A. Wilde[1,2] — [1]Physik Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Zentrum für Quantum Engineering (ZQE), Technische Universität München, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Technische Universität München, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Germany

CrB_2 exhibits antiferromagnetic order below $T_N = 89$ K [1]. Applying pressure leads to the suppression of magnetic order and the onset of superconductivity [2,3,4]. We report ab initio calculations of CrB_2 for different pressures and discuss possible mechanisms leading to the suppression of magnetic order and the onset of superconductivity. In addition we discuss the electronic structure for different possible magnetic ground states and their compatibility with neutron scattering experiments [4] and quantum oscillation measurements [5,6].
[1] A. Bauer et al., PRB 90, 064414 (2014).
[2] C. Pei et al., arXiv:2109.15213 (2021).
[3] S. Biswas et al., PRB 108, L020501 (2023).
[4] A. Regnat, PhD thesis, TUM (2019).
[5] M. Brasse et al., PRB 88, 155138 (2013).
[6] S. Sauther, PhD thesis, TUM (2021).

TT 7.10 Mon 17:30 H31

Calculating core-hole valence electron interactions from *ab initio* — •Felix Sorgenfrei[1], Olle Eriksson[1,2], and Patrik Thunström[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability (WISE), Uppsala University, Uppsala Sweden

One common approach to simulating X-ray absorption spectra (XAS) for strongly correlated systems is the cluster model, where a model Hamiltonian is described with numerous free parameters. However, when different parameter sets yield the same spectra, drawing definitive conclusions becomes challenging. To overcome this, approaches integrating density functional theory (DFT) or DFT+ methods with the cluster model have been developed, allowing most parameters to be determined *ab initio*. Nonetheless, the Coulomb interaction between the core-hole and valence electrons (U_{cv}) remains undetermined from *ab initio* calculations. In this talk, I will present a method to calculate the screened core-valence interaction using *ab initio* linear response DFT, offering a more rigorous and predictive framework for XAS simulations.

TT 7.11 Mon 17:45 H31

SOLAX: A Python solver for fermionic quantum systems with neural network support — Louis Thirion[1], Philipp Hansmann[1], and •Pavlo Bilous[2] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany

We present a new Python library SOLAX [1] designed for configuration interaction (CI) calculations of fermionic quantum many-body systems which require high dimensional expansions in Slater determinant bases. The provided Python classes allow to conveniently encode basis sets, quantum states, and operators within the second quantization formalism. The JAX-based GPU-accelerated back-end performs efficiently the quantum mechanical operations necessary to determine many-body quantum states in finite-size Hilbert spaces.

Along with these core functionalities, SOLAX integrates a neural-network (NN) support for the CI calculation for otherwise prohibitively large expansions in Slater determinant basis sets. We show how NN can be used in SOLAX to identify a priori unknown subsets of the most important Slater determinants and iteratively obtain high-quality approximative many-body quantum states. Our recent developments include also NN-supported construction of spectral functions, which we plan to provide in future versions of SOLAX.

[1] L. Thirion, P. Hansmann, and P. Bilous, arXiv:2408.16915 (2024).

TT 8: Measurement Technology and Cryogenics

Time: Monday 15:00–17:45 Location: H32

TT 8.1 Mon 15:00 H32

64-pixel Magnetic Micro-Calorimeter array to study X-ray transitions in muonic atoms — •Daniel Kreuzberger, Andreas Abeln, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, Daniel Hengstler, Andreas Reifenberger, Adrian Striebel, Daniel Unger, Julian Wendel, and Peter Wiedemann — for the QUARTET Collaboration, Kirchhoff Institute for Physics, Heidelberg University

The QUARTET collaboration aims to improve the knowledge on the absolute nuclear charge radii of light nuclei from Li to Ne. We use a low temperature Metallic Magnetic Calorimeter (MMC) array for high-precision X-ray spectroscopy of low-lying states in muonic atoms. MMCs are characterized by a high resolving power of several thousand and a high quantum efficiency in the energy range up to 100 keV. Conventional solid-state detectors do not provide sufficient accuracy in this energy range. A high statistics measurement with lithium, beryllium and boron has recently been performed at the Paul Scherrer Institute. We present the experimental setup and the performance of the detector used. We discuss the first preliminary spectra and systematic effects in this measurement. The high statistics data in combination with the achieved energy resolution and calibration accuracy should allow a more precise characterization of the muonic X-ray lines. With the knowledge gained, a significant improvement in the determination of nuclear charge radii is expected.

TT 8.2 Mon 15:15 H32

Magnetocaloric upgrade for the Quantum Design PPMS® — •Marvin Klinger, Jorginho Villar Guerrero, Anna Klinger, Tim Treu, Anton Jesche, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg

Achieving millikelvin temperatures presents significant challenges in experimental physics. While many laboratories operate liquid helium cryostats at 2 K, reaching very low temperatures traditionally requires dilution refrigeration - a technique demanding both specialized expertise and substantial resources. We developed an upgrade for the Quantum Design Physical Property Measurement System (PPMS®) that overcomes these limitations. Our system employs adiabatic demagnetization refrigeration (ADR) to achieve temperatures well below 50 mK for multiple hours. The exceptional performance stems from novel quantum ADR materials that overcome disadvantages of traditional hydrated paramagnetic salts [1]. The upgrade consists of a user-friendly insert that integrates seamlessly with existing PPMS® systems. Its modular design allows researchers to easily swap the low-temperature assembly to accommodate different experimental needs, currently supporting electrical transport, stress/strain, and heat capacity measurements. This versatility and accessibility can make sub-50 mK measurements available to a broader scientific community without the complexity of dilution refrigeration.

[1] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025)

TT 8.3 Mon 15:30 H32

The noise-o-meter: A novel device to disentangle noise sources in superconducting devices — •Lukas Münch, Daniel Hengstler, Matthew Herbst, David Mazibrada, Andreas Reifenberger, Markus Renger, Christian Ständer, Rui Yang, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

In many applications of superconducting devices, different intrinsic noise sources are limiting the ultimate performance of the device. Our new device allows to conveniently disentangle the noise of the read-out chain, and to distinguish between magnetic flux noise and other noise sources. It consists of a microfabricated Wheatstone-like bridge of four superconducting inductors, two of which are filled with a sample material, which is read out via a pair of two-stage dc-SQUID read-out chains. The device can be operated in two modes. In the passive mode, the output signals of both read-out chains are cross-correlated, which allows the measurement of the total noise of all intrinsic noise sources within a sample material. In the active mode, the bridge is driven by an AC current to measure the samples complex susceptibility and, therefore, specifically the samples magnetic noise via the fluctuation-dissipation theorem. We used this setup to characterize SiO_2, Ag:Er and Au:Er films in a large temperature range from 20 to 800 mK. We discuss our design considerations and present the results of these measurements. Furthermore, we address the current performance limits of $S_\Phi = 30\,\mathrm{n}\Phi_0/\sqrt{\mathrm{Hz}}$ in passive mode and around 10 ppm for the concentration of magnetic impurities in active mode.

TT 8.4 Mon 15:45 H32

Broadband EPR Spectroscopy of $LiYF_4$ doped with Rare-Earth Ions — •Ana Strinic[1,2,3], Patricia Oehrl[1,2,3], Georg Mair[1,2], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Walther-Meißner-Institute, Bavarian Academy of Sciences and Humanities, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

We report on the study of hyperfine transitions of rare-earth ions doped into the host crystal $LiYF_4$ (RE^{3+}:$^7LiYF_4$) using broadband EPR spectroscopy at millikelvin temperatures. While the studied crystals are intentionally doped with ^{167}Er or ^{143}Nd, we identify impurity traces of other rare-earth ions from their EPR-transitions, based on previously published spin Hamiltonian parameters [1]. Taking into account the electron Zeeman, the hyperfine, and the quadrupole interactions, the high resolution spectra allow for the determination of refined spin Hamiltonian parameters for ^{167}Er and ^{143}Nd, as well as for the identified impurities. Our results demonstrate the advantage of using broadband EPR for material research, not only because precise information on the interactions of the spin system can be obtained, but also because the material purity can be tested. This study is relevant for quantum memory applications, as high purity materials are associated with achieving long coherence times [2].

[1] J. P. Sattler, J. Nemarich, Phys. Rev. B 4, 1, (1971);
[2] M. Le Dantec et al., Sci. Adv. 7, eabj9786 (2021).

TT 8.5 Mon 16:00 H32

Electro-optic cavities: Towards local measurement of light-matter coupling — •Michael S. Spencer[1], Joanna M. Urban[1], Maximilian Frenzel[1], Niclas S. Mueller[1], Olga Minakova[1], Martin Wolf[1], Alexander Paarmann[1], and Sebastian F. Maehrlein[1,2,3] — [1]FHI Berlin — [2]HZDR — [3]TU Dresden

Cavity quantum electrodynamics is expected to provide a unique direction for tailoring ground- and excited-state properties in correlated materials. Bringing this together with high-field driving in the terahertz (THz) spectral range opens the door to explore low-energy, field-driven cavity electrodynamics. Despite this potential, leveraging field-driven material control in bulk cavities is hindered by the lack of direct retrieval of intra-cavity fields. Here, we demonstrate novel active cavities, consisting of a Fabry-Pérot cavity filled with an electro-optic crystal, which measure their intra-cavity electric fields on ultrafast timescales. With these, we demonstrate quantitative retrieval of the cavity modes in amplitude and phase. We furthermore design a tunable multi-layer cavity, enabling deterministic design of hybrid cavities for future field-resolved polaritonic systems. Our theoretical modeling reveals the origin of the avoided crossings embedded in the intricate mode dispersion upon cavity tuning and enable fully-switchable polaritonic effects within arbitrary materials hosted by the hybrid cavity. Electro-optic cavities will therefore serve as in-situ probes of light-matter interactions across all coupling regimes, laying the foundation for field-resolved intra-cavity quantum electrodynamics.

15 min. break

TT 8.6 Mon 16:30 H32

Two-stage Pulse Tube Cryocooler with intermediate heat exchanger for accessing regenerator cooling capacity — •Bernd Schmidt[1,2], Jack-André Schmidt[1,2], Xaver Herrmann[1,2], Jens Falter[1], Dirk Dietzel[1,2], and André Schirmeisen[1,2] — [1]TransMIT GmbH, Center for Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics, University of Giessen, Germany

Two-stage PTCs achieve minimum temperatures of 2.2 K and have found their way even into sensitive applications where they compete with conventional LHe-bath cryostats. The 1st stage of a PTC is providing quite large cooling power at higher temperatures, ideal to cool radiation shields and precool peripheral elements. In addition, the cooling capacity of the regenerator is often used for precooling. This raises the question how the cooling capacity of a regenerator can best be harnessed. We present a cryocooler design [1], where an additional heat exchanger was incorporated into the 2nd stage regenerator.

This intermediate cooling stage allows to extract 4-5 W of cooling power at temperatures of 8-9 K for a standard two-stage PTC with a cooling capacity of 1.6 W at 4.2 K. The experimental data shows that applying the additional heating power does not adversely influence the performance of the second stage cold

flange. The achieved cooling powers and temperatures are, for instance, ideally suited to cool superconducting wires in current quantum systems.

[1] J. Falter et al., submitted to Cryogenics (preprint: https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4814535)

TT 8.7 Mon 16:45 H32

Experimental investigations of a frequency optimized Pulse Tube Cryocooler cooldown — •Jack Schmidt[1,2], Bernd Schmidt[1,2], and Andre Schirmeisen[1,2] — [1]Justus-Liebig-Universität Gießen — [2]TransMIT GmbH

Working in research often requires lower temperatures to achieve material effects such as superconductivity. This is achieved by using cryogenic liquids or closed cycle cryocoolers. Later have sub genres of working principle and provide different positive and negative aspects. We focus on the usage of Gifford-McMahon-type pulse tube cryocoolers which provide temperatures down to 2.2 K with the usage of Helium. The cooling power at 4.2 K scales up to 5 Watts nowadays with an electrical input power of the compressor around 25 kW. [1] As for mechanical stability the cryostats often become bulky and heavy. Including temperature isolation of the cold parts the cooldown times become very large. As the cryocoolers are mostly optimized for ongoing low temperature operation the cooling process lacks adaptations for an ideal cooldown. Other findings on this topic suggest to adjust valves and frequency. [2] Here we present our findings on the cooling process of a cryocooler to reduce cooldown time while adjusting the frequency. We were able to reduce the cooling time of the cryocooler by 9 % , applying electrical heat the cooldown is reduced by 10 %.

[1] X. Hao et al., Development of a 5 W/4.2 K two-stage pulse tube cryocooler. CEC/ICMC, C2Or3A-03 (2023);
[2] R. Snodgrass et al., Nat. Commun. 15, 3386 (2024).

TT 8.8 Mon 17:00 H32

Photoelectron characterization of a Cold field emitter for Ultrafast TEM — •Tim Dauwe[1,2], Nora Bach[1,2], Rudolf Haindl[1,2], Armin Feist[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) combines high spatial resolution with capabilities to image structures in the ultrafast temporal regime. This development was substantially advanced by creating femtosecond photoelectron pulses at modified Schottky tip emitters [1]. Further progress is expected by utilizing cold field emission guns (CFEG), which offer particularly high brightness and a narrower kinetic energy spectrum. In this contribution, we present a characterization of laser-triggered photoemission from a CFEG. We use a recent gun design allowing for laser access to the emitter (see Ref. [2]) and analyze beam characteristics in the linear photoemission regime. The CFEG is shown to support sub-nanometer probes and allows for photoelectron energy widths below 0.3eV. We emphasize the characterization of the spectral shape as a function of gun settings and compare it to theoretical models. Our experiments provide new insights for implementing and understanding photoemission from a CFEG, which will promote UTEM experiments at high resolution.

[1] A. Feist et al., Ultramicroscopy, 176 (2017)
[2] A. Schröder et al., arXiv:2410.23961 (2024)

TT 8.9 Mon 17:15 H32

Erbium dopants as luminescence thermometers in nanophotonic silicon waveguides — •Kilian Sandholzer, Stephan Rinner, Justus Edelmann, and Andreas Reiserer — Technical University of Munich, TUM School of Natural Sciences, and Munich Center for Quantum Science and Technology (MCQST), Garching, Germany

The demand for fast and accurate temperature measurements in nanophotonic silicon devices grows as integrated structures for applications become more complicated and denser in classical and quantum technologies. Established approaches use sensors attached close to the components, which limits spatial resolution and increases the footprint of devices [1]. We propose and implement luminescence-based thermometry using directly integrated erbium emitters within nanophotonic silicon waveguides [2]. Coverage from 2 K to 295 K is achieved using two different effects: The thermal activation of non-radiative decay channels via impurities is used for temperatures above 200 K, and the population dynamics of crystal field and spin levels caused by phononic thermalization at lower temperatures. We achieve relative thermal sensitivities of 0.22(4) %/K at room temperature, increasing to 420(50) %/K at 2 K. Combined with spatially selective implantation, our method promises precise thermometry from ambient to cryogenic temperatures with a few-nanometer resolution.

[1] Y. Ma, B. Dong, and C. Lee, Nano Convergence 7, 12 (2020)
[2] K. Sandholzer et al., arXiv (2024)

TT 8.10 Mon 17:30 H32

Fast, accurate and local temperature control using qubits — •Riya Baruah[1], Pedro Portugal[1], Joachim Wabnig[2], and Christian Flindt[1,3] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [2]Nokia Bell Labs, Cambridge, United Kingdom — [3]RIKEN Center for Quantum Computing, Wakoshi, Saitama 351-0198, Japan

Many quantum technologies operate in the subkelvin regime. It is therefore desirable to develop practical tools and methods for the precise control of the temperature in nanoscale quantum systems. Here, we present a proposal for fast, accurate, and local temperature control using qubits, which regulate the flow of heat between a quantum system and its thermal environment [1,2]. The qubits are kept in a thermal state with a temperature that is controlled in an interplay between work done on the qubits by changing their energy splittings and the flow of heat between the qubits and the environment. Using only a few qubits, it is possible to control the thermal environment of another quantum system, which can be heated or cooled by the qubits. As an example, we show how a quantum system at subkelvin temperatures can be significantly and accurately cooled on a nanosecond timescale.

[1] P.Portugal, F.Brange, C.Flindt, Phys. Rev. Res. 4, 043112 (2022).
[2] R.Baruah, P.Portugal, J.Wabnig, C.Flindt, arXiv:2410.04796 (2024).

TT 9: Correlated Magnetism – Low-Dimensional Systems

Time: Monday 15:00–18:15 Location: H33

TT 9.1 Mon 15:00 H33

Pressure and quantum magnetism: Insights from brochantite $Cu_4SO_4(OH)_6$ — •Victoria Ginga[1], Bin Shen[2], Ece Uykur[3], Nico Giordano[4], and Alexander Tsirlin[1] — [1]Felix Bloch Institute, University of Leipzig, Germany — [2]EP VI, EKM, University of Augsburg, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Germany

Brochantite $Cu_4SO_4(OH)_6$, a widespread natural copper sulfate mineral, exemplifies a low-dimensional quantum magnet due to its geometrically frustrated $S = 1/2$ Cu^{2+} chains. The crystal structure of brochantite ($P2_1/n$) consists of edge-sharing zigzag double chains forming corrugated sheets in the *ab*-plane, with dissimilar Cu-O-Cu bridges fostering complex magnetic interactions. Ferromagnetic ordering within the Cu1-Cu2 and Cu3-Cu4 chains coexists with antiferromagnetic coupling between the chains, thus creating a delicate balance that can be affected by external pressure. We show that brochantite develops antiferromagnetic ordering below $T_N \approx 6$ K at ambient pressure. High-pressure X-ray diffraction data show that the monoclinic structure of brochantite remains stable up to at least 33 GPa, but individual structural parameters and especially bond angles are modified by pressure, thus affecting magnetic frustration in the compound. Magnetization measurements under pressure reveal changes in the Neel temperature and in the position of the susceptibility maximum. Our findings highlight brochantite as a platform for studying the interplay of structural and magnetic properties under extreme conditions.

TT 9.2 Mon 15:15 H33

μSR-investigation of clinoatacamite $Cu_2Cl(OH)_3$ — •Carolin Kastner[1], Fabrice Bert[2], Thomas J. Hicken[3], Jonas A. Krieger[3], Hubertus Luetkens[3], Aaron Schulze[1], Dirk Menzel[1], F. Jochen Litterst[1], Leonie Heinze[4], Kirrily C. Rule[5], Anja U. B. Wolter[6], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]SQM, Université Paris-Saclay, Orsay, France — [3]PSI, Villigen, Switzerland — [4]FZ Jülich GmbH, JCNS at MLZ, Garching, Germany — [5]ANSTO, Kirrawee, Australia — [6]IFW Dresden, Dresden, Germany

Interest in the natural mineral clinoatacamite $Cu_2Cl(OH)_3$ arose due to its chemical and structural relationship to herbertsmithite, a candidate material featuring a quantum spin liquid state on the kagome lattice. In clinoatacamite, the Cu^{2+} spins form a system of distorted kagome layers with three inequivalent antiferromagnetic in-plane couplings and weaker ferromagnetic interlayer exchange. This gives rise to a complex magnetic phase diagram which contains a sequence of magnetic transitions of unknown symmetry.

Here, we present a study of the magnetic phase diagram of single-crystalline clinoatacamite using muon spin spectroscopy (μSR) to gain insight into the microscopic details of the different magnetic phases. For our investigation, the natural, single-crystalline samples were extensively pre-characterized by magnetization and specific heat. We will discuss our findings in the context of the local site symmetry of the different Cu ions.

TT 9.3 Mon 15:30 H33

Complex magnetic excitations in the alternating ferro-antiferromagnetic chain vompound $Cu_2(OH)_3Br$ — •Kirill Povarov[1], Yurii Skourskii[1], J. Wosnitza[1,2], David Graf[3], Zhiying Zhao[4], and Sergei Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, HZDR, Dresden — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]National High Magnetic Field Laboratory, Tallahassee — [4]Fujian Institute of Research of Structure of Matter, Fujian

We report the intricate spectrum of magnetic excitations in the mixed-chain quantum magnet $Cu_2(OH)_3Br$. Electron spin resonance (ESR) measurements in the frequency range between 0.1 and 1 THz reveal two distinct types of excitations: Low-energy modes of antiferromagnetic resonance (AFMR), and a high-energy excitation multiplet. The latter was argued to stem from mixing between the spinons and magnons, based on the results of zero-field neutron spectroscopy [1]. Peculiarities of their behavior in magnetic fields up to 16 T are discussed.

This work was supported by the Deutsche Forschungsgemeinschaft through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - *ct.qmat* (EXC 2147, project No. 390858490) and the SFB 1143, as well as by HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

[1] Zhang *et al.*, PRL **125**, 037204 (2020).

TT 9.4 Mon 15:45 H33

Synthesis and physical properties of the quasi-spin chain compound Li_2CuO_2 — •Ashiwini Balodhi[1,2] and Min Gyu Kim[2] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI 53201, USA

Li_2CuO_2 serves as an excellent model system for investigating low-dimensional magnetism, owing to its simple $CuOi_4$ square planar coordination along the b-axis (orthorhombic structure). Previous studies on both polycrystalline and single-crystal samples have revealed an antiferromagnetic (AFM) transition at $T_N \sim 9$ K, accompanied by a canted AFM spin structure at T = 2.6 K. To probe the intrinsic magnetic properties of Li_2CuO_2, we synthesized this material using the flux method. We will present detailed magnetic, and heat capacity measurements on flux-grown samples. Magnetization and heat capacity data confirm a long-range antiferromagnetic transition at T_N = 9.3 K. In contrast to earlier studies reporting ferromagnetic components at low temperatures, our results do not indicate any evidence of ferromagnetic ordering in low temperature regime.

This work is supported by the University of Wisconsin-Milwaukee.

[1] A. Balodhi, M. G. Kim, Crystals 14, 288 (2024).
[2] A. Balodhi, M. G. Kim. J.Magn.Magn.Mater. 611, 172617 (2024).

TT 9.5 Mon 16:00 H33

Sub-Kelvin magnetic susceptibility insights into the spin chain system $YbAlO_3$ — •Lipsa Behera[1,2], Javier Landaeta[2], Konstantin Semeniuk[2], and Elena Hassinger[1,2] — [1]TUD Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Low dimensional quantum magnets offer a rich platform to explore intriguing physics such as Tomonaga-Luttinger liquid, incommensurate phases and quantum phase transitions. What makes them special is the constraint in dimensionality leading to strong correlations. $YbAlO_3$ is an example of a quasi-one-dimensional spin chain system that can be described as a S = 1/2 Heisenberg chain with smaller Ising-like interchain interactions. At 1K it shows a typical spinon spectrum. At low temperature, the phase diagram presents an antiferromagnetic phase below 0.9 K, that changes into a longitudinal spin density wave including a MS/3 plateau, transverse antiferromagnetic phase and the field polarised state with H ||a. Recent thermal conductivity and magnetostriction measurements uncovered a previously unobserved MS/5 plateau phase at B = 0.7 T, motivating detailed sub-kelvin magnetic susceptibility studies. Here, we report ac susceptibility measurements down to 25 mK, which not only reproduces the known phase diagram to a good extent, but also confirm the presence of the magnetization plateau Ms/5. Furthermore, it reveals additional anomalies, embedded in the incommensurate phase, adding up to the complex magnetic behavior of this material.

TT 9.6 Mon 16:15 H33

Evidence of spin-phonon charge coupling in the quasi-1D Ising spin chain system α-CoV_2O_6 — •Debismita Naik and Pradip Khatua — Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal 741246, India

The quasi-one-dimensional Ising spin chain system α-CoV_2O_6 exhibits fascinating magnetic properties at lower temperatures. The DC magnetization and specific heat confirm the antiferromagnetic long-range ordering temperature T_N = 15 K. From the specific heat, the calculated magnetic entropy above T_N suggests short-range ordering in this low-dimensional compound. The temperature-dependent XRD supports the key finding of magnetoelastic coupling, which is crucial for linking the electrical and magnetic dipoles. Temperature-dependent Raman spectroscopy reveals the presence of spin-phonon coupling below T_N. Additionally, the study highlights an unusual evolution of the Raman modes above T_N which appears to be linked to short-range magnetic ordering. The renormalization of Raman modes and lattice anomalies near T_N illustrate spin-lattice coupling via magnetoelastic and spin-phonon interactions leads to interplay between spin, charge, and phonon degrees of freedom in α-CoV_2O_6. To support the intriguing phenomena, the theoretical charge density difference maps suggest the formation of electrical dipoles between Co and O atoms below T_N arises from p-d hybridization.

15 min. break

TT 9.7 Mon 16:45 H33

Crystal structure, electronic structure and magnetism in the binary compound Cr_3Se_4 — •Helge Rosner[1], Seojin Kim[1], Yurii Prots[1], Vincent Morano[2], Oksana Zaharko[2], Jörg Sichelschmidt[1], Marcus Schmidt[1], and Michael Baenitz[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, 5232 Villigen PSI, Switzerland

Cr_3Se_4 crystallises in a monoclinic lattice, structurally closely related to the rhombohedral chalcogenite delafossite-like systems $ACrX_2$ with A = Na, Cu, Ag and X = S, Se. In contrast to these intrinsically semiconducting materials with a nonmagnetic monovalent A site, in Cr_3Se_4 the distorted triangular $CrSe_2$ layers are separated by a formally trivalent and magnetic ion. In consequence, the inter-layer distance is strongly reduced, making the system more three dimensional, and thus strongly increasing the magnetic ordering temperature.

Here, we present a joint experimental and theoretical study of the binary material Cr_3Se_4, including thermodynamic measurements, high resolution XRD, neutron scattering and density functional band structure calculations. Our data consistently demonstrate that the metallic system undergoes an antiferromagnetic ordering at about 160 K which is strongly coupled to the crystal lattice. The band structure calculations show that the conduction bands originate from strongly hybridised Cr-Se states with sizeable spin-orbit interaction. In a detailed comparison, we will highlight the similarities and differences between Cr_3Se_4 and the chalcogenite delafossites.

TT 9.8 Mon 17:00 H33

First-principles phonon study of $AgCrS_2$, $AgCrSe_2$, and $AgCrTe_2$ — •Seo-Jin Kim, Jörg Sichelschmidt, Michael Baenitz, Yurii Prots, Markus Schmidt, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We study the elastic and dynamic stability of layered triangular lattice systems $AgCrS_2$, $AgCrSe_2$, and $AgCrTe_2$ using density functional theory (DFT). These systems share the same structure but exhibit different properties. Multiferroic $AgCrS_2$ undergoes an additional structural transition to a monoclinic phase and exhibits a collinear double-stripe antiferromagnetic ground state below T_N = 42 K. $AgCrSe_2$ shows noncollinear cycloidal magnetic ordering below T_N = 32 K. To investigate the interplay between magnetism and structure, we analyze the elastic constants and phonon dispersions of these compounds. Our findings reveal that the on-site Coulomb repulsion and additional symmetry alterations in the Cr layer are crucial for achieving dynamical stability in $AgCrS_2$. Furthermore, we analyze $AgCrSe_2$ and $AgCrTe_2$ to understand the general trends in elastic and dynamic properties with chalcogen variation.

TT 9.9 Mon 17:15 H33

Magnetic-field tuning of the spin dynamics in the van der Waals antiferromagnet $CuCrP_2S_6$ (CCPS) — •Joyal John Abraham[1,2], Sebastian Selter[1], Yuliia Shemerliuk[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2,3], Vladislav Kataev[1], and Alexey Alfonsov[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden — [3]Institute for Solid State and Materials Physics and Würzburg- Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062

Magnetic van der Waals (vdW) materials have recently attracted significant attention due to their tunable magnetic properties, easy exfoliation, and possible integration into spintronic devices. In this work, we explore with electron spin resonance (ESR) spectroscopy the spin dynamics of the vdW antiferromagnetic (AFM) compound CCPS featuring interpenetrating antipolar Cu^{1+} and (AFM) Cr^{3+} sublattices. Above the AFM ordering temperature $T_N \approx 30$ K ESR reveals prominent ferromagnetic (FM) spin correlations that persist far above T_N, suggesting an intrinsically two-dimensional character of the spin dynamics in CCPS. At $T < T_N$, a complex field dependence of collective excitations of the AFM-ordered spin-lattice was observed featuring two non-degenerate magnon gaps at $H = 0$. A remarkable tuning of the excitations from the AFM-type to the FM-type with increasing field strength was demonstrated. Application of the linear spin wave theory enabled us to quantify the exchange and anisotropic constants. Furthermore, this unusual crossover of AFM-FM excitations is explained using the obtained energy parameters.

TT 9.10 Mon 17:30 H33

Investigation of the insulator to metal transition in the 2d van der Waals magnet $FePSe_3$ — •Saicharan Aswartham, Masoumeh Rahimkhani, Andreas Kreyssig, and Anna Böhmer — Experimentalphysik IV, Ruhr- Universität Bochum, 44801 Bochum, Germany

Layered magnetic van der Waals (vdW) materials offers an interesting playground for the investigation of correlated electronic ground states in two dimensions. $FePSe_3$ belongs to the family of transition metal phosphorus trichalcogenides $TMPX_3$ with an antiferromagnetic ground state with T_N=108 K. Interestingly, under the application of external pressure FePSe3 undergoes insulator to metal transition. Here, we present detailed synthesis and physical properties of $Fe_{1-x}TM_xPSe_3$ with different transition metal substitution. We furtheraim to investigate spin cross over behaviour with the application of chemical pressure in $FePSe_3$.

[1] Wang et al., Nat. Commun. 9, 1914 (2018).
[2] Selter et al., Phys. Rev. Mater. 5, 073401 (2021).

TT 9.11 Mon 17:45 H33

Modelling low-energy spin excitation measurements in field-induced phases of the spin-ladder antiferromagnet $BiCu_2PO_6$ — Patrick Pilch[1], Kirill Amelin[2], •Gary Schmiedinghoff[3], Anneke Reinold[1], Changqing Zhu[1], Kirill Yu. Povarov[4], Sergei Zvyagin[4], Hans Engelkamp[5], Yin-Ping Lan[6], Guo-Jiun Shu[6], Fang-Cheng Chou[7], Urmas Nagel[2], Toomas Rõõm[2], Götz S. Uhrig[1], Benedikt Fauseweh[1,3], and Zhe Wang[1] — [1]TU Dortmund, 44227 Dortmund, Germany — [2]NICPB, 12618 Tallinn, Estonia — [3]DLR, 51147 Cologne, Germany — [4]HZDR, 01328 Dresden, Germany — [5]Radboud University, 6525 ED Nijmegen, The Netherlands — [6]Taipei Tech, Taipei 10608, Taiwan — [7]NTU, Taipei 10617, Taiwan

We report on terahertz spectroscopic measurements and subsequent theoretical modelling of quantum spin dynamics on single crystals of a spin-1/2 frustrated spin-ladder antiferromagnet $BiCu_2PO_6$ as a function of applied external magnetic fields. Anisotropic spin triplon excitations are observed, which split in applied magnetic fields with a quantum phase transition at $B_{c1} = 21.4\,T$ for fields applied along the crystallographic *a* axis.

We theoretically model the magnetic field dependence of the triplon modes by using continuous unitary transformations to determine an effective low energy Hamiltonian. Through an exhaustive parameter search we find numerically optimized parameters to very well describe the experimentally observed modes, which corroborate the importance of significant magnetic anisotropy in the system.

The talk focuses on the theoretical analysis of the experimental data.

TT 9.12 Mon 18:00 H33

Evidence of multiple phase transition in $Sr_2BB'O_6$ — •Aprajita Joshi, Shalini Badola, Akriti Singh, and Surajit Saha — Indian Institute of Science Education and Research Bhopal, India

The manifestation of phase transition is well mimicked by the lattice, thus by phonons, which requires its correlation with other degrees of freedom (spins, phonons etc.). Often, one can study the behavior of associated phonons with external perturbation to get more insight into the ground state of the material. Thus, any changes in the phase can be tracked with the external stimuli. Keeping this in mind, we explored the structural and magnetic attributes of $Sr_2BB'O_6$ with the help of Raman spectroscopy, using temperature as an external perturbation. The obtained phonon parameter shows the signature of a series of structural phase transitions. Magnetic measurements reveal that it also stabilizes in an antiferromagnetic ground state. An apparent deviation in Raman modes was seen around both the magnetic transitions, acting as a signature of spin-phonon coupling in the system. Additionally, temperature-dependent Raman gave insight into the local distortion in the lattice arising in the magnetically ordered state. This was also corroborated by temperature-dependent XRD measurements.

TT 10: Topological Semimetals

Time: Monday 15:00–17:45 Location: H36

TT 10.1 Mon 15:00 H36

Uniaxial pressure tuning of the anomalous Hall effect in Mn_3Ge — •Gustavo Lombardi[1], Leonardo Oparacz Kutelak[2], Mario Moda Piva[1], Vinicius Estevo Silva Frehse[3], Guilherme Calligaris[2], Ricardo Donizeth dos Reis[2], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Brazilian Synchrotron Light Laboratory, 13083-100, Campinas, Brazil — [3]Center for Electronic Correlations and Magnetism, 86159, Augsburg, Germany

The hexagonal Heusler compound Mn_3Ge exhibits an antiferromagnetic structure in which the Mn spins are arranged in a 120° triangular configuration characteristic of a Kagome lattice in the *ab* plane. These Kagome layers are periodically stacked along the *c* axis. This structure gives rise to a large anomalous Hall effect (AHE) due to a non-vanishing Berry curvature. Uniaxial pressure provides an effective method for tuning the AHE in Mn_3Ge. Our results reveal that applying stress along the *a* direction, which induces a distortion in the *ab* plane, significantly modifies the Hall signal. In contrast, stress applied along the *c* axis has no visible effect on the Hall signal. These results, combined with previous hydrostatic pressure data [1], suggest that the strong variations in the AHE are due to changes in the magnetic order in the *ab* plane. We also find that the application of hydrostatic and uniaxial pressure leads to different modifications of the magnetic order, the former inducing an out-of-plane tilt of the Mn spins, while the latter induces rotations of the Mn spins within the *ab* plane.

[1] R. D. Dos Reis et al., Phys. Rev. Mater. **4**, 51401 (2020).

TT 10.2 Mon 15:15 H36

Terahertz-light induced dynamics in the magnetic Weyl semimetal Mn_3Sn — •Anneke Reinold[1], Sergey Kovalev[1], Tomohiro Uchimura[2], Shunsuke Fukami[2], and Zhe Wang[1] — [1]Department of Physic, TU Dortmund University, Germany — [2]Laboratory for Nanoelectronics and Spintronics, Research Institute of Electrical Communication, Tohoku University, Sendai, Japan

We present a time-resolved spectroscopic study of the strong terahertz (THz) field-driven dynamics in the chiral-structured non-collinear Kagome antiferromagnet Mn_3Sn, a material renowned for anomalous transport properties, topological effects, and promising spintronic applications [1]. The driven charge and spin nonequilibrium dynamics are probed by optical transmission and Faraday rotation with a sub-picosecond time resolution for various experimental conditions. By varying THz and optical polarization, sample orientation, and sample temperature, we carry out a comprehensive investigation of the THz field-driven nonequilibrium dynamics, in order to figure out the contributions due to different mechanisms. Our findings provide insight into the THz field-driven spin dynamics in this Kagome antiferromagnet and demonstrate its potential for THz spintronic applications.

[1] J. Han, T. Uchimura et al., Nat. Phys. **20**, 1110 (2024).

TT 10.3 Mon 15:30 H36

Anomalous Hall and Nernst effect in the Weyl semimetal $Ta_{1+x}Ru_{1-x}Te_4$ — •Mahdi Behnami[1,2,3], Dmitri Efremov[1], Grigory Shipunov[1], Saicharan Aswartham[1], Vilmos Kocsis[1], Marina Putti[3,4], Bernd Büchner[1,2], Helena Reichlova[1,2,5], and Federico Caglieris[4] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Physics, University of Genoa, 16146 Genova, Italy — [4]CNR-SPIN, 16152 Genova, Italy — [5]Institute of Physics ASCR, v.v.i., Cukrovarnick a 10, 162 53, Praha 6, Czech Republic

The anomalous Nernst effect is a transverse thermoelectric phenomenon driven by a temperature gradient perpendicular to both the heat current and the magnetic order vector. This effect is particularly valuable for probing the topological nature of materials, as it exhibits greater sensitivity to the Berry curvature near the Fermi energy compared to the anomalous Hall effect. In this study, we report that the type-II Weyl semimetal $Ta_{1+x}Ru_{1-x}Te_4$ exhibits both anomalous Hall and Nernst effects. These phenomena can be attributed to the finite Berry curvature generated by the Weyl points in this material.

TT 10.4 Mon 15:45 H36

Electronic transport and classification for topological nodal planes — •Moritz M Hirschmann[1,2], Kirill Alpin[1], Raymond Wiedmann[1], Niclas Heinsdorf[1,3], Wan Yee Yau[1,4], Andreas Leonhardt[1], Douglas H Fabini[5], Johannes Mitscherling[1,6,7], and Andreas P Schnyder[1] — [1]MPI FKF, Stuttgart, Germany — [2]RIKEN CEMS, Wako, Japan — [3]UBC, Vancouver, Canada — [4]MPI CBG, Dresden, Germany — [5]MIT, Cambridge, USA — [6]UC, Berkeley, USA — [7]MPI PKS, Dresden, Germany

Nodal planes are the two-dimensional generalization of nodal points/lines [1], and like them, they may carry a topological charge, for which we devise a symmetry-based classification. When a single or a pair of two nodal planes are topological, Fermi arcs connect the pockets of Weyl points and nodal planes on the surface. While this is similar to Weyl semimetals, their transport properties differ. We find that the large degeneracy of nodal planes is susceptible to a time-reversal breaking that contributes to the anomalous Hall effect. Further, perturbed nodal planes generically enhance the quantum metric contributing to the interband part of the optical conductivity. As an application, we study the hexagonal van der Waals material $CoNb_3S_6$, which exhibits such topological

nodal planes. Recently, this compound has gained interest due to its All-in-All-out magnetic order that exhibits a non-trivial spin-space symmetry [2]. Here, the topological nodal planes dominate the anomalous Hall and Nernst effects.
[1] Nature 594, 374 (2021).
[2] arXiv:2403.01113 (2024).

TT 10.5 Mon 16:00 H36

Quantum geometry of topological nodal planes in Kondo systems — •Yannis Ulrich[1], Andreas Schnyder[1], and Laura Classen[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Department of Physics, Technical University of Munich, D-85748 Garching, Germany

The geometric properties of the Hilbert space of Bloch states, such as the Berry curvature or quantum metric, play an important role in understanding topological semimetals. They are also fundamental for the understanding of various physical responses, including the (non-)linear Hall effect and (magneto-)optical conductivities. In this talk, I investigate the quantum geometry of two-dimensional topological band degeneracies, i.e., topological nodal planes, with a flat dispersion. Such nodal planes naturally arise in Kondo materials with screw rotation symmetries. Using a periodic Anderson model, I show how nodal planes in these Kondo materials can be tuned via pressure or temperature to be close to the Fermi level with a nearly flat dispersion. I show that such flat nodal planes exhibit a substantial quantum geometry, which in turn leads to nontrivial signatures in the (non-)linear Hall responses. Derivations of the Hall conductivities are presented in the manifestly gauge-invariant language of projectors, emphasizing their advantages in this type of calculation.

TT 10.6 Mon 16:15 H36

Finite-size topological phases from semimetals — •Adipta Pal[1,2] and Ashley M. Cook[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany

Topological semimetals are some of the topological phases of matter most intensely-studied experimentally. The Weyl semimetal phase, in particular, has garnered tremendous, sustained interest given fascinating signatures such as the Fermi arc surface states and the chiral anomaly, as well as the minimal requirements to protect this three-dimensional topological phase. Here, we show that thin films of Weyl semimetals (which we call quasi-(3-1)-dimensional, or q(3-1)d) generically realize finite-size topological phases distinct from 3d and 2d topological phases of established classification schemes: response signatures of the 3d bulk topology co-exist with topologically-protected, quasi-(3-2)d Fermi arc states or chiral boundary modes due to a second, previously-unidentified bulk-boundary correspondence. We show these finite-size topological semimetal phases are realized by Hamiltonians capturing the Fermiology of few-layer Van der Waals material MoTe2 in experiment. Given the broad experimental interest in few-layer Van der Waals materials and topological semimetals, our work paves the way for extensive future theoretical and experimental characterization of finite-size topological phases.

15 min. break

TT 10.7 Mon 16:45 H36

Phonon-mediated surface superconductivity in Weyl semimetals — •Kristian Maeland and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

Recent experiments show that Weyl semimetals can host surface superconductivity in the Fermi arcs, while remaining metallic in the bulk. We study a lattice model of a Weyl semimetal to see if phonons are a candidate pairing mechanism to explain this phenomenon. Specifically, we study the pairing mechanism in detail on the surface and in the bulk. Furthermore, we make predictions about the critical temperature and the momentum dependence of the gap function.

TT 10.8 Mon 17:00 H36

The Weyl-Mott point: Topological and non-Fermi liquid behavior from an isolated Green's function zero — •Rafael Alvaro Flores Calderon[1] and Chris Hooley[2] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187 Dresden, Germany — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 2TT, United Kingdom

We present a model in which a Hatsugai-Kohmoto interaction is added to a system of fermions with a Weyl point in their non-interacting dispersion relation, and analyze its behavior as a function of the chemical potential. We show that the model exhibits a Weyl-Mott point, a single isolated Green's function zero, and that this implies an emergent non-Fermi-liquid state at the border of the metallic regime and a gapped topological state for the insulating one. The Weyl-Mott point inherits the topological charge from the original Green's function pole, and is therefore naturally associated with a strongly correlated chiral anomaly.

TT 10.9 Mon 17:15 H36

Observation of quasiparticle lifetime oscillations in WSi_2 — •Ivan Volkau[1], Nico Huber[1], Leo Maximov[1], Andreas Bauer[1,3], Christian Pfleiderer[1,2,3], and Marc A. Wilde[1,3] — [1]Technical University of Munich (TUM) — [2]MCQST, Munich — [3]TUM Zentrum für Quantum Engineering

The observation of quasiparticle lifetime oscillation (QPLOs) in CoSi [1] raises the question whether they are a generic feature observable in many materials or if they require a specific band structure. Here, we report the observation of QPLOs in WSi_2, which has recently generated great interest due to its remarkable characteristics in its transport properties, such as axis-dependent conduction polarity [2] and extremely large magnetoresistance [3]. We present Shubnikov-de Haas (SdH) and de Haas-van Alphen measurements, performed at different orientation of magnetic field up to 18 T and temperatures down to 1.5 K. We analyze the oscillation frequencies, their angular dependence, and their temperature dependence. The detected combination frequencies in the SdH effect exhibit characteristics consistent with QPLOs theory providing another example where the influence of QPLOs is observed.
[1] Nature 621, 276 (2023).
[2] Chem. Mater. 35, 4228 (2023).
[3] Phys. Rev. B 102, 115158 (2020).

TT 10.10 Mon 17:30 H36

Anomalous photo-Nernst effect and impact of disorder in $HfTe_5$ films — Maanwinder Singh[1,2], Tobias Meng[3], and •Christoph Kastl[1,2] — [1]Walter-Schottky-Institute, Technical Unversity of Munich, Germany — [2]Munich Center for Quantum Science and Technology — [3]Institute of Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

We discuss optoelectronic transport in thin films of $HfTe_5$, which is a non-magnetic, weakly gapped semimetal at the border of a weak to strong topological insulator transition. We find that focused photoexcitation results in strong a transversal response at finite magnetic field, which we describe in terms of a Berry curvature driven anomalous photo-Nernst effect of three-dimensional massive Dirac fermions [1]. We further use Raman microscopy to reveal significant microscale disorder and strain in contacted films, which has important implications for the interpretation of transport experiments in $HfTe_5$ due to the sensitivity of its electronic structure to external strain [2].
[1] Singh et al., Adv. Phys. Res. 3, 2300099 (2024).
[2] Singh et al., ACS Nano 18, 18327 (2024).

TT 11: Superconductivity: Poster

Time: Monday 15:00–18:00 Location: P4

TT 11.1 Mon 15:00 P4

Chiral and nematic superconductivity in monolayer $NbSe_2$ — •Anton Bleibaum[1], Julian Siegl[1], Wen Wan[2], Marcin Kurpas[3], John Schliemann[1], Miguel M. Ugeda[2,4,5], Magdalena Marganska[1], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [3]Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland — [4]Centro de Física de Materiales, Paseo Manuel de Lardizábal 5, 20018 San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao 48013, Spain

Superconductivity emerges when there is an effective attractive electron-electron interaction. As proposed by Kohn and Luttinger in 1965, screening of the Coulomb interaction can give rise to long-range Friedel oscillations providing regions of attractive interaction which allow for Cooper pairing. In $NbSe_2$, Coulomb repulsion is sufficient to induce superconductivity, when accounting for screening on the triangular lattice. Using momentum resolved gap equations, we find two quasi-degenerate nematic solutions near the critical temperature T_c. In agreement with tunneling spectroscopy experiments, a complex linear combination forms a fully gaped chiral phase well below T_c. When we allow for an in-plane magnetic field, we find an equal spin pairing component.

TT 11.2 Mon 15:00 P4

Exfoliation and STM/STS Investigations of Monolayer $NbSe_2$ S/F Systems — •Tiark Tiwary[1], Marcel Strohmeier[1], Elke Scheer[1], and Angelo Di Bernardo[1,2] — [1]University of Konstanz, 78457 Konstanz, Germany — [2]University of Salerno, Via Giovanni Paolo II, 132, 84084 Fisciano (SA), Italy

Two dimensional materials have become of great interest in the recent years, because of their promise to enable novel electronic functionality by choosing suitable material combinations. A typical feature of 2D superconductors is their anisotropy of the critical field which is most pronounced in the monolayer limit. To understand more about the behaviour of Ising superconductivity in monolayer $NbSe_2$, STM/STS measurements were performed. To this end, gold-assisted exfoliation was used to obtain large monolayer on a Ti/Au surface. The measurements largely confirmed the previous reports [1, 2] on monolayer $NbSe_2$. To develop devices for superconducting spintronics, the interplay between a ferromagnet and monolayer $NbSe_2$ is investigated. Multiple techniques to gain $NbSe_2$ monolayer were explored. The exfoliation of small monolayers on a Co surface could be achieved.

[1] Wan et al., Adv. Mater. 34, 2206078 (2022);
[2] Kuzmanović et al., Phys. Rev. B **106**, 184514 (2022).

TT 11.3 Mon 15:00 P4

Cavity Mediated Control on Study of Transient THz Field on Superconductors — Angela Montanaro, Giacomo Jarc, •Nitesh Khatiwada, and Daniele Fausti — Friedrich-Alexander-Universität Erlangen-Nürnberg

Cavity QED has emerged as a new stimulus for studying phase transition in quantum materials. A recent study[1] demonstrating changes in critical temperature for metal insulator phase transition mediated by cavity electrodynamics in 1T-TaS_2 has inspired us to investigate cavity mediated phase transition in superconductors.

[1] Nature 622, 487 (2023).

TT 11.4 Mon 15:00 P4

THz spectroscopy on superconducting ZrN thin films — •Ozan Saritas[1], Frederik Bolle[1], Martin Dressel[1], Roman Potjan[2], Marcus Wislicenus[2], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Fraunhofer Institute for Photonic Microsystems (IPMS), Center Nanoelectronic Technologies (CNT), Dresden, Germany

The recent large-scale preparation of superconducting ZrN thin films is of interest for potential quantum technology applications [1]. Therefore, here we use THz frequency domain spectroscopy to investigate the superconducting electrodynamics of ZrN thin films, with thickness between 20 nm and 50 nm, grown on 300 mm-standard silicon substrates. We have measured the transmission and phase shift of THz radiation passing through the ZrN films, and we have obtained the frequency-dependent dielectric function. We thus acquired characteristic material quantities such as the temperature-dependent superconducting energy gap $2\Delta(T)$ and superfluid density $n_s(T)$. With decreasing thickness, there is a clear trend towards a lower critical temperature T_c, a reduced $2\Delta(T = 0)$, and a lower $n_s(T = 0)$. While the overall behavior is similar to BCS predictions, thinner films exhibit values for the ratio $2\Delta(T = 0)/(k_B T_c)$ that deviate more from the canonical value.

Additionally, a novel analysis of the temperature-dependent shift of Fabry-Perot transmission resonance frequencies of superconducting thin-film samples was performed.

[1] R. Potjan *et al*, Appl. Phys. Lett. **123**, 172602 (2023)

TT 11.5 Mon 15:00 P4

Terahertz investigations on superconducting nitride thin films — •Yayi Lin[1], Frederik Bolle[1], Janine Lorenz[2], Marcello Guardascione[2], Marc Neis[2], Thomas J. Smart[2], Martin Dressel[1], Rami Barends[2], Pavel Bushev[2], F. Stefan Tautz[2], Felix Lüpke[2], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Jülich, Germany

In recent years, superconducting nitride thin films have garnered significant attention, for example for applications in quantum electronics. Due to the wide range of accessible kinetic inductance, high critical temperature, and correspondingly large energy gap, these materials are readily utilized in microwave resonators, low-temperature amplifiers, and quantum circuits.

We use terahertz (THz) spectroscopy to probe the electrodynamics of superconducting NbTiN ($T_c > 10$ K) and TiN ($T_c > 3$ K) thin films at frequencies below and above their superconducting energy gaps. We combine THz frequency-domain spectroscopy and THz time-domain spectroscopy to cover the frequency range from 100 GHz to 3 THz. We present key properties of several nitride thin films such as critical temperature (T_c), complex optical conductivity ($\hat{\sigma}$), energy gap (2Δ), superfluid density (n_s), and kinetic inductance (L_k). Of particular interest is the absolute value of the superconducting energy gap, which allows comparison with other spectroscopic techniques and predictions based on BCS theory.

TT 11.6 Mon 15:00 P4

Nanoscale Characterization of Defects in Superconducting Nitrides — •Janine Lorenz[1,2,3], Amin Karimi[1], Yorgo Hadad[1], Rami Barends[1], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,4] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen Universität, Germany — [4]II. Physikalisches Institut, Universität zu Köln, Germany

Due to their elevated critical temperature and high kinetic inductance, Nitride supercondcutors are promising candidates for microwave resonators and low-noise amplifiers that are essential for useful quantum computing. We aim to improve structural and superconducting properties of our 11 nm NbTiN thin films grown by sputter deposition. By implementing a post-deposition thermal annealing protocol in Nitrogen/Hydrogen gas atmosphere we achieve an increase in critical temperature from initially 11.5 K to 18 K. In this work, we apply scanning probe techniques to investigate surface superconductivity and defects that appear as Yu-Shiba-Rusinov states of treated and untreated thin films.

TT 11.7 Mon 15:00 P4

Superconductivity of Reduced Indium Tin Oxide — •Luca Hofmeister, Jan Pusskeiler, Gabriele Untereiner, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Deutschland

Indium tin oxide (ITO) is a transparent semiconductor commonly used in photovoltaics and flat screen displays. It is possible to induce low temperature superconductivity in ITO via electrochemical reduction in a NaCl solution. [1,2]

We reduced multiple ITO samples at a constant reduction current and measured the temperature dependence of their two-point resistance with a microwave Corbino spectrometer. Depending on the reduction time, the T_c ranges from 2.2 K to 3.7 K, forming a superconducting dome.

Reduction induces a color change of the ITO, which loses some of its transparency for increasing reduction times. Nevertheless, ITO retains some transparency even after very long reduction, thereby making ITO a candidate for usage as a transparent superconducter.

[1] A. E. Aliev *et al.*, Appl. Phys. Lett. **101**, 252603 (2012);
[2] E. Batson *et al.*, Supercond. Sci. Technol. **36**, 055009 (2023).

TT 11.8 Mon 15:00 P4

Structural properties of $YBa_2Cu_3O_7$ thin film nanopatterns generated by focused He-ion-beam irradiation — •Robin Hutt[1], Cesar Magen[2], Christoph Schmid[1], Jan Ullmann[1], Simon Koch[1], Javier Pablo-Navarro[2], Ross Carter[1], Paul Zimmermann[1], Frank Schreiber[1], Dieter Koelle[1], Reinhold Kleiner[1], Ivan Zaluzhnyy[1], and Edward Goldobin[1] — [1]Universität Tübingen, Germany — [2]INMA, Universidad de Zaragoza - CSIC, Spain

Irradiation of a $YBa_2Cu_3O_7$ (YBCO) thin film with a focused He ion beam (He-FIB) with spot size $\lesssim 10$ nm changes its properties on the nanoscale. A moderate irradiation dose D supresses the critical temperature T_c locally, thus allowing us to "draw", e.g., Josephson barriers, while a high D destroys (amorphizes) the crystal locally, letting us create highly resistive walls (edges of devices and holes) in one fabrication run. We report on the irradiation of YBCO thin films by He-FIB using single lines and rectangular areas with different doses and investigate the result using transmission electron microscopy (TEM). We visualize the crossover to amorphization at the critical dose D_c and the growth of the amorphous track width with D. Using a simple model, we obtain the value of D_c and FIB spot size with a good accuracy. In the areas irradiated by $D < D_c$ we use strain analysis of the TEM images to detect subtle changes in the crystal structure. This is complemented by spatially-resolved X-ray diffraction data that indicate the swelling of the film in c-direction in irradiated regions. Finally, these observations are correlated with electric transport properties of irradiated areas.

TT 11.9 Mon 15:00 P4

$YBa_2Cu_3O_7$ thin films on Si substrates for SQUID-on-lever scanning probe microscopy — •Simon Koch, Alexander Koller, Christoph Schmid, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany

Scanning SQUID microscopy (SSM) is a powerful technique for imaging magnetic fields or dissipation processes. The use of the high-T_c cuprate superconductor $YBa_2Cu_3O_7$ (YBCO) combined with custom made Si atomic force microscopy (AFM) cantilevers could enable SSM in the Tesla range and at temperatures up to ~ 80 K with high spatial resolution. However, YBCO has a complex crystal structure and a small coherence length, which leads to a high sensitivity to defects on the atomic scale. High quality YBCO films can only be obtained by epitaxial growth on lattice-matched substrates. Therefore, the challenge with this approch is the integration of YBCO thin films on Si wafers. In recent years, epitaxial $SrTiO_3$ (STO) with perovskite crystal structure has been realized on Silicon [1] and epitaxial STO-on-Si commercial substrates are now available. STO is lattice-matched to YBCO, and therefore provides an ideal starting point for the project.

We present our process for the fabrication of YBCO thin films on STO-on-Si substrates, based on pulsed laser deposition (PLD) and discuss the optimization of growth conditions. We further present our preliminary results regarding film quality and electrical characterization of fabricated structures.

[1] Abel *et al.*, Nature Mater. **18**, 42-47 (2019).

TT 11.10 Mon 15:00 P4

Disorder dependent properties of superconductors — •Marvin Zibula and Götz Seibold — Institut für Physik B-TU Cottbus-Senftenberg, Erich-Weinert Straße 1, 03046 Cottbus

We study the properties of disordered superconductors within the attractive Hubbard model and a disorder potential which interpolates between diluted impurities and Anderson-type disorder with a random potential at each lattice site. In the latter case, we reproduce the results from Ghosal et al. [1], corresponding to the formation of superconducting islands that are not correlated to the underlying charge distribution. However, such a correlation becomes effective upon reducing the impurity concentration. Our results are important for recent optical experiments related to the nonlinear first harmonic response which are more compatible with the diluted model.

[1] A.Ghosal, M.Randeria, N.Trivedi, Phys.Rev.B 65, 014501 (2001)

TT 11.11 Mon 15:00 P4

Influence of strong correlations on impurity-induced TRSB in a (s+id)-wave superconductor — •Marius Paul and Götz Seibold — BTU Cottbus

In numerical simulations of the extended Hubbard model with nearest-neighbor attraction, which is an actively investigated model for high-Tc-superconductors, there has been made observations of time reversal symmetry breaking in the form of loop currents in the last few years [1,2]. Those loop currents emerge mainly in the vicinity of an $s + id$-state when nonmagnetic disorder is present in the superconductor. While previous work has focused on the investigation of this phenomenon within the Bogoljubov-de Gennes approximation, we will discuss here the influence electronic correlations on the stability of the loop currents. This is accomplished via the time-dependent Gutzwiller approximation extended towards the inclusion of pairing correlations.

[1] Z.-X.Li, S. Kivelson, D.-H.Lee, npj Quantum Mater. 6, 12 (2021).
[2] C.N.Breiø, P.J.Hirschfeld, B.M.Andersen, PRB 105, 014504 (2022).

TT 11.12 Mon 15:00 P4

Constraints on the theoretical modeling of hole-doped La_2CuO_4 — •Qiwei Li, Xuejing Zhang, and Eva Pavarini — Peter Grünberg Institute-2, Forschungszentrum Jülich, Jülich, Germany

The low-energy electronic properties of hole-doped La_2CuO_4 are believed to be well captured by the single-band Hubbard model describing x^2-y^2 electrons. This finds support, e.g., on Fermi surface and angle resolved photoemission experiments. Here we show that this imposes constraints on the microscopic description of the system.

TT 11.13 Mon 15:00 P4

Nonlinear THz-spectroscopy of $PdCoO_2$ and LBCO: Probing c-axis dynamics and collective excitations — •Shuhan Wang[1], Tim Priessnitz[2], Min-Jae Kim[1,2], Liwen Feng[1,2], Gideok Kim[2], Bernhard Keimer[2], and Stefan Kaiser[1,2] — [1]TUD Dresden University of Technology, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Layered quantum materials offer a unique platform for studying anisotropic transport and collective excitations. Using THz-High-Harmonics Generation, we investigate the c-axis responses of $PdCoO_2$ and $La_{2-x}Ba_x$ CuO_4 (LBCO) grown on offcut substrates. $PdCoO_2$ shows exceptionally large THz second harmonic and third harmonic generation [1] while LBCO shows distinct features linked the superconducting Higgs response and the Josephson plasma resonance. We will discuss the features referenced to the linear response of these systems measures with THz time domain spectroscopy.

[1] T. Priessnitz et al., arXiv:2409.07872

TT 11.14 Mon 15:00 P4

Higgs collective mode in superconductors: in- and out-of equilibrium — •Sida Tian[1], Rafael Haenel[1,2], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart — [2]Quantum Matter Institute, University of British Columbia, Vancouver V6T 1Z4, Canada

Collective modes in superconductors encode rich information about the superconducting state. Experimentally probing them requires THz lasers that push the system away from equilibrium. We present a theory of non-equilibrium response based on Keldysh formalism, and introduce a recent developed experimental technique of Non-equilibrium Antistokes Raman Scattering. We further comment on the influence of higher-order fluctuations to collective modes, which will change the collective mode mass. This implies that in circumstances where quantum corrections become relevant such as strong coupling, the Higgs mode will move inside the pair breaking gap.

TT 11.15 Mon 15:00 P4

Nematic susceptibility in heavily hole-doped iron based superconductors — •Franz Eckelt[1], Xiaochen Hong[2], Vilmos Kocsis[3], Vadim Grinenko[4], Bernd Büchner[2], Christian Hess[1], Chul-Ho Lee[5], and Kunihiro Kihou[5] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]College of Physics and Center of Quantum Materials and Devices, Chongqing University, 401331 Chongqing, China — [3]Leibnitz-Institut for Solide State and Materials Research, 01069 Dresden, Germansy — [4]Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 201210, China — [5]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8568, Japan

We investigate the elastoresistivity of heavily hole doped iron-based superconductor $Ba_{1-x}K_xFe_2As_2$ in the range x=0.68-0.98 using a piezoelectric measurement technique. We observe a divergent increase in elastoresistance along the [110] direction during cooling for all samples the amplitude of which possesses a strong non-montonic doping dependence. We discuss our results in terms of nematic fluctuations, Fermi surface effects near a Lifshitz transition, and a potential orbital-selective Mott transition.

TT 11.16 Mon 15:00 P4

The Search for 1144 Phases under Pressure — •Leonard Essich, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe University Frankfurt, Germany

Alternative stacking of 122 Fe-based pnictides has enabled the synthesis of the 1144 phase $ABFe_4As_4$ (A = alkali, B = alkaline earth). Examples include $CaKFe_4As_4$, where a *half-collapsed* tetragonal phase emerges under pressure, and $EuRbFe_4As_4$ or $EuCsFe_4As_4$, where Eu magnetism coexists with superconductivity [1,2]. Theoretical studies predict the stability of further 1144 Fe-arsenides and an extension to phosphides ($AB(TM)_4P_4$ where TM = Fe, Ru, Co, or Ni). Notably, $CaKRu_4P_4$ has been successfully synthesised [1]. This work investigates the synthesis of other 1144 phases under high-pressure conditions, designed to support the incorporation of smaller phosphorus atoms on arsenic lattice positions. Multi-anvil presses offer precise pressure and temperature control, large sample sizes, and adaptable setups for crystal growth research. In this contribution, we present the capabilities of a multi-anvil press, the challenges encountered during sample preparation, and outline the pathway to synthesising 1144 phases. A Walker-type module, previously utilized in our laboratory, contains a 6-8 anvil configuration within a steel cylinder [3]. The choice of pressure-transmitting medium and internal configuration is crucial to achieving the desired outcome in these experiments.

[1] B. Q. Song *et al.*, Phys. Rev. Materials **5**, 094802 (2021)
[2] U. S. Kaluarachchi *et al.*, Phys. Rev. B **96**, 140501 (2017)
[3] A. A. Haghighirad *et al.*, Cryst. Growth Des. **8**, 1961 (2008)

TT 11.17 Mon 15:00 P4

Two-Gap Superconductivity in the Noncentrosymmetric La_3Se_4 — F Košuth[1,2], N Potomová[2], Z Pribulová[1], J Kacmarčík[1], •M Naskar[3], D S Inosov[3], S Ash[4], A K Ganguli[5], J Soltýs[6], V Cambel[6], P Szabó[1], and P Samuely[1] — [1]Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences, SK04001 Košice, Slovakia — [2]Centre of Low Temperature Physics, Faculty of Science, P. J. Šafárik University, SK-04001 Košice, Slovakia — [3]Institut für Festkörper und Materialphysik, Technische Universität Dresden, D-01069 Dresden, Germany — [4]Institute for Solid State Research, Leibniz IFW Dresden, D-01069 Dresden, Germany — [5]Department of Chemistry, Indian Institute of Technology Delhi, New Delhi 110016, India — [6]Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava SK84104, Slovakia

Point-contact Andreev reflection spectroscopy at low temperatures and high magnetic field has been carried out on the noncentrosymmetric superconductor La_3Se_4 (T_c = 8 K). Two superconducting energy gaps Δ_1 and Δ_2, with $2\Delta_1/k_BT_c$ = 5.8 and $2\Delta_2/k_BT_c$ = 2.3, are directly observed in certain spectra. The effects of temperature and magnetic fields help to distinguish a two-gap structure, even in the more common spectra where only a single gap is visible at low temperatures, indicated by a pair of maxima around zero bias. The presence of two-gap superconductivity, consistent with the results from point-contact Andreev reflection spectroscopy, is further confirmed by heat capacity and Hall probe magnetization measurements.

TT 11.18 Mon 15:00 P4

Positive Evidence for Bogoliubov-Fermi Surfaces in Al/InAs Hybrids — •Simon Feyrer[1], Ignacio Lobato[1], Vjeko Dimic[1], Michael Prager[1], Dominique Bougeard[1], Matthias Kronseder[1], Giorgio Biasiol[4], Carlos Balseiro[2], Liliana Arrachea[2], Marco Aprili[3], Christoph Strunk[1], and Leandro Tosi[1,2] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Argentina — [3]Laboratoire: Physic des Solides, Université Paris-Saclay, France — [4]IOM CNR, Laboratorio TASC, Area Science Park Basovizza, Trieste, Italy

We present measurements of a lumped element microwave resonator made out of hybrid Al/InAs superconductor/semiconductor 2D heterostructures. In our

device, the inductor is a narrow wire taylored in the material, dominating the kinetic inductance contribution. The resonance frequency depends on temperature, on power and strongly on in-plane magnetic field. We have observed a change of behavior as the magnetic field becomes larger than B*, consistent with a contribution of the superconducting 2DEG in the InAs affected by the spin-orbit coupling [1]. Using resonators with different geometries we discuss the correlation between the observed anisotropy and the crystal orientation.
[1] D. Phan et al., Phys. Rev. Lett. 128, 107701 (2022).

TT 11.19 Mon 15:00 P4

Proximity induced superconductivity in non-collinear antiferromagnets (NCAFMs) — •Anshuman Padhi[1], Prajwal Rigvedi Madhusudan Rao[1], Ajin Joy[2], Ajesh K Gopi[1], Jiho Yoon[1], Jae-Chun Jeon[1], Banabir Pal[1], and Stuart S. P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, 06120, Halle (Saale), Germany — [2]Indian Institute of Science, 560012, Bengaluru, India

Conversion of spin-singlet Cooper pairs to spin-polarised triplet Cooper pairs has been a significant achievement of proximity induced superconducting hybrids. But they often require multilayed stack of mismatched magnetisation interfacing the superconducting condensate, leading to lower tunability, less flexibility on the choice of materials and lesser densities of converted triplet Cooper pairs. Recently, usage of non-collinear antiferromagents have been shown to host long-ranged supercurrents and owing to their atomic distribution of spins in a Kagome lattice are a prime candidate for triplet superconductivity. In this study we aim to fundamentally understand the proximity effect into two-phases of a Mn-based antiperovskite, by analysing the field-dependence of the critical temperature of the superconducting thin-film interfacing them. The unique spin-texture of such materials, with broken inversion symmetry and the presence of uncompensated moments too, can lead to interesting physics w.r.t. the Andreev levels. Thus we fabricate S/I/NCAFM tunneling devices and perform electrical tunneling measurements to study the probable Andreev levels and the impact of the spin-states on them. This exploratory work aims at a deeper level of understanding of Cooper pair interactions in NCAFMs.

TT 11.20 Mon 15:00 P4

Interaction of supercurrents in multiterminal graphene Josephson junctions — •Paul Maier, Romain Danneau, and Detlef Beckmann — Institut für Quantenmaterialien und Technologien, Karlsruher Institut für Technologie

Topological states are predicted to exist in the Andreev bound state spectrum of multiterminal Josephson junction with four or more terminals [1]. Superconductor graphene hybrid structures are especially suitable to realize such devices due to the gate tunability of graphene and the low contact resistance necessary to form Andreev bound states. Understanding the distribution of supercurrent in graphene multiterminal Josephson junctions is one step in the search for these states. We report on the experimental investigation of transport in a four-terminal graphene Josephson junction. We observe magnetic interference patterns in two-terminal measurements and critical current contours in multi-terminal measurements, and compare the results to theoretical simulations.
[1] R.-P. Riwar et al., Nat. Commun. 7, 11167 (2016).

TT 11.21 Mon 15:00 P4

Control of Andreev Reflection via a Single-Molecule Orbital — •Lorenz Meyer[1], Jose L. Lado[2], Nicolas Néel[1], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Department of Applied Physics, Aalto University, 02150 Espoo, Finland

Charge transport across a single-molecule junction fabricated from a normal-metal tip, a phthalocyanine, and a conventional superconductor in a scanning tunneling microscope is explored as a function of the gradually closed vacuum gap. The phthalocyanine (2H-Pc) molecule and its pyrrolic-hydrogen-abstracted derivative (Pc) exhibit vastly different behavior. Andreev reflection across the 2H-Pc contact exhibits a temporary enhancement that diminishes with increasing conductance. The hybridization of 2H-Pc with the tip at contact formation gives rise to a molecular magnetic moment that is Kondo-screened in the tip. In contrast, the single-Pc junction lacks Andreev reflection in the same conductance range. Spectroscopy experiments and supporting nonequilibrium Green function calculations highlight the importance of a molecular orbital close to the Fermi energy for rationalizing the observations.

Funding by the DFG through KR 2912/18-1 and KR 2912/21-1 is acknowledged.

TT 11.22 Mon 15:00 P4

Real-space mapping of Yu-Shiba-Rusinov states around magnetic defects on superconducting surfaces — •Raffaele Aliberti[1,2], Samir Lounis[1,4], Philipp Rüssmann[1,3], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]RWTH Aachen, Aachen, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [4]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Interfacing magnetic impurities with superconductors generally gives rise to Yu-Shiba-Rusinov (YSR) bound states. Using first-principles, we study the case of Mn impurities deposited on a superconducting Ta (110) surface. We explore both the orbital nature and amplitude of the induced YSR states while investigating their spatial extent, which is characterized by an oscillatory and anisotropic behavior as function of distance with respect to the Mn impurities.In particular, we study the interplay of intrinsic electronic structure properties of the hosting superconductor and that of the impurities, which impacts the resulting "cloud" of YSR states.

We employ the Kohn-Sham Bogoliubov-de Gennes method within the all-electron full-potential relativistic Korringa-Kohn-Rostoker Green function method [1] interfaced with the AiiDA infrastructure for high-throughput automation [2].

TT 11.23 Mon 15:00 P4

Stochastic resonance realized with a superconducting magnetic impurity state — •Philipp Maier[1], Björn Kubala[1,2], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University — [2]German Aerospace Center (DLR), Ulm

The phenomenon of stochastic resonance was originally studied in the context of climatic changes and has since been observed in a variety of systems, both classical and quantum. Here, we employ this phenomenon to infer the rates of tunneling processes in the course of quantum electronic transport [1,2]. We theoretically investigate the emergence of stochastic resonance in superconducting junctions, focusing on a system where one electrode hosts a Yu-Shiba-Rusinov state – a discrete bound state within the superconducting gap induced by the magnetic exchange interaction between a magnetic impurity and its superconducting host. Applying the framework of full counting statistics, we demonstrate that stochastic resonance manifests as the reduction of the Fano factor and a resonance of the tunneling current. The frequency of the resonance reveals information about the rate of microscopic electronic processes, e.g. the process responsible for quasiparticle-occupation parity breaking.
[1] M. Hänze et al., Sci. Adv. 7 (2021)
[2] T. Wagner et al., Nat. Phys. 15 (2019)

TT 11.24 Mon 15:00 P4

Dynamical simulations of single photon detection in superconducting nanowires — •Carlos Alberto Diaz Lopez[1], Joachim Ankerhold[1], Björn Kubala[1,2], and Ciprian Padurariu[1] — [1]Institute of Complex Quantum Systems, University of Ulm, Ulm, Germany — [2]German Aerospace Center (DLR), Ulm, Germany

We use a Python simulation package py-TDGL [1] based on modified Ginzburg-Landau theory [2] to simulate the dynamics of the superconducting condensate in a thin nanowire during the detection of a single-photon. The detection event is modeled phenomenologically as a hot-spot formation: the photon is modeled as an initially localized increase in the electronic temperature, with a Gaussian spatial profile that diffuses outwards while also dissipating in time. Our simulations successfully reproduce the characteristic time-dependent voltage peaks measured in superconducting nanowire single-photon detectors, while providing an accompanying movie-like dynamics of the superconducting order parameter. We propose a method to enhance the prominence of the voltage peaks by optimizing the applied DC current and the intensity of an externally-applied perpendicular magnetic field, with the goal of enabling the detection of single-photons in a broader frequency spectrum.
[1] L.Bishop-Van Horn, Comput.Phys.Commun**291**, 108799 (2023).
[2] L. Kramer, R. J. Watts-Tobin, Phys. Rev. Lett. **40**, 1041 (1978).

TT 11.25 Mon 15:00 P4

Simulations of heating effects in dual Shapiro step circuits — •Matthias Meiring, Fabian Kaap, Sergey Lotkhov, and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig

So-called dual Shapiro steps are quantised current steps separated by $2ef$, with e the elementary charge and f the rf drive frequency. They have recently gained renewed interest due to successful experimental demonstrations [1,2,3]. These dual Shapiro steps could bear the potential for a novel quantum current standard. Our measurements of dual Shapiro steps in an Al/AlO_x/Al dc-SQUID connected to a circuit made of high-kinetic-inductance granular aluminium and high-ohmic oxidised titanium revealed an electron temperature, which is substantially higher compared to the case without rf drive. We evaluate thermal heating phenomena in the measured chip layout and present adapted circuit designs, which should reduce heating effects and enhance the step size. Achieving this will lead to more prominent dual Shapiro steps and could thus pave the way to a new quantum current standard based on superconducting circuits.
[1] R.S.Shaikhaidarov et al., Nature 608 (2022).
[2] N. Crescini et al., Nat. Phys. 19 (2023).
[3] F. Kaap et al., Nat. Commun. 15 (2024).

TT 11.26 Mon 15:00 P4

Broadband kinetic inductance of high impedance superconductors — •Jan Pusskeiler[1], Martin Dressel[1], Thomas Valentin[2], Ameya Nambisan[2], Simon Geisert[2], Ioan Pop[1,2], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Physikalisches Institut and IQMT, KIT

Kinetic inductance quantifies the intrinsic phase-shifted electrodynamics of superconductors and lies at the heart of superconducting quantum electronics operating at microwave frequencies. Determining the complex impedance Z of disordered and granular superconductors in a frequency range from 10 kHz to 20 GHz using a broadband Corbino reflectometer allows direct observation of the kinetic inductance as a linear contribution to the reactance, $\mathrm{Im}(Z) = L_{\mathrm{kin}} \cdot \omega$. By obtaining the broadband kinetic inductance at temperatures deep in the superconducting state, from 1.15 K up to the critical temperature T_c, we can extrapolate the zero-temperature kinetic inductance.

We study granular aluminum as a high-kinetic inductance superconductor featuring a superconducting dome in the low-temperature phase diagram as a function of normal-state resistivity ρ_{dc}. We report kinetic inductances ranging from 20 pH/sq to 2 nH/sq for granular aluminum thin films with resistivities between 120 $\mu\Omega$cm and 6100 $\mu\Omega$cm. We calculate the superfluid stiffness and observe a $1/\rho_{\mathrm{dc}}$ dependance, as also reported in [1]. Furthermore, we observe absorption features that we interpret as signatures of collective modes of the superfluid condensate.

[1] U. S. Pracht *et al.*, Phys. Rev. B **93**, 100503(R) (2016)

TT 11.27 Mon 15:00 P4

Characterization of photoresists for deep UV direct writing lithography — •Niels Fiedler[1], Andreas Reifenberger[1], Lukas Münch[1], Alexander Stoll[1], Ludwig Hoibl[2], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kirchhoff Institute for Physics, Heidelberg University — [2]Heidelberg Instruments Mikrotechnik GmbH

Photoresists are integral to the precise pattern transfer processes required for fabricating micro- and nanoscale devices. The structuring of photoresists with optical maskless lithography systems has proven to be extremely versatile and efficient in research and development. Within the framework of the SuperLSI project, Heidelberg Instruments is developing a maskless lithographic platform incorporating a 266 nm Deep UV optical system, designed to achieve patterning resolutions as fine as 200 nm. Identification and thorough characterization of photoresists compatible with the lithographic platform is required. We focus on the performance of a positive (DuPont UV5-0.6) and negative (micro resist technology ma-N 2405) photoresist for the fabrication of superconducting sub-500 nm features. Structural fidelity, etch resistance, and developer compatibility with superconducting materials, such as niobium and aluminum, are evaluated. Achieving reduced linewidths advances quantum sensors like SQUIDs by enabling smaller Josephson junctions (JJs). Initial results for cross-type JJs with areas below 1 μm^2 highlight the potential of optical maskless lithography for flexible wafer-scale fabrication of superconducting devices.

TT 11.28 Mon 15:00 P4

Chemical-mechanical polishing process for the fabrication of cross-type Nb/Al-AlOx/Nb Josephson tunnel junctions — •A. Stoll, N. Fiedler, L. Münch, D. Hengstler, A. Reifenberger, A. Fleischmann, and C. Enss — KIP, Heidelberg University

Josephson tunnel junctions (JJs) are the basic elements of many superconducting electronic devices such as qubits or superconducting quantum interference devices (SQUIDs). Since many applications demand numerous JJs, a reliable wafer-scale fabrication process yielding reproducible, high-quality junctions is essential.

We present the microfabrication process of cross-type Nb/Al-AlOx/Nb Josephson tunnel junctions, emphasizing chemical-mechanical polishing (CMP) for planarization within SiO_2. A layer of SiO_2 is deposited over the structured trilayer, and CMP is used to polish away excess SiO_2, resulting in a planar, smooth, and uniform surface that enhances the accuracy and reliability of the junctions. Quality checks were conducted on junctions of various sizes, as well as the influence of support-like structures around junctions, to evaluate performance and scalability. Electrical characterizations demonstrate high-quality superconducting properties, validating the efficacy of CMP in the planarization of Josephson junction trilayers

This method enhances the scalability and integration of Josephson junctions in complex superconducting circuits, contributing to advancements in quantum computing and superconducting electronics.

TT 11.29 Mon 15:00 P4

High-quality niobium Josephson junctions for superconducting mm-wave qubits — •Urs Strobel[1], Benedict Rothmund[1], Lucas Radke[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut for Quantum Materials and Technologies (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Millimeter-wave quantum circuits require a superconductor with an energy gap above 100 GHz , which exceeds the energy gap of the widely used aluminum. Niobium offers much more suitable properties in this frequency range. Implemented in thin film technology on low loss substrates, high quality niobium Josephson junctions should complement the capacitors and inductors required for quantum circuits. We have developed Nb/Al-AlO_x/Nb trilayer Josephson junctions suitable for quantum circuits and characterized them at cryogenic temperatures. We present dc and mm-wave measurement data obtained with these junctions. In addition, we discuss design considerations for prospective mm-wave transmon qubits.

TT 11.30 Mon 15:00 P4

Building a Quantum Wheatstone Bridge — •Thilo Krumrey[1], Alex Kreuzer[1], Hossam Tohamy[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]IQMT, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Today's qubits, while still quite noisy, are sufficiently coherent for non-computing applications. We are exploring the possibility of using an arrangement of superconducting qubits to study the quantum version of the Wheatstone resistance bridge[1]. It would allow for comparative measurements of coupling energies using the interference of an excitation gradient across strongly coupled qubits. We propose an implementation of a quantum Wheatstone bridge using superconducting quantum circuits with quarton flux qubits. Here, the large positive anharmonicity and the tunability [2] of the operating frequency are beneficial for our application. We will present circuit simulations results based on the proposed design and compare them with measurements of the circuit at mK temperatures.

[1] K. Poulsen *et al.*, PRL **128**, 240401 (2022).
[2] F. Yan *et al.*, arXiv:2006.04130v1.

TT 11.31 Mon 15:00 P4

Charge Sensitivity of a Quantum Phase Slip Transistor — •Marius Frohn[1], Jan Nicolas Voss[1], Hannes Rotzinger[1,2], and Alexey Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Quantenmaterialien und Technologien (IQMT), Karlrsruher Institut für Technologie, Karlsruhe, Germany

Superconducting quantum phase slip (QPS) devices are high-impedance circuits that are promising for quantum sensing applications or the realisation of a current standard. For example, the QPS transistor is a dual circuit to the SQUID and is therefore sensitive to charge rather than flux. We study QPS transistors fabricated from two strongly coupled granular aluminium nanowires. This allows us to use intrinsic electromigration[1] to fine-tune the Coulomb blockade voltage in situ. The current-voltage characteristics at different gate biases and wire resistances provide insight into the charge sensitivity and operating range of the QPS transistor. We present the results of experiments on superconducting nanowire circuits at mK temperatures.

[1] J. N. Voss, Y. Schön, M. Wildermuth, D. Dorer, J. H. Cole, H. Rotzinger and A. V. Ustinov, ACS Nano **15** (2021)

TT 11.32 Mon 15:00 P4

Characterization of Nb Air Bridges for Superconducting Quantum Computing — •Amanda Scoles[1,2], Niklas Bruckmoser[1,2], Leon Koch[1,2], Ivan Tsitsilin[1,2], David Bunch[1,2], Julius Feigl[1,2], Lea Richard[1,2], Vera Bader[1,2], Lasse Södergren[1,2], Christian Schneider[1,2], and Stefan Filipp[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany

Superconducting qubits are a promising platform for the realization of practical quantum computing. The short gate times, comparatively long lifetimes, and relatively straightforward fabrication process, when compared to other systems, indicate an encouraging future for superconducting quantum circuits. Nevertheless, further optimization of both the fabrication and calibration processes is necessary to fully realize the potential of this platform. In particular, there is a need to enhance qubit coherence, reliability and scalability, which are the current main limitations of this technology.

In this work we investigate Nb air bridges, which provide flexibility in routing of control lines and facilitate the scaling of qubit numbers in planar geometries. We investigate the optimal fabrication parameters in order to maximize the yield of such structures. Additionally, we assess the quality factors of superconducting resonators in the vicinity of air bridges as well as daisy chains of air bridges, to determine the additional loss induced by the air bridge process.

TT 11.33 Mon 15:00 P4

Chiral High-Fidelity State Transfer with Thouless Pumping in Superconducting Circuits — •Lukas Vetter[1,2], Federico Roy[1,2], Jacquelin Luneau[1,2], João H Romeiro[1,2], Max Werninghaus[1,2], Christian MF Schneider[1,2], Peter Rabl[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Scienes, Department of Physics — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften

Efficient and robust techniques for state transfer and entanglement generation are vital for the progress of quantum technologies. Thouless pumping enables the topologically protected chiral transfer of excitations in quantum systems, however, dispersion during the protocol leads to losses in transfer fidelity. Here, we introduce a protocol for high-fidelity state transfer based on Thouless Pumping with Bloch Oscillations to suppress dispersion. Our protocol enables the transfer of single and multi-excitation Fock states and Bell states with high fidelity while being robust against perturbations of the Hamiltonian. We describe the effect of Bloch Oscillations using semi-classical equations of motion and show that changing the pumping cycle enables the generation of distant Bell pairs. We experimentally implement our results on a superconducting qubit device by realizing the pumping on a tunable coupler architecture. Our work paves the way for using Thouless pumping in quantum information processing, with applications in topologically robust entanglement generation and multi-qubit gates.

We acknowledge financial support from GeQCoS, MUNIQC-SC, MCQST, OpenSuperQPlus100, and the Munich Quantum Valley.

TT 11.34 Mon 15:00 P4

Vacuum Correlations in Superconducting Quantum Circuits — •Gesa Dünnweber[1,2,3] and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

When the quantum vacuum is subjected to time-varying boundary conditions, its inherent fluctuations can be parametrically amplified to create photonic excitations. This phenomenon, known as the dynamical Casimir effect, has been experimentally realized in superconducting quantum devices. Building on these results, we theoretically investigate the correlations induced in such circuits by quantum vacuum interactions. In particular, we analyze a system featuring controlled time-dependence across multiple components and consider potential technological applications.

TT 11.35 Mon 15:00 P4

Gate tunable superconductivity in Al/STO hybrid structures — •Jay Schmidt, Simon Reinhardt, Matthias Kronseder, Nicola Paradiso, and Christoph Strunk — Deptartment of Exp. and Appl. Physics, University of Regensburg, Germany

We present a systematic study on the gate-tunable superconducting properties of Al thin films epitaxially deposited on STO substrates. As a quantum paraelectric, STO exhibits an exceptionally high $\varepsilon \approx 7000$, enabling substantial charge modulation at the Al/STO interface. Metal deposition on STO induces oxygen vacancy formation within the substrate, contributing double electron donors that create an interface 2DEG. Based on measurements of the Hall-effect we extract charge carrier densities in the Al/STO system that are comparable to those in pristine Al films and significantly surpass those observed in LAO/STO 2DEGs. This finding indicates that charge transport is predominantly mediated by Al carriers. $T_C(n)$ and $B_C(T, n)$ exhibit strong tunability under an applied gate voltage with variations up to 15% and 50%, respectively. Notably, the observed T_C values ($\approx$ 0.92 - 1.06 K) are lower than those of pristine Al thin films ($\approx$ 1.4 K) but exceed those of STO, suggesting a bilayer system of superconductors with distinct gap energies coupled through proximity effects. We further investigate the superfluid stiffness, which turns out to be also highly gate-tunable with variations up to 15%. These results underline the potential of Al/STO heterostructures as a versatile platform for studying tunable superconducting phenomena.

TT 11.36 Mon 15:00 P4

Design of a Gate Tunable $\lambda/4$ Josephson Parametric Amplifier in an Al/InAs Hybrid Superconductor/Semiconductor Heterostructure — •Vjeko Dimić[1], Simon Feyrer[1], Alexander Kirchner[1], Giorgio Biasiol[2], Christoph Strunk[1], and Leandro Tosi[1,3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]CNR-Istituto Officina dei Materiali Laboratorio TASC, Italy — [3]Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Argentina

We present the design of a Josephson parametric amplifier based on a distributed $\lambda/4$ microwave resonator fabricated on a hybrid Al/InAs heterostructure. The 2DEG hosted in the InAs is used to tailor SNS junctions which terminate the resonator and can be tuned using an electrostatic gate deposited on top [1]. We characterize the microwave response of $\lambda/4$ resonators, the losses and the tunability of the resonance frequency resulting from the gate modulation of the Josephson inductance. We show how amplification can be obtained by pumping the gate electrode at twice the resonance frequency.

[1] W. Strickland et al., Phys. Rev. Appl. 19, 034021 (2023).

TT 11.37 Mon 15:00 P4

Design of granular aluminum based kinetic inductance traveling wave parametric amplifiers — Daniel Valenzuela, Christoph Kissling, •Victor Gaydamachenko, Fabian Kaap, Sergey Lotkhov, and Lukas Grünhaupt — Physikalisch-Technische Bundensanstalt, Bundesallee 100, 38116 Braunschweig

Superconducting traveling wave parametric amplifiers (TWPA) are a key ingredient in readout chains, which benefit greatly from lowest possible added noise and several GHz of bandwidth. In the case of kinetic inductance based TWPAs (KI-TWPA), the non-linear kinetic inductance of disordered superconducting thin films is used to enable three- and four-wave mixing processes for signal amplification. A key challenge for the design of KI-TWPAs is to ensure an impedance of 50 Ohm. In addition, unwanted frequency conversion processes have to be phase mismatched, while those generating amplification need to be retained. We tackle both challenges using so-called artificial coplanar waveguides with a multiperiodic capacitance variation. Here, we discuss the design of granular aluminum (grAl) KI-TWPA, our fabrication and process, and show initial experimental results.

TT 11.38 Mon 15:00 P4

Advanced Josephson travelling wave parametric amplifyer analysis with non-linear circuit simulations — •Lars Aaron Anhalt[1,2,3], Daniil Bazulin[1,2], Gleb Krylov[1,2], Yongjie Yuan[4], Diego Contreras[1,2,3], Christian Gnandt[1,2,3], Michael Haider[4], Kirill Fedorov[1,2,5], and Stefan Filipp[1,2,5] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]School of Natural Sciences, Technical University of Munich, 85748 Garching — [3]Ludwig-Maximilians-Universität in Munich, 80539 Munich — [4]TUM School of Computation, Information and Technology, Technical University of Munich, 85748 Garching — [5]Munich Center for Quantum Science and Technology, 80799 Munich

Broadband, quantum-limited microwave amplifiers are crucial for efficient and fast readout, which enables scaling of superconducting quantum processors. Josephson travelling wave parametric amplifiers (JTWPAs) are the most common solution in the field, providing amplification via copropagation of a pump tone with a signal in a nonlinear medium composed of Josephson junctions. Unwanted conversion processes, as well as stringent requirements on the fabrication processes, still pose challenges to their successful implementation. Here, we demonstrate how circuit simulation with WRSpice can help with the interpretation of experimental measurements of particular JTWPA designs and facilitate further improvements. Our simulations prove to be applicable to a wide range of circuit designs and varying parameters, reproducing competing conversion processes that go beyond analytical results from commonly used coupled mode equations.

TT 11.39 Mon 15:00 P4

Observing measurement-induced transitions in a transmon qudit — •Philippe Gigon[1,2], Zihao Wang[3], Benjamin D'Anjou[1], Alexandre Blais[1], and Machiel Blok[3] — [1]Université de Sherbrooke — [2]Walther-Meißner-Institut — [3]University of Rochester

Numerous experiments have shown that high-power dispersive transmon readout can lead to unexpected state transitions. Significant theoretical efforts have been made to describe these transitions using a simplified model, avoiding the need to account for the full Lindbladian dynamics of the coupled resonator-transmon system [1,2,3,4]. In this study, we employ a semi-classical effective drive model combined with Floquet theory and compare its predictions with experimental results from a transmon qudit. The high controllability and the readout capabilities of the qudit make it the perfect tool to study measurement-induced transitions. Our findings reveal that the semi-classical model accurately predicts critical photon numbers, identifies the states involved in the transitions, and quantifies the affected population.

[1] D. Sank et al., Phys. Rev. Lett. 117, 190503 (2016).
[2] M. Khezri et al., Phys. Rev. Appl. 20, 054008 (2023).
[3] R. Shillito et al., Phys. Rev. Appl. 18, 034031 (2022).
[4] M. F. Dumas et al., Phys. Rev. X 14, 041023 (2024).

TT 11.40 Mon 15:00 P4

Collective behavior of qubits coupled to a common wave-guide — •Johannes Friedrich[1,2], Gerhard Huber[1,2], Joan Agustí[1,2], Gesa Dünnweber[1,2], Christian Schneider[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften

The behavior of multiple qubits coupled to a common waveguide cannot be understood as the additive behavior of single qubits. Since the waveguide can mediate an all-to-all interaction between qubits via propagating photons, collective radiant states, such as superradiant, subradiant, and twilight states, can be

formed [1,2]. Using superconducting qubits offers control over multiple system parameters such as individual qubit frequency, coupling and spacing and enables the realization of 1D waveguides with large coupling to decoherence ratios, parameters difficult to achieve in atomic systems. Here, we explore parameter regimes beyond time and spatial uniform couplings, providing insights into designing quantum devices with controllable radiative properties.

We acknowledge financial support from GeQCoS, MUNIQC-SC, MC-QST, OpenSuperQPlus100, the Munich Quantum Valley and the Deutsche Forschungsgemeinschaft.

[1] Y. Ke, et al., Phys. Rev. Lett. 123, 253601 (2019).
[2] B. Kannan et al., Nature 583 (2020).

TT 11.41 Mon 15:00 P4

Design of fluxonium qubits inductively coupled to granular aluminum based readout resonators — •Li-Wei Chang, Asen Georgiev, Fabian Kaap, Sergey Lotkhov, Mark Bieler, and Lukas Gruenhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The fluxonium qubit is a specific type of superconducting qubit, which has garnered significant interest due to its coherence time in the milli-second range, high gate fidelities on the order of 99.9%, and a large anharmonicity up to several GHz. Recent years have also seen a surge in material studies related to this type of qubit, with a particular focus on high kinetic inductance materials such as granular aluminum (grAl). Three basic components form a fluxonium qubit: a Josephson junction, a capacitor, and a so-called superinductor with an impedance larger than the resistance quantum $R_Q = \hbar/4e^2$. We discuss our circuit parameters chosen via numerical simulations to implement a fluxonium with a transition frequency of 0.6 GHz ~ 12 GHz depending on the external magnetic field. To enable dispersive readout, we employ a granular aluminum based readout resonator. This configuration not only provides substantial inductance but also allows inductive coupling to the qubit. We present our methodology to design the circuit parameters, including the dispersive shift, quality factor, and T1 Purcell decay

TT 11.42 Mon 15:00 P4

Understanding loss channels in fluxonium qubits through high-impedance LC resonators — •Matthias Zetzl[1,2,3], Johannes Schirk[1,2,3], Florian Wallner[1,2,3], Ivan Tsitsilin[1,2,3], Niklas Bruckmoser[1,2,3], Christian Schneider[1,2,3], and Stefan Filipp[1,2,3] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Munich, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Current quantum systems based on superconducting qubits are limited by their rate of information loss. Therefore, identifying and mitigating the sources of decoherence of individual qubits is key to improve the performance of these systems. Here, we investigate loss mechanisms in Josephson junction arrays, which are commonly used to implement protected qubits such as "fluxonium" or "zero-pi" qubits. To probe these loss channels, we characterize high-impedance lumped-element LC resonators, comprised of two charge islands connected by a Josephson junction array. While this architecture closely resembles that of "fluxonium" qubits, it allows for a more straightforward characterization by direct transmission measurements of the resonators. By extracting the internal quality factor of the resonators, we can assess the fabrication quality of the junctions in a fast and efficient way, providing a useful tool for all junction based components.

TT 11.43 Mon 15:00 P4

dc-SQUIDs with distributed lossy lines to damp LC resonances — •Nicolas Kahne, Anna Ferring-Siebert, Daniel Hengstler, Fabian Krämer, David Mazibrada, Lukas Münch, Alexander Stoll, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

SQUIDs are sensitive superconducting magnetic flux to voltage converters, whose operation is based on the Josephson effect. In particular at mK temperatures this sensitivity can be degraded by LC-resonances in inductances and capacitances of different structures of the SQUID design. To damp the resonances and reduce their influence on the SQUID characteristics, lumped-element resistors are commonly placed into the SQUID circuitry, which need precise simulations to determine the appropriate resistance values and positions.
In this contribution we show results for a dc-SQUID with a new damping strategy, using lossy lines for the input coil and the feed lines. For the input coil we use a thin gold layer which is fabricated in a bilayer process underneath the superconducting coil. For the parallel pair feed lines, on the other hand, we damp inductively through large areas of gold on top which are galvanically decoupled by an insulating layer. We compare the different damping schemes for single dc-SQUIDs and two-stage dc-SQUID setups, regarding the resonance features in their SQUID characteristics and noise contributions. For future designs we also plan tests with SQUID-washers made of lossy lines.

TT 11.44 Mon 15:00 P4

Mapping Locations of Two Level Defects in Superconducting Quantum Circuits — •David Mazibrada[1], Johannes Schwenk[1], Jürgen Lisenfeld[1], Hannes Rotzinger[1,2], Philip Willke[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Institut for Quantum Materials and Technologies, 76131 Karlsruhe, Germany

The development of superconducting quantum circuits has drawn attention to the study of microscopic two-level systems (TLS), as they are a source of decoherence and instability of qubits. Individual TLS can be manipulated using microwave signals, but their specific locations in quantum circuits remain largely unclear. We intend to manipulate the TLS using the electric field of an atomic force microscope tip [1]. This approach should allow us to gain insights into the microscopic nature of the TLS. We will present the assembled atomic force microscope setup and show characterisation data of quantum circuits measured at millikelvin temperatures.

[1] M. Hegedüs, et al., arXiv:2408.16660v1 (2024)

TT 11.45 Mon 15:00 P4

Fully tunable C-shunted Flux Qubits for TLS Research — •Benedikt Berlitz[1], Alexey V. Ustinov[1,2], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, Karlsruhe Institute of Tech- nology (KIT), Karlsruhe, Germany — [2]IQMT, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Material defects forming two-level-systems (TLS) present a source of decoherence and unwanted degrees of freedom in superconducting quantum systems. The qubits in turn can be used as a tool to study the properties of TLS. We fabricated fully tunable, capacitively shunted superconducting flux qubits specifically to be used as TLS detectors, aiming for good coherence in a wide accessible qubit frequency range. The goal is to gather comparable data of many defects located within the same device. We describe design, fabrication and measurements of the fabricated samples. Studying TLS with these tools will enhance our understanding of the underlying physics of TLS in amorphous ma- terials and hopefully reveal a path to achieving higher coherence with superconducting qubits.

TT 11.46 Mon 15:00 P4

Identification of Noise Sources in Superconducting Microstructures — •Markus Renger, Anton Jarecka, Daniel Hengstler, Matthew Herbst, David Mazibrada, Lukas Münch, Andreas Reifenberger, Christian Ständer, Rui Yang, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

Improving the performance of superconducting devices often means identifying and eliminating different noise sources. Many noise sources are independent of the specific experimental set-up and transferable across many device categories such as qubits, SQUIDs, and superconducting detectors. We have constructed a stand-alone device with which we can analyze specific noise sources in a representative manner. This device consists of a Wheatstone-like bridge of four micro-fabricated superconducting inductors, two of which filled with sample material, and a pair of two-stage dc-SQUID read-out chains. We can use the method of cross-correlation, to derive the total noise contribution of our device, or AC-drive the Wheatstone bridge to measure the complex AC susceptibility of the sample material. Our experiments are performed at temperatures between $T = 20$ mK and $T = 800$ mK in the frequency range from $f = 100$ mHz to $f = 100$ kHz. We discuss the design of the experimental holder with excellent thermal coupling and shielding. We present the results of multiple measurements on thin films of SiO_2, Ag:Er, as well as Au:Er and perform a detailed comparison. In addition, we demonstrate our device's ability to probe the dynamics of magnetic moments in the sample material.

TT 11.47 Mon 15:00 P4

Dual Tone Spectroscopy of Atomic Tunneling Systems — •Jan Blickberndt, Anton Jarecka, Moritz Maur, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

Atomic Tunneling Systems (TSs) are intrinsic to disordered structures and thin films, inevitably impacting microstructured devices by causing noise and decoherence in all kinds of applications ranging from Josephson Junctions to cryogenic detector readout chains. Understanding the dynamics of these random fluctuators is essential to mitigate their deteriorative effects on superconducting quantum devices. To investigate the non-equilibrium dielectric behavior of TSs under electric bias, we developed a novel LC resonator setup based on a Wheatstone bridge design. This configuration features two resonance branches that share a common dielectric host material in their capacitors, thereby probing the exact same ensemble of TSs. By applying an external bias field via a cover electrode, we can modulate the energy states of the TSs, enabling their transition between the two resonance modes which allows us to explore ensemble properties as well as the non-linear dynamics of two-level systems. Our current experiments confirm the functionality of the device. To complement the experimental work, we developed a Monte Carlo simulation framework to validate and extend our findings.

TT 11.48 Mon 15:00 P4

Dynamic Control of Dielectric Loss in Amorphus Solids at Low Temperatures — •Marc Hyps, Christian Ständer, Jan Blickberndt, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

The main influence on the low temperature behaviour of amorphous solids is determined by atomic tunneling systems (TSs). TSs can be described by the phenomenological standard tunneling model (STM). The STM assums the TSs to be broadly distributed in their energy splitting. Experimental investigations of atomic tunneling systems gained recent interest due to their deteriorative effects in superconducting quantum devices, such as increased noise and decoherence. We use newly designed and microfabricated superconducting LC-resonator to study the dielectric rf-response of an amorphous sample in the presence of an electric bias field. The bias field is applied via an electrode placed above the resonator chip wich modifies the energy splitting of the TSs. With this setup we are able to prove the non-equillibrium Landau-Zener dynamics with two different measurement protocols. Aditionally we apply two symetrically detuned pump tones. These resulted in an inversion of the population difference between ground and exited state, hence gain. Also an additional loss contribution was found, hinting towards a coupling to nuclear quadrupol moments.

TT 11.49 Mon 15:00 P4

Enhancement of Low Temperature Dielectric Loss through Vibrational Bias — •Jonathan Herbrich, Christian Ständer, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

At low temperatures low energy excitations are present in amourphous solids, due to atomic tunneling systems (TSs), leading to different properties compared to their crystalline counterparts. These TSs can be expressed as two level systems with a flatly distributed energy splitting. These properties are well described by the phenomenological standard tunneling modell (STM). Due to their negative influence like noise and decoherance on superconducting quantum devices, these TSs are a subject of recent investigations.

Lately we investigated the dielectric rf-response of an amourphous sample while slowly varying an electric bias field. A microfabricated superconducting LC-resonator, using the sample as a substrate, was used for these measurements. In recent measurements a mechanical strain field was used instead of the electric one. The field is applied by bending the sample with a piezoelectric actuator. As a result, the energy splitting of the TSs is modified, as these couple to the strain field via the deformation potential. Our measurements can be described in a framework based on Landau-Zener transition, origianally developed for the description of electrically biased resonators.

TT 11.50 Mon 15:00 P4

Superconducting Qubits for Measurements with Infrared Photons — •Jonathan Huschle[1], Markus Griedel[1,2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institut for Technology (KIT) — [2]Institut for Quanten Materials and Technologies (IQMT), Karlsruhe Institut for Technology (KIT)

In superconductors, the impact of photons with energy higher than the energy gap leads to breaking of Cooper pairs, which increases noise level and introduces additional dissipation at microwave frequencies. The coherence of superconducting qubits is particularly sensitive to this influence and can be used as a detector. In the qBriqs project, we develop a setup and measurement protocol for far-infrared photons and identify the influence of broken Cooper pairs using a modified transmon qubit[1]. Here, the capacitance of the qubit is reduced, resulting in an increased charge noise sensitivity. We present the qubit design and measurements at mK temperatures.

[1] B. G. Christensen *et al.*, Phys. Rev. B 100, 140503 (2019).

TT 11.51 Mon 15:00 P4

Round Robin of the European "Metrology for Superconducting Qubits" (MetSuperQ) Project — •Paul Kugler — KIT, Karlsruhe, Deutschland

Project presentation: The MetSuperQ project addresses the urgent need for metrology support in superconducting circuits, a leading technology for practical quantum computers. The qubit round robin aims to enhance qubit coherence times by studying external influences through round robin measurements at multiple institutes and laboratory settings. This initiative will demonstrate qubit readout and benchmarking, disentangle intrinsic from external sources of decoherence, and raise awareness about the reliability of qubit characterization. By closing the gap in metrology support, this project paves the way for fault-tolerant quantum computers and their scalability.

TT 11.52 Mon 15:00 P4

Quantum Secret Sharing in Multipartite Microwave Networks — •Karolina Weber[1,2], Wun Kwan Yam[1,2], Simon Gandorfer[1,2], Florian Fesquet[1,2], Kedar E. Honasoge[1,2], Maria-Teresa Handschuh[1,2], Achim Marx[1], Rudolf Gross[1,2,3], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Quantum secret sharing (QSS) is a quantum cryptography scheme that provides an unconditionally secure way to exchange information in multipartite networks. Here, information about a secret quantum state is shared with n receivers, where the original secret state can be reconstructed if and only if a sufficient number of receivers collaborate. The remaining receivers do not acquire enough information for reconstruction, thereby protecting the secret state from losses, noise, or malicious conspiracies. We experimentally implement the QSS protocol with coherent states in a microwave network with $n = 3$ parties using continuous-variable entanglement and analyze the achieved reconstruction fidelities for different scenarios. We observe that the reconstruction fidelity with 2 collaborating parties exceeds the no-cloning limit, thus, proving the unconditional security of the QSS protocol. Finally, we consider an extension of this experiment towards sharing of qubit states and its applications to blind quantum computing.

TT 11.53 Mon 15:00 P4

Simulation of Non-Markovian Waveguide QED Systems with Tensor-Network Techniques — •Ze Xu — Walther-Meißner-Institute

The coupling of atoms or other two-level emitters to the quantized electromagnetic field is typically modeled using a Markovian master equation, which accounts for both dissipative and coherent photon-mediated interactions. However, this description breaks down in extended optical networks or slow-light waveguides, where significant propagation delays lead to strongly retarded, i.e., non-Markovian, interactions between the emitters. This regime of light-matter interactions remains largely unexplored due to the complexity of modeling non-Markovian effects in a fully quantized framework. In this poster, I will discuss the application of tensor-network techniques for simulating non-Markovian waveguide QED systems with strongly driven emitters, focusing specifically on the case of so-called giant atoms under critical coupling conditions.

TT 11.54 Mon 15:00 P4

Evaluating Spin Ensembles Based on Phosphorus Donors for Quantum Memory Applications — •Andreas Dunaev[1,2], Patricia Oehrl[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Solid-state spin ensembles show great potential for applications in quantum memory devices due to their long coherence times and compatibility with superconducting quantum circuits [1]. Crucial requirements for the application as a memory platform are that the stored information can be accessed and the storage capacity can actively be reset [2]. Here, we discuss an electron spin ensemble of phosphorus donors in silicon coupled to a superconducting resonator in this context. In detail, we present the characterization of this coupled system and demonstrate the storage of classical pulses using a Hahn-echo pulse sequence at temperatures of 4K, moderate magnetic fields, and GHz frequencies. In addition, we introduce the concept of an active reset of the spin ensemble using infrared light. We compare our findings to an input-output model.

[1] A. Morello *et al.*, Adv. Quantum Technol. **3**, 2000005 (2020)
[2] J. O'Sullivan *et al.*, Phys. Rev. X **12**, 041014 (2022)

TT 11.55 Mon 15:00 P4

Remote Cooling of Spin-ensembles through a Spin-mechanical Hybrid Interface — •Wang Yang[1], Durga Dasari[1], and Joerg Wrachtrup[1,2] — [1]3. Physikalisches Institut, ZAQuant, University of Stuttgart, Allmandring 13, 70569 Stuttgart, Germany — [2]Max Planck Institute for solid state research, Heisenbergstraße 1, 70569 Stuttgart, Germany

We present a protocol for the ground-state cooling of a tripartite hybrid quantum system, in which a macroscopic oscillator acts as a mediator between a single probe spin and a remote spin ensemble. In the presence of weak dispersive coupling between the spins and the oscillator, cooling of the oscillator and the ensemble spins can be achieved by exploiting the feedback from frequent measurements of the single probe spin. We explore the parameter regimes necessary to cool the ensemble, the oscillator, or both to their thermal ground states. This novel cooling protocol shows that, even with only weak dispersive coupling, energy transfer-like effects can be obtained by simply manipulating the probe spin. These results not only contribute to the development of a practical solution for cooling/polarizing large spin ensembles, but also provide a relatively simple means of tuning the dynamics of a hybrid system. The proposed protocol thus has broader implications for advancing various quantum technology applications, such as macroscopic quantum state generation and remote sensing.

TT 11.56 Mon 15:00 P4

Towards SQUID Optomechanical Devices based on $YBa_2Cu_3O_7$ — •Timo Märklin, Kenny Fohmann, Michael Schöllhorn, Mohamad El Kazouini, Christoph Schmid, Benedikt Wilde, Dieter Koelle, Reinhold Kleiner, and Daniel Bothner — Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany

Integrating a superconducting quantum interference device (SQUID) into a superconducting microwave resonator yields a circuit with a flux-tunable resonance frequency. By additionally releasing a part of the SQUID loop from the substrate such that it can oscillate mechanically, one obtains a SQUID optomechanical device in which microwave photons interact with phonons of the mechanical oscillator. If their interaction rate is sufficiently high, one can prepare non-classical states in the mechanical resonator which could build the foundation for experiments testing quantum gravity.

Today's standard material for superconducting frequency-tunable resonators is aluminum. However, the low critical field of aluminum in the range of some 10 mT severely limits the interaction rates achievable in SQUID optomechanical devices, as the interaction rate is directly proportional to an externally applied magnetic field. Therefore, we investigate the high-T_c superconductor $YBa_2Cu_3O_7$ (YBCO) regarding its suitability for SQUID optomechanics, since its high critical field beyond 10 T promises interaction rates higher than those achieved so far. This poster presents our recent progress along the path towards SQUID optomechanical devices based on YBCO.

TT 11.57 Mon 15:00 P4

Analysis of the Mechanical Properties of Nanomechanical String Resonators based on NbTiN — •Burak Bülbüloğlu[1,2], Korbinian Rubenbauer[1,2], Thomas Luschmann[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Opto- and electromechanical systems play an intricate part in the fields of quantum sensing and transduction. Aluminum (Al) is a popular material platform in the field of cavity-optomechanics due to its low internal loss rates at microwave frequencies and self-limiting oxide. However, the operation of Al is limited by its critical temperature ($T_c \approx 1.2\,K$ in the bulk). We explore Niobium Titanium Nitride (NbTiN) as an alternative candidate for opto- and electromechanical systems based on thin film technology. NbTiN has a T_c of up to 17 K in bulk and can be used as a material for planar superconducting microwave quantum circuits. Moreover, it has a higher critical current density compared to Al and, thus, can support a larger photon number or microwave drive power. Here, we present doubly-clamped NbTiN nanomechanical string resonators and investigate their mechanical properties. We find stress levels on par with annealed Al, positioning NbTiN strings as a promising platform for the implementation of nano-electromechanical circuits operating at elevated temperatures.

TT 11.58 Mon 15:00 P4

Cavity Optomechanics with a Carbon Nanotube Nanomechanical Resonator — •Katrin Burkert, Akong Loh, Furkan Özyigit, Fabian Stadler, Anton Weber, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Carbon nanotubes (CNTs) are the smallest and lightest nanomechanical resonators. Suspended between Ti/Au electrodes and gated, they can act simultaneously as beam resonators with large Q and as quantum dots. We have realized optomechanical coupling of a SWCNT nanomechanical resonator to a microwave cavity and quantified it through optomechanically induced transparency measurements [1,2]. The nonlinearity of Coulomb blockade in the CNT was exploited to significantly enhance the coupling strength, reaching $g_0 \sim 100$ Hz [1,2]; also back-action of the CNT on the microwave cavity has been demonstrated [1,2]. Ongoing work is directed towards strong coupling and ground state cooling of the nanomechanical resonator. This requires improvements of the microwave cavity [3] and the transfer assembly procedure. Suspended CNTs have been proposed as long-lived nano-electromechanical qubits [4], a topic of high current research interest [5].

[1] S. Blien et al., Nat. Commun. 11, 1636 (2020).
[2] N. Hüttner et al., PR Appl. 20, 064019 (2023).
[3] N. Kellner et al., PSSB 260, 2300187 (2023).
[4] F. Pistolesi et al., PRX 11, 031027 (2021).
[5] Y. Yang et al., Science 386, 783 (2024).

TT 11.59 Mon 15:00 P4

Dissipative Microwave Optomechanics with a Carbon Nanotube — •Anton Weber, Katrin Burkert, Akong Loh, Niklas Hüttner, and Andreas K. Hüttel — Institut for Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

High-frequency nanomechanical resonators are valuable for many measurement applications. We investigate a high quality factor mechanical resonator consisting of a suspended carbon nanotube. The nanotube is actuated by applying an external radiofrequency signal. Its motion can modulate its conductance, allowing for electrical detection [1]. In order to transfer this type of experiment from time-averged, dc measurement to fast GHz detection, the nanotube can be integrated into a microwave reflectometry setup at low temperature. A Quartz tuning-fork based carbon nanotube transfer is used to insert the bottom-up grown CNTs into the top-down designed circuit geometry [2]. The specific electronic and mechanical properties of CNTs require adaptation to the microwave circuit; a stub tuner, formed from coplanar waveguides (CPWs), is used for this purpose. They are particularly suitable for high impedance CNTs, as their resonant frequencies and impedance behavior can be precisely controlled by their geometry. The nanotube vibration modulates the signal reflection, effectively resulting in a dissipatively coupled microwave optomechanical system [3].

[1] G. A. Steele et al., Science 325, 5944 (2009).
[2] S. Blien et al., PSSB 255, 180018 (2018).
[3] F. Elste et al., Phys. Rev. Lett. 102, 207209 (2009).

TT 11.60 Mon 15:00 P4

Simulation model on the trigger time in superconducting single-photon detectors — •Tim Janocha, Someshvaran Udayakumar, Stefan Kaiser, and Riccardo Bassoli — Technische Universität Dresden, Dresden, Deutschland

Superconducting nanowire single-photon detectors (SNSPDs) are promising quantum communication devices due to their high efficiency, low dark count rates and minimal timing jitter. Here we present a simulation model on the trigger time between photon absorption and detection triggering. Within the framework of the proposed model, the influence of the photon energy, bias current, and strip width are investigated and their influence on the device performance is discussed.

TT 11.61 Mon 15:00 P4

Towards X-ray Spectroscopy with sub-eV Absolute Energy Calibration up to 100 keV — •A. Striebel, A. Abeln, A. Brunold, D. Kreuzberger, D. Unger, D. Hengstler, A. Reifenberger, A. Fleischmann, L. Gastaldo, and C. Enss — Kirchhoff Institute for Physics, Heidelberg University

Metallic magnetic calorimeters (MMCs) are energy-dispersive X-ray detectors which provide an excellent energy resolution over a large dynamic range combined with a very good linearity. MMCs convert the energy of each incident photon into a temperature pulse which is measured by a paramagnetic temperature sensor. The resulting change of magnetisation is read out by a SQUID magnetometer.

To investigate electron transitions in U^{90+} within the framework of the SPARC collaboration, we developed the 2-dimensional maXs-100 detector array. It features 8x8 pixels with a detection area of 1 cm^2, an absorber thickness of 50 μm, a photo efficiency of 18 % at 100 keV, an energy resolution of 40 eV at 60 keV and was successfully operated in a recent beamtime at CRYRING@FAIR. To increase the photo efficiency to above 35 % at 100 keV we develop a new maXs-100 detector with 100 μm thick absorbers.

Currently, the absolute energy calibration is limited not by the detector itself, but by the Struck SIS3316 analog-to-digital converter. We present a technique to precisely determine the ADCs' non-linearity using an Analog Devices EVAL-ADMX1002B ultra low-distortion sine wave generator. This allows to correct for the non-linearity. We discuss the effect of this correction on actual MMC spectra.

TT 11.62 Mon 15:00 P4

Towards Large-Area 256-Pixel MMC Arrays for High Resolution X-ray Spectroscopy — •Andreas Abeln, Daniel Hengstler, Daniel Kreuzberger, Andreas Reifenberger, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

Metallic Magnetic Calorimeters (MMCs) are energy-dispersive cryogenic particle detectors. Operated at temperatures below 50 mK, they provide very good energy resolution, high quantum efficiency as well as high linearity over a large energy range. In many precision experiments in X-ray spectroscopy the photon flux is small, thus a large active detection area is desirable. Therefore, we develop arrays with increasing number of pixels.

In this contribution we present a detector setup featuring a novel dense-packed 16 × 16 pixel MMC array. The pixels provide a total active area of 4 mm × 4 mm and are equipped with 5 μm thick absorbers made of gold. This ensures a stopping power of at least 50 % for photon energies up to 20 keV. The expected energy resolution is 1.4 eV (FWHM) at an operating temperature of 20 mK. For the cost-effective read-out of the 128 detector channels we envisage the flux-ramp multiplexing technique. We present first results of the detector characterization obtained utilizing parallel 2-stage dc-SQUID read-out chains. We discuss the detector performance, focusing on the thermal behavior within the detector as well as to the thermal bath.

TT 11.63 Mon 15:00 P4

MMC-Based Photon and Phonon Detector for Scintillating Crystals at mK **Temperatures** — •Ioana-Alexandra Nitu, Christian Enss, Andreas Fleischmann, Daniel Hengstler, Ashish Jadhav, Cagla Mahanoglu, Andreas Reifenberger, Christian Ritter, and Loredana Gastaldo — Kirchhoff Institute for Physics, Heidelberg University

Scintillating crystals at mK temperatures are used in the search for neutrinoless double beta decay ($0\nu\beta\beta$) and Dark Matter, because they provide the means to discern the interaction of heavy particles, such as α particles, from light ones, such as electrons. The discrimination is achieved by measuring the temperature increase of the crystal and the emitted light simultaneously. This approach is used in the AMoRE experiment where $LiMoO_4$ crystals are employed to search for $0\nu\beta\beta$.

We present the design concept of an integrated photon and phonon (P2) detector, based on low temperature metallic magnetic calorimeters (MMCs). This detector is to be microfabricated on a 3-inch Si wafer; the central wafer area is used for the detection of the scintillation light, while the outer area contains three double-meander MMC detectors to monitor temperature changes in the crystal. We pursue the optimisation of the design and discuss the challenges in the microfabrication of the photon and phonon detector. Preliminary results are presented and compared to the expected performance.

TT 11.64 Mon 15:00 P4

MMC-based X-ray Detector for Transitions in light Muonic Atoms — •Peter Wiedemann, Andreas Abeln, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, Daniel Hengstler, Daniel Kreuzberger, Andreas Reifenberger, Adrian Striebel, Daniel Unger, and Julian Wendel — for the QUARTET Collaboration, Kirchhoff Institute for Physics, Heidelberg University

High energy resolution X-ray spectroscopy of muonic atoms is used for the determination of charge nuclear radii. The QUARTET collaboration aims to improve the accuracy of nuclear charge radii of light elements from Li to Ne up to one order of magnitude by using Metallic Magnetic Calorimeter (MMC) arrays. These Detectors have already demonstrated excellent energy resolution and energy calibration with sub-ev prevision. We present the result obtained with the newly developed MMC array optimized to reach a quantum efficiency of 98% at 19 keV with 4 eV ΔE_{FWHM} We Discuss the performance achieved with this new MMC array at the light of precision X-ray spectroscopy of muonic lithium, beryllium and boron.

TT 11.65 Mon 15:00 P4

Towards Phonon Detection in Superfluid Helium with MMCs — •Axel Brunold, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

The search for light dark matter requires innovative detection techniques that can probe weakly interacting particles with exceptional sensitivity. One promising approach involves studying elastic scattering interactions between dark matter particles and helium atoms at millikelvin temperatures.

As part of the "Direct search Experiment for Light dark matter", DELight, a pilot experiment is conducted to investigate the behavior of metallic magnetic calorimeters (MMCs) submerged in liquid helium. MMCs have previously demonstrated the capability to detect photons with high energy resolution and linearity; this experiment seeks to explore how these properties translate to the detection of phonons. In this setup, a small copper cell (300 ml) is cooled to below 1 K within a ^{3}He/^{4}He dilution refrigerator and filled with ^{4}He. The liquid helium level, while filling and later on operating the MMC, is monitored with an LC circuit-based level meter. At these millikelvin temperatures, ^{4}He is deep in its superfluid phase, enabling a long mean free path for phonons and rotons. A resistive heater is used to excite phonons, which are then collected by an MMC on a 5 mm x 5 mm silicon substrate. This contribution presents the setup and first results.

TT 11.66 Mon 15:00 P4

MOCCA: A 4k-pixel Molecule Camera for the Position and Energy Resolved Detection of Neutral Molecule Fragments — •Abdullah Özkara[1], Christian Enss[1], Andreas Fleischmann[1], Lisa Gamer[2], Loredana Gastaldo[1], Daniel Hengstler[1], Christopher Jakob[2], Daniel Kreuzberger[1], Ansgar Lowack[1], Oldřich Novotnỳ[2], Andreas Reifenberger[1], Dennis Schulz[1], and Andreas Wolf[2] — [1]Kirchhoff Institute for Physics, Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg

The MOCCA detector is a 4k-pixel high-resolution molecule camera based on metallic magnetic calorimeters and read-out with SQUIDs that is able to detect neutral molecule fragments with keV kinetic energies. It will be deployed at the Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg, a storage ring built to prepare and store molecular ions in their rotational and vibrational ground states, enabling studies on electron-ion interactions. To reconstruct the reaction kinematics, MOCCA measures the energy and position of the molecule fragments incidenting on the detector, even with multiple particles hitting the detector simultaneously.

For readout, the signals of the 64 pixels of each row are added up and a triggered pixel is identified by its unique signal decay time. Two pixel rows are connected to the same SQUID with opposite polarity. This allows the use of only 32 SQUID channels to read out all 4094 pixels of the detector. We present an improved readout scheme using an exponential decay time spacing. In addition, we compare simulations of this scheme to measured data.

TT 11.67 Mon 15:00 P4

Characterization of Ti/Au Bilayer at mK — •Martin Schwendele, Christian Enss, Andreas Fleischmann, Daniel Hengstler, Ashish Jadhav, Lukas Münch, Andreas Reifenberger, and Loredana Gastaldo — Kirchhoff Institute for Physics, Heidelberg University

Low temperature microcalorimeters reach high energy resolution in a wide energy range thanks to very sensitive thermometers. Magnetic penetration depth thermometers (MPTs) would represent a very interesting alternative with respect to commonly used metallic magnetic calorimeteres (MMCs) and transition edge sensors (TESs).

We present the study of Ti/Au bilayers, typically used in TES as sensible material for MPTs. Films with different ratios between the superconducting layer and the normal conducting layers have been produced using sputtering technique. We discuss the dependence of the transition temperature as a function of the thickness ratio as well as the estimation of the penetration depth as a function of temperature.

TT 12: Quantum Transport and Quantum Hall Effects (joint session HL/TT)

Time: Monday 16:45–18:15 Location: H15

TT 12.1 Mon 16:45 H15

kdotpy: A Python application for k·p band structure simulations of zincblende semiconductors — •Wouter Beugeling[1,2], Florian Bayer[1,2], Christian Berger[1,2], Jan Böttcher[3], Leonid Bovkun[1,2], Christopher Fuchs[1,2], Maximilian Hofer[1,2], Saquib Shamim[1,2], Moritz Siebert[1,2], Li-Xian Wang[1,2], Ewelina M. Hankiewicz[3], Tobias Kiessling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik (TP4), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The software project kdotpy aims at simulations of electronic band structures of semiconductor devices with k·p theory. The application implements the widely used Kane model, capable of reliable predictions of transport and optical properties for a large variety of topological and non-topological materials with a zincblende crystal structure.

In this presentation, I present the core functionality and features of kdotpy. I will explain how we have implemented principles of modern software engineering and good scientific practice in this project.

TT 12.2 Mon 17:00 H15

End states in zigzag Haldane model nanoribbons — Simone Traverso, Maura Sassetti, and •Niccolò Traverso Ziani — Physics Department, University of Genova, Italy

As topological materials based on the graphene lattice become experimentally realizable in materials such as germanene, the physics of the bound states that characterize them at step edges and in quasi one-dimensional settings becomes relevant.

In this context, the appearance of topological bound states in zigzag Haldane nanoribbons will be addressed [1]. A reentrant topological phase diagram is found. Together with numerical results, a low energy theory extending the Jackiw-Rebbi paradigm will be presented.

[1] S. Traverso, M.Sassetti, N. Traverso Ziani, NPJ Quantum Materials 9, 9 (2024).

TT 12.3 Mon 17:15 H15

Time-reversal invariant Chalker-Coddington model and the real-space renormalisation group — •Syl Shaw and Rudolf A. Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

The Chalker-Coddington model has been utilised to great success in understanding the plateau transitions in the quantum Hall effect. Since the model's incep-

tion, it has been extended to a time-reversal invariant symmetry class to describe the quantum-spin Hall effect. Here we adapt a real-space renormalisation group method[1] to respect time-reversal symmetry and use it investigate the phase diagram of the quantum-spin Hall effect. We aim to find distinct phases as a function of both saddle-point height, z and spin-mixing angle ϕ. At the phase boundary between insulator and metal, we compute the value of the critical exponent of the localisation length, ν, with the same real-space renormalisation technique. [1] S. Shaw, R. A. Römer Physica E 165, 116073 (2025)

TT 12.4 Mon 17:30 H15

Utilizing Silicon Qubit Devices for Quantum Electrical Metrology — •Dustin Wittbrodt[1], Johannes Christian Bayer[1], Lars Schreiber[2,3], Janne Lehtinen[4], Marcelo Jaime[1], and Frank Hohls[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]Forschungszentrum Juelich, Juelich, Germany — [4]SemiQon Technologies Oy, Espoo, Finland

The 2019 redefinition of the SI system established fixed values for fundamental constants such as the elementary charge (e) and the Planck constant (h), enabling the quantum realization of the units of Ampere, Volt, and Ohm. While the quantum realization of Volt and Ohm is well-established, the realization of the Ampere, whether directly through Single Electron Pumps (SEPs) or indirectly via the Volt and Ohm, has yet to achieve the same level of accuracy. Moreover, further device applications in practical circuits require paralelization approaches to achieve higher current outputs. The international project "Advanced Quantum Technology for Metrology of Electrical Currents" (AQuanTEC) aims to upscale SEPs beyond the 1 nA threshold. To achieve this, AQuanTEC explores several strategies, including the use of silicon devices first designed for spin qubit realization. These devices are highly promising due to their potential scalability, driven by ongoing advancements in integrating large numbers of qubits.

TT 12.5 Mon 17:45 H15

Surface state dominated transport in HgTe topological insulator devices — •Maximilian Hofer[1,2], Christopher Fuchs[1,2], Lena Fürst[1,2], Tobias Kiessling[1,2], Wouter Beugeling[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Topological Insulators, Am Hubland, 97074 Würzburg, Germany

Recently grown three dimensional topological insulators based on tensile strained HgTe exhibit an exceptionally high mobility and very low intrinsic carrier density. The high quality material has made it possible to study the Landau level dispersion at low magnetic fields and identify four distinct transport regimes. We demonstrate that while a contribution from the topological surface states to transport measurements is expected across the full experimentally accessible density range, there exists only a narrow density regime for which the electronic transport is exclusively carried by the topological surface states. We present the corresponding phase diagram for pure topological surface state transport depending on layer thickness and carrier concentration. For thick HgTe films grown pseudomorphically strained on CdTe, the total carrier density needs to be kept between 1.8×10^{11} cm^{-2} and 2.6×10^{11} cm^{-2} to remain in the pure surface state region and avoid contributions from bulk states. The experimental observations are supported by eight band $\boldsymbol{k} \cdot \boldsymbol{p}$ band structure calculations.

TT 12.6 Mon 18:00 H15

Designing a quantum sorter based on two-dimensional topological insulators — •Amanda Teodora Preda[1,2], Iulia Ghiu[2], Lucian Ion[2], Andrei Manolescu[3], and George Alexandru Nemnes[1,2] — [1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, Magurele- Ilfov, 077125, Romania — [2]University of Bucharest, Faculty of Physics, Atomistilor 405, Magurele-Ilfov, 077125, Romania — [3]Department of Engineering, Reykjavik University, Menntavegur 1, Reykjavik IS-102, Iceland

The idea of a quantum sorter emerged in quantum information, a field that aims to exploit quantum effects and manipulate qubits for information processing. In theory, it was proven that one can propose a universal quantum sorter for any arbitrary observable. To this point, suitable experimental schemes of implementation for this proposal were explored mainly in quantum optics. In our study, we introduce a solid-state version of a quantum sorter, based on a multi-terminal mesoscopic device with multiple output ports, that aims to separate the incoming states by both their spin and transversal mode. In order to maximize the state-separation efficiency of such a device, we chose to exploit the unique transport properties of topological insulators. Employing the tight-binding based simulation package Kwant, we modeled a device that meets the criteria of an irreversible quantum sorter, using the well-established BHZ Hamiltonian to simulate a multi-terminal quantum system made up of both trivial and topological materials.

TT 13: Focus Session: Magnetic Phenomena from Phonon Chirality and Angular Momentum II (joint session MA/TT)

The magnetic moment of the electron lies at the heart of magnetism and spintronics. However, recent research has unveiled the angular momentum and magnetic moment of chiral phonons as fundamental quantities in their own right. These chiral phonons give rise to a plethora of novel lattice phenomena analogous to electronic effects, such as the phonon Hall and phonon Zeeman effects. Moreover, they play a critical role in angular momentum transfer on ultrafast timescales, as seen in the Einstein-de Haas effect. Chiral phonons can also generate effective magnetic fields reaching the tesla scale, inducing magnetization in antiferromagnetic, paramagnetic, and even nonmagnetic materials - a phenomenon reminiscent of the Barnett effect. These advancements showcase phonon chirality and angular momentum as powerful emerging tools for generating and controlling magnetism. This focus session aims to highlight the latest breakthroughs in chiral-phonon magnetism and foster connections between the rapidly evolving field of chiral phononics and the broader magnetism research community.

Coordinators: Dominik M.Juraschek, Eindhoven University of Technology, d.m.juraschek@tue.nl; Martina Basini, ETH Zürich, m.basini@ethz.ch

Time: Tuesday 9:30–12:45 Location: H16

TT 13.1 Tue 9:30 H16

Continuous-wave terahertz spectroscopy on chiral phonons — •Ji Eun Lee, Luca Eisele, Artem Pronin, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

We apply continuous-wave frequency-domain terahertz spectroscopy to study chiral phonons at low frequencies. As samples, we use thin films of materials with soft phonon modes, such as SrTiO3 and (doped) PbTe. Our experimental method utilizes both, measurements of transmission with circular-polarized light and Faraday-rotation experiments. In the talk, our approach to the measurements and preliminary results will be summarized.

TT 13.2 Tue 9:45 H16

Spin-lattice coupling in multiscale modeling: from angular momentum transfer to chiral phonons — •Markus Weissenhofer[1,2], Philipp Rieger[1], Sergiy Mankovsky[3], Akashdeep Kamra[5], MS Mrudul[1], Hubert Ebert[3], Ulrich Nowak[4], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]Freie Universität Berlin, Berlin, Germany — [3]Ludwig Maximilian Universität, München, Germany — [4]Universität Konstanz, Konstanz, Germany — [5]Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Kaiserslautern, Germany

Transfer and manipulation of angular momentum is a key aspect in spintronics. Recently, it has been shown that angular momentum transfer between spins and lattice is possible on ultrashort timescales [1]. To contribute to the understanding of this transfer, we have developed a theoretical multiscale framework for spin-lattice coupling, which is linked to ab-initio calculations on the one hand and magnetoelastic continuum theory on the other [2], allowing for the study of a wide range of magnetomechanical phenomena. Here I will discuss how this framework can be used to calculate magnon-phonon coupling parameters, emphasizing the importance of a Dzyaloshinskii-Moriya type interaction for angular momentum transfer [2] and revealing the existence of chiral phonons in iron arising from a chirality-selective coupling [3]. [1] Tauchert al., Nature 602, 73 (2022); Luo et al., Science 382, 698 (2023). [2] Mankovsky et al., PRL 129, 067202 (2022); Weißenhofer et al., PRB 108, L060404 (2023). [3] Weißenhofer et al., arXiv:2411.03879.

TT 13.3 Tue 10:00 H16

Chiral phonon-induced magnetization reversal in 2D ferromagnets — •Daniel Bustamante Lopez[1] and Dominik Juraschek[2] — [1]Department of Physics, Boston University, Boston, Massachusetts 02215, USA — [2]Department of Applied Physics and Science Education, Eindhoven University of Technology, Eindhoven, Netherlands

In our previous work, we explored magnonic rectification, where a coherently excited chiral phonon generates an effective magnetic field capable of inducing quasistatic magnetization in antiferromagnetic materials. In this study, we extend this concept to ferromagnetic materials, demonstrating that phononic magnetic fields can achieve permanent magnetization reversal. We focus on two-dimensional chromium-based ferromagnetic crystals, including CrI3, CrGeTe3, and CrCl3, and investigate reversal mechanisms such as damping switching and precessional switching. Our findings reveal that phononic magnetic fields enable robust and permanent magnetization reversal within nanoseconds, highlighting their potential for ultrafast magnetic control.

TT 13.4 Tue 10:15 H16

Chiral phonons in coupled magnon-phonon band structure — •Yelyzaveta Borysenko, Daniel Schick, and Ulrich Nowak — University of Konstanz, Konstanz, Germany

Coupling of spin and lattice degrees of freedom in magnetic materials is a key aspect for angular momentum based information processing. During ultrafast demagnetization, spin angular momentum can be transferred into the lattice creating chiral phonons even in simple centrosymmetric materials [1]. Spin-lattice coupling mechanisms involved in such processes can be approached using first principles calculations, which allow to determine leading energy terms for angular momentum exchange for different materials [2, 3]. Coupled spin-lattice dynamics is then described constructing angular momentum-conserving Hamiltonian linked to ab initio calculated model parameters [4].

Here, we linearize the equations of motion and calculate coupled magnon-phonon dispersions. We discuss how different coupling terms, e.g., of anisotropy or Dzyaloshiskii-Moriya type, can modify magnon and phonon dispersions, open up energy gaps, lift the degeneracy of modes, and lead to avoided crossings in the band structure.

[1] S. R. Tauchert et al., Nature 602, 73 (2022); [2] S. Mankovsky et. al., Phys. Rev. Lett. 129, 067202 (2022); [3] J. Hellsvik et al., Phys. Rev. B 99, 104302 (2019); [4] M. Weißenhofer et al., Phys. Rev. B 108, L060404 (2023)

TT 13.5 Tue 10:30 H16

Phonon Inverse Faraday effect from electron-phonon coupling — •Natalia Shabala and Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

The phonon inverse Faraday effect describes the emergence of a DC magnetization due to circularly polarized phonons. From time-dependent second order perturbation theory and electron-phonon coupling we develop a microscopic formalism for phonon inverse Faraday effect. We arrive at a general and material-independent equation [1]. Using this equation for ferroelectric soft mode in $SrTiO_3$ gives an estimate of effective magnetic field which is consistent with recent experiments [2]. Hence, our approach is promising for shedding light into the microscopic mechanism of angular momentum transfer between ionic and electronic angular momentum, which is expected to play a central role in the phononic manipulation of magnetism.

[1] N. Shabala and R. M. Geilhufe, Accepted to PRL, arXiv:2405.09538, 2024
[2] M. Basini et al., Nature 628, 534 (2024)

TT 13.6 Tue 10:45 H16

Temperature dependent magnon-phonon coupling in YIG/GGG heterostructures — •J. Weber[1,2], M. Cherkasskii[3], F. Engelhardt[3,4,5], S.T.B. Goennenwein[6], S.Viola Kusminskiy[3,5], S. Geprägs[1], R. Gross[1,2,7], M. Althammer[1,2], and H. Huebl[1,2,7] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Munich, Germany — [3]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [4]Department of Physics, University Erlangen-Nuremberg, Erlangen, Germany — [5]Max Planck Institute for the Science of Light, Erlangen, Germany — [6]Department of Physics, University of Konstanz, Germany — [7]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Magnon-phonon coupling in heterostructures has recently gained interest in the context of angular momentum conversion and angular momentum transport via phonons. A typical experimental setting is a bilayer system, where the magnetization dynamics of a magnetic thin film interacts with the elastic standing wave excitations of a non-magnetic bulk crystal. So far, bulk acoustic wave resonators consisting of a ferrimagnetic yttrium iron garnet (YIG) film deposited on a crystalline gadolinium gallium garnet (GGG) substrate have been studied at room temperature due to the favorable magnetic damping properties of YIG [1]. We present a temperature dependent analysis of the magnon-phonon coupling of a YIG/GGG bulk acoustic wave resonator.

[1] K. An et al., Phys. Rev. B **101**, 060407, (2020).

15 min. break

TT 13.7 Tue 11:15 H16

Modeling of the preparation and conservation of coherent phonon (pseudo) angular momentum — •Olga Minakova[1], Maximilian Frenzel[1], Carolina Paiva[2], Joanna M. Urban[1], Michael S. Spencer[1], Martin Wolf[1], Dominik M. Juraschek[2,3], and Sebastian F. Maehrlein[1,4,5] — [1]FHI Berlin — [2]Tel Aviv University — [3]Eindhoven University of Technology — [4]HZDR — [5]TU Dresden

The angular momentum of lattice vibrations - phonon angular momentum - is an underexplored degree of freedom in solid-state systems. Recent experiments have shown that circularly-polarized THz pulses can coherently excite degenerate phonon modes, enabling the preparation of phonon angular momentum states. THz-Kerr effect spectroscopy provides a means to monitor these states by directly measuring vectorial phonon trajectories. To interpret such experiments, it is essential to understand the symmetry properties of the phonon modes that influence the driving and probing processes, as well as the conservation of angular momentum in the crystal lattice. Here, we model the generation and detection of coherent phonon angular momentum, revealing how crystal symmetry dictates the selection rules in the lattice. We show that the form of the Raman tensors associated with the phonon explains the phonon helicity observed in experiments, linking the discrete rotational symmetry of the material to the conservation of pseudo angular momentum in lattice vibrations.

TT 13.8 Tue 11:30 H16

Spin-spin interaction via chiral phonons — •Daniel Schick[1], Markus Weissenhofer[2,3], Akashdeep Kamra[4], and Ulrich Nowak[1] — [1]University of Konstanz, Konstanz, Germany — [2]Uppsala University, Uppsala, Sweden — [3]Free University of Berlin, Berlin, Germany — [4]University of Kaiserslautern-Landau, Kaiserslautern, Germany

Coupling between the magnetic degrees of freedom and phonons has emerged as a topic of great importance for explaining various magnetic phenomena, like ultrafast demagnetization processes [1], and the possibility to affect magnetization dynamics via phonon pumping [2]. We develop a tool to study spin-lattice coupling in atomistic simulations, which conserves total angular momentum. This allows us to precisely retrace the transfer of angular momentum between the spin and lattice systems. We demonstrate the emergence of an effective spin-spin interaction mediated by chiral phonons. This effect can arise from thermal phonons as follows. A spin may precess after coupling to a phonon, with this precession producing chiral phonons, which in turn, affect other spins. A similar effect can be achieved by driving a spin to induce chiral phonons. We discuss the dependence of this interaction on the temperature and strength of the spin-lattice interaction and discuss our findings within the context of phonon-enhanced magnon transport phenomena.

[1] S. R. Tauchert, et. al., Nature **602**, 73 (2022)
[2] R.Schlitz et. al. Phys. Rev. B **106**, 014407 (2022)

TT 13.9 Tue 11:45 H16

Ultrafast generation of multicolor chiral phonons in magnetic and ferroelectric materials — •Omer Yaniv[1] and Dominik M. Juraschek[2] — [1]Tel Aviv University, Tel Aviv, Israel — [2]Eindhoven University of Technology, Eindhoven, Netherlands

Terahertz pulses are powerful tools capable of initiating coherent vibrational motions in solids. Circularly polarized pulses can further excite chiral phonons. Such phonons carry an angular momentum and are able to generate magnetic moments leading to a varying range of phenomena, including the phonon Hall, phonon Zeeman, and phonon inverse Faraday effects. Our study investigates the coherent driving of phonons using multicolor laser pulses, leading to Lissajous trajectories of the atoms. We demonstrate the generation of such multicolor chiral phonons in BaTiO3, a task that presents significant challenges due to the requirement of an exact 1:2 phonon frequency ratio. Achieving this precise ratio is crucial for the generation of closed atomic Lissajous loops. However, we overcome this challenge by creating phonon polaritons with shifted frequencies through the use of optical cavities. This approach allows us to surpass the limitations imposed by the strict phonon frequency ratio. By carefully tuning the cavity parameters, we demonstrate a new pathway for controlling lattice vibrations at ultrafast timescales. We also explore how multicolor phonons tune magnetic properties in monolayer CrI3, a 2D material with strong spin-orbit coupling and ferromagnetism. By manipulating phonon dynamics, we examine the interaction between lattice vibrations and magnetic order.

TT 13.10 Tue 12:00 H16

Chiral Phonons induced by Magnon-Phonon Coupling — •Hannah Bendin[1], Alexander Mook[2], Ingrid Mertig[1], and Robin R. Neumann[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Johannes Gutenberg University, Mainz, Germany

Chiral phonons, the quasiparticles of circularly polarized lattice vibrations, have recently been investigated due to a range of emerging phenomena. Notably, chiral phonons carry nonzero angular momentum. However, the systems in which they occur still require extensive research. Chiral phonons may, for example, be

found in lattices with broken inversion symmetry. Alternatively, they can be induced by the coupling to magnons, the quasiparticles of spin excitations, thereby lifting time-reversal symmetry.

Here, we analyze how magnetoelastic coupling gives rise to magnon-phonon hybridization, which, in turn, generates phonon angular momentum. Conversely, we show how the phonon angular momentum and the spin of the magnons affects their coupling strength. This interplay between magnons and chiral phonons allows for the tunability of the phonon angular momentum.

TT 13.11 Tue 12:15 H16

Ultrafast laser-induced carrier and magnetization dynamics in $SrTiO_3$ from real-time time-dependent DFT — •Andri Darmawan, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Recent experimental studies indicate electric-field-driven ferroelectricity [1] and multiferroicity [2] in the paradigmatic nonmagnetic band insulator $SrTiO_3$ in the terahertz regime. Following a comprehensive study of the optical [3] and x-ray absorption [4] spectra including quasiparticle and excitonic effects, here we explore the response of $SrTiO_3$ to laser excitation. Using real-time time-dependent density functional theory (RT-TDDFT) as implemented in the Elk code, we investigate both linear and circular polarized laser pulses. A complex site- and orbital-dependent temporal dynamics is observed with opposite sign of fluctuations at O and Ti sites and charge transfer from O $2p$ to Ti $3d$ states for linearly polarized light, that breaks dynamically inversion symmetry. Notably, circularly polarized pulses induce a finite transient magnetic moment which is absent for linearly polarized pulses. Funding by DFG within CRC1242 (project C02) and computational time at magnitUDE, amplitUDE and the Leibniz Supercomputer Center (project pr87ro) are gratefully acknowledged.

[1] T.F. Nova et al., Science 364, 1075 (2019)

[2] M. Basini et al., Nature 628, 534 (2024)

[3] V. Begum, M.E. Gruner and R. Pentcheva, Phys. Rev. Mater. 3, 065004 (2019)

[4] V. Begum-Hudde et al., Phys. Rev. Res. 5, 013199 (2023)

TT 13.12 Tue 12:30 H16

Phonon pumping in ferromagnet/nonmagnetic insulator hybrid systems — •Richard Schlitz[1], Luise Holder[1], Johannes Weber[2,3], Mikhail Cherkasskii[4], Fabian Engelhardt[4], Julie Střihavková[5], Matthias Althammer[2,3], Silvia V. Kusminskiy[4,6], Hans Huebl[2,3,7], and Sebastian T. B. Goennenwein[1] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Walther-Meißner-Institut, BAdW, Garching, Germany — [3]School of Natural Sciences, TUM, Garching, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [5]Faculty of Mathematics and Physics, Charles University, Prague — [6]Max Planck Institute for the Science of Light, Erlangen, Germany — [7]Munich Center for Quantum Science and Technology, München, Germany

In ferromagnetic thin films, magnetization dynamics, e.g., driven by ferromagnetic resonance, can coherently couple to phonons. If a ferromagnetic film is deposited on a crystalline substrate with polished parallel faces, the sample stack forms a bulk acoustic resonator, leading to characteristic modifications of the magnetic resonance signal.

In this work, we show that the magnetoelastic coupling can mediate the hybridization of the coherent magnetization dynamics with longitudinal and transverse phonons, with a particular dependence on the orientation of the magnetic field. We extract the magnetoelastic coupling parameters and compare them with theoretical expectations. Our results show that both longitudinal and transverse phonons can be efficiently excited, depending on the magnetic field orientation.

TT 14: Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)

Time: Tuesday 9:30–13:15 Location: H18

TT 14.1 Tue 9:30 H18

Topological orbital Hall effect caused by skyrmions and antiferromagnetic skyrmions — •Lennart Schimpf, Ingrid Mertig, and Börge Göbel — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The topological Hall effect is a hallmark of topologically non-trivial magnetic textures such as magnetic skyrmions. It quantifies the transverse electric current once an electric field is applied and occurs as a consequence of the emergent magnetic field of the skyrmion. Likewise, an orbital magnetization is generated. Here we show that the charge currents are orbital polarized even though the conduction electrons couple to the skyrmion texture via their spin [1]. The topological Hall effect is accompanied by a topological orbital Hall effect even for s electrons without spin-orbit coupling. As we show, antiferromagnetic skyrmions and antiferromagnetic bimerons that have a compensated emergent field [2], exhibit a topological orbital Hall conductivity that is not accompanied by charge transport and can be orders of magnitude larger than the topological spin Hall conductivity.

[1] B. Göbel, L. Schimpf, I. Mertig, arXiv pre-print: 2410.00820

[2] B. Göbel, I. Mertig, O. Tretiakov, Physics Reports 895, 1 (2021)

TT 14.2 Tue 9:45 H18

Optimization of orbital torques in ferrimagnets and their relationship with Gilbert damping — •shilei ding, william legrand, hanchen wang, mingu kang, paul noel, and pietro gambardella — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Application of an electric field can induce a non-equilibrium orbital angular momentum in conductive materials whose electronic bands have a k-dependent orbital character. This phenomenon can lead to the current-induced accumulation of orbital momenta in nonmagnetic layers, which can then diffuse into neighboring magnetic layers and interact with the local magnetization through spin-orbit coupling, giving rise to orbital torques. Conversely, the excitation of spin precession in a magnetic layer can give rise to an orbital current, resulting in orbital pumping and dissipation of angular momentum in the nonmagnetic layer. In the first part, I will present the efficacy of converting orbital to spin momenta in ferrimagnetic materials, specifically in the RE-TM ferrimagnet GdyCo100-y. This work underscores the mechanisms that facilitate orbital-to-spin conversion within a magnetic layer at the atomic level. In the second part, I will discuss how the Gilbert damping parameter correlates to spin and orbital torques in magnetic layers adjacent to Pt and CuOx layers, respectively. I will show that CoFe/CuOx bilayers exhibit a favorable combination of efficient orbital torque and minimal increase in Gilbert damping, which is promising for the implementation of orbital torque oscillators with reduced damping compared to spin torque oscillators.

TT 14.3 Tue 10:00 H18

Orbital magnetoresistance in insulating antiferromagnets — •Christin Schmitt[1], Sachin Krishnia[1], Edgar Galíndez Ruales[1], Takashi Kikkawa[2], Duc Tran[1], Timo Kuschel[1], Eiji Saitoh[2], Yuriy Mokrousov[1,3], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, 55128 Mainz, Germany — [2]Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Insulating antiferromagnetic and ferrimagnetic materials are promising candidates for spintronic devices due to their intrinsic properties such as low damping [1]. Recently, orbital angular momentum (OAM) has emerged as a crucial concept in condensed-matter physics. Theoretical and experimental studies have highlighted that the orbital Hall effect (OHE) can enable orbital currents with efficiency orders of magnitude higher than that of spin Hall effects [2]. Here, we investigate magneto-resistance effects in magnetic systems [2,3]. We find that in TmIG the transverse magnetoresistance signal is increased significantly upon replacing Pt, a spin-current generator, by Cu*, a pure orbital-current generator. Further, we explore antiferromagnets with orbital magnetoresistance effects as pure orbital current is crucial for next generation pure orbitronics devices using abundant, cheap and environmentally friendly materials. [1] R. Lebrun, et al., Nature, 561, 222-225 (2018). [2] S. Ding, et al., Phys. Rev. Lett. 125, 177201 (2020). [3] S. Ding et al., Phys. Rev. Lett. 128, 067201 (2022).

TT 14.4 Tue 10:15 H18

Non-reciprocity in magnon mediated charge-spin-orbital current interconversion — •Sachin Krishnia[1], Omar Ledesma-Martin[1], Edgar Galindez-Ruales[1], Felix Fuhrmann[1], Duc Tran[1], Rahul Gupta[1], Marcel Gasser[1,2], Dongwook Go[1,2], Gerhard Jakob[1], Yuriy Mokrousov[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In magnetic systems, angular momentum is carried by the spin and orbital degrees of freedom. Non-local devices can be used to study angular momentum transport. They consist of parallel heavy-metal nanowires placed on top of magnetic insulators like yttrium iron garnet (YIG), facilitating the transmission of information by magnons, generated by the accumulation of spin at the interface, created via the spin Hall effect (SHE) and detected via the inverse SHE (iSHE). It has been demonstrated that these processes have comparable efficiencies when the role of the detector and injector is reversed, which points to reciprocity of the processes. However, we show that by adding Ru as a source of direct and inverse orbital Hall effect (OHE), the system no longer exhibits this reciprocity. Specifically, the generation of magnons via the combination of SHE and OHE

and detection via the iSHE is found to be about 35% more efficient than the inverse process for our system [1]. [1] O. Ledesma et al., arXiv:2411.07044 (2024).

TT 14.5 Tue 10:30 H18

Detection of dynamic x-ray magnetic linear dichroism in NiO — •Timo Kuschel[1], Johannes Demir[1], Olga Kuschel[2], Joachim Wollschläger[2], and Christoph Klewe[3] — [1]Bielefeld University, Germany — [2]Osnabrück University, Germany — [3]Advanced Light Source (ALS), Berkeley, USA

Spin transport through thin antiferromagnetic layers such as NiO has been studied by ferromagnetic resonance (FMR) spin pumping [1], spin Seebeck effect [2], non-local magnon spin transport [3] and x-ray detected FMR (XFMR) [4]. In all these experiments, the spin current has been identified in an adjacent Pt layer [1-3] or FeCo film [4] via inverse spin Hall effect or dynamic x-ray magnetic *circular* dichroism, respectively, after having the NiO layer already passed.

In this contribution, we study Fe_3O_4/NiO/Pt [5] by XFMR and present the identification of dynamic x-ray magnetic *linear* dichroism (XMLD) [6] at the Ni L edges directly in the NiO layer for FMR spin pumping in the adjacent Fe_3O_4 layer. We will analyze the XFMR response depending on the NiO thickness. Further, we will discuss coupling phenomena at the NiO-Fe_3O_4 interface vs. spin transport through the NiO layer as the origin of the dynamic XMLD response.

[1] H. L. Wang et al., Phys. Rev. Lett. 113, 097202 (2014)
[2] W. Lin et al., Phys. Rev. Lett. 116, 186601 (2016)
[3] G. R. Hoogeboom et al., Phys. Rev. B 103, 144406 (2021)
[4] M. Dabrowski et al., Phys. Rev. Lett. 124, 217201 (2020)
[5] L. Baldrati et al., Phys. Rev. B 98, 014409 (2018)
[6] C. Klewe et al., New J. Phys. 24, 013030 (2022)

TT 14.6 Tue 10:45 H18

Manipulating the sign of the interlayer exchange coupling — •Nathan Walker — The Open University, Milton Keynes, UK

We demonstrate, using computer simulations and a non-equilibrium Greens function approach, that the sign of the out-of-equilibrium interlayer exchange coupling (ooeIEC) changes in the presence of an external bias. The system consists of a double barrier connected to an exchange coupled ferromagnetic trilayer. We find a strongly non-linear dependence of the spin current on voltage which results in the exchange coupled tri-layer switching between parallel and antiparallel configurations. Our results are in excellent agreement with earlier theoretical calculations, which predict an approximately 2π topological phase change of the (equilibrium) IEC. We believe that this could act as an energy efficient mechanism for magnetic switching which does not rely on spin-transfer torque (STT). There are potential applications to magnetoresistive random-access memory (MRAM), one of the principal contenders for a universal memory.

TT 14.7 Tue 11:00 H18

Harnessing Orbital Hall Effect in Spin-Orbit Torque MRAM — •J. Omar Ledesma Martin[1,2], Rahul Gupta[1], Chloé Bouard[2], Fabian Kammerbauer[1], Iryna Kononenko[1], Sylvain Martin[2], Gerhard Jakob[1,3], Marc Drouard[2], and Mathias Kläui[1,3] — [1]1 Institute of Physics, Johannes Gutenberg University Mainz, 55099, Mainz, Germany — [2]Staudingerweg 7 — [3]Department of Physics, Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491, Trondheim, Norway

There is considerable potential in the Orbital Hall Effect (OHE) and the Spin Hall Effect (SHE) as electrical means for controlling the magnetization of spintronic devices. Here Ru stands out exhibiting an orbital Hall conductivity four times greater than the spin Hall conductivity of Pt. [1] This work assesses the efficiency of four distinct stacks in devices with perpendicular Magnetic Tunnel Junctions (MTJ). Following the formula Ta/OHE/Pt/[Co/Ni]x3/Co/MgO/CoFeB/Ta/Ru, where the OHE materials are Ru, Nb, and Cr. Additionally, a sample with Pt instead of OHE serves as a reference. The results demonstrate an improvement for the Ru samples, exhibiting higher damping-like torque and significantly lower switching current density compared to both the other samples and the Pt reference. These findings, including first-principle calculations, underscore the potential of Ru as an OHE material for enhancing the performance and power consumption of spintronic devices.

[1] R. Gupta et al., arXiv:2404.02821 (2024). Nature Comm. In press (2024)

15 min. break

TT 14.8 Tue 11:30 H18

Spin and orbital Hall effect in metal systems: extrinsic vs. intrinsic contributions — •Sergiy Mankovsky and Hubert Ebert — LMU of Munich, 81377 Munich, Germany

Kubo's linear response formalism has been used to study the orbital Hall effect (OHE) for non-magnetic undoped and doped metallic systems, focusing on the impact of different types of disorder. Corresponding first-principles calculations of the orbital Hall conductivity (OHC) were performed making use of the KKR Green function method that allows in particular to monitor the impact of the vertex corrections on the OHC. The doping- and temperature-dependence of the OHC have been investigated and compared with corresponding results for the spin Hall conductivity (SHC). The temperature dependent properties of the OHC and SHC determined by thermally induced lattice vibrations (in non-magnetic materials) and spin fluctuations (in magnetic systems) have been accounted for making use of the alloy analogy model. For elemental systems at finite temperature a dominating role of the intrinsic contribution to the temperature-dependent OH and SH conductivities is found. In contrast, the OH and SH conductivities of doped systems at low temperatures are dominated by the SOC-driven extrinsic contributions strongly decreasing at higher temperatures due to the increasing impact of the electron-phonon scattering.

TT 14.9 Tue 11:45 H18

Simulations of spin transport in YIG — •Ben Schwanewedel, Moumita Kundu, and Ulrich Konstanz — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Being synthesized first in 1957, YIG has the lowest Gilbert damping among all known materials. This makes it interesting for spintronic applications and long-range spin transport. In YIG's complex unit cell Fe atoms occupy 20 sublattices leading to 20 magnon bands between 0 and 25 THz. We develop an atomistic spin model for YIG based on exchange interactions from Ref. [1], which were determined through neutron scattering. Further parameters were adapted from Ref. [2]. We varify our study through investigation of the magnon dispersion and comparing it to the results of Ref. [1].

We use atomistic spin dynamics simulations for the model above based on the stochastic Landau-Lifshitz-Gilbert equation to unravel its spin dynamics and spin transport properties. The spin transport is triggered by thermal gradients and and local magnetic fields and it is analyzed using an observable which is proportional to the magnon population. Also, magnon dispersions far from equilibrium are evaluated and discussed.

[1] Princep, Andrew J., et al. "The full magnon spectrum of yttrium iron garnet." npj Quantum Materials 2.1 (2017): 63.

[2] Barker, Joseph, and Gerrit EW Bauer. "Thermal spin dynamics of yttrium iron garnet." Physical review letters 117.21 (2016): 217201.

TT 14.10 Tue 12:00 H18

Orbital Hall effect accompanying quantum Hall effect — •Börge Göbel and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

The quantum Hall effect emerges when two-dimensional samples are subjected to strong magnetic fields at low temperatures: Topologically protected edge states cause a quantized Hall conductivity in multiples of e^2/h. Here we show that the quantum Hall effect is accompanied by an orbital Hall effect [1]. Our quantum mechanical calculations fit well the semiclassical interpretation in terms of "skipping orbits". The chiral edge states of a quantum Hall system are orbital polarized akin to an orbital version of the quantum anomalous Hall effect in magnetic systems. The orbital Hall resistivity scales quadratically with the magnetic field making it the dominant effect at high fields.

The discussion can be generalized to systems with effective magnetic fields: The topological Hall effect caused by the emergent field of topological spin textures, such as magnetic skyrmions, is accompanied by an orbital Hall effect, as well [2].

[1] B. Göbel, I. Mertig, Phys. Rev. Lett. 133, 146301 (2024)
[2] B. Göbel, L. Schimpf, I. Mertig, arXiv pre-print: 2410.00820

TT 14.11 Tue 12:15 H18

Large Spin Hall Angle in Mn-based Antiferromagnetic Alloys — •Nabil Menai[1], Martin Gradhand[2], and Derek Stewart[3] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, BS8-1TL, UK — [2]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [3]Western Digital Research Center, San Jose, California 95119, USA

Antiferromagnets (AFMs) have emerged as crucial materials for spintronic technologies for their ability to host spin-dependent transport phenomena, despite their zero net magnetization. Their robustness against external magnetic fields and ultrafast spin dynamics make them ideal for efficient spin-charge interconversion. In this theoretical study, we use density functional theory and Greens function methods to investigate the transport properties of Mn-based binary alloyed AFMs. Our focus is on the total spin Hall conductivity (SHC), accounting for both the intrinsic contributions from Berry curvature and the extrinsic effects from skew scattering and side-jump mechanisms. The objective is to identify AFM materials that exhibits a high spin Hall angle (SHA); with an efficient charge-to-spin Hall current conversion ratio. Our results reveal that doping MnPt with Ir significantly enhances the SHA, achieving a value of 8% at room temperature. In contrast, doping with Pd offers temperature stability with lower SHA values. Additionally, we examine the effects of substituting Mn atoms with magnetic transition metals such as Fe and Ni. These findings underscore the potential of antiferromagnetic alloys for efficient spin current generation.

TT 14.12 Tue 12:30 H18

Competing ordinary and Hanle magnetoresistance in Pt and Ti thin films — •Sebastian Sailler[1], Giacomo Sala[2], Denise Reustlen[1], Richard Schlitz[1], Min-Gu Kang[2], Pietro Gambardella[2], Sebastian T.B. Goennenwein[1], and Michaela Lammel[1] — [1]Department of Physics, University of Konstanz — [2]Department of Materials, ETH Zurich

One of the key elements in spintronics research is the spin Hall effect, allowing to generate spin currents from charge currents. A large spin Hall effect is observed in materials with strong spin orbit coupling, e.g. Pt. Recent research suggests the existence of an orbital Hall effect, the orbital analogue to the spin Hall effect, which also arises in weakly spin orbit coupled materials like Ti, Mn or Cr. In any of these materials, a magnetic field perpendicular to the spin or orbital accumulation leads to additional Hanle dephasing and thereby the Hanle magnetoresistance. Here, we studied the magnetoresistance (MR) of Pt thin films over a wide range of thicknesses. Careful evaluation shows that the MR of our textured samples is dominated by the so-called ordinary MR, while the Hanle effect does not play a significant role. Analyzing the intrinsic properties of Pt films deposited by different groups, we find that next to the resistivity, also the structural properties of the film influence which MR dominates. We further show that this correlation can also be found in orbital Hall active materials like Ti. We conclude that in all materials exhibiting a spin or orbital Hall effect, the Hanle MR and the ordinary MR coexist, and that the sample's purity and crystallinity determines which MR dominates.

TT 14.13 Tue 12:45 H18

Orbital Hanle magnetoresistance in Mn thin films — •Min-Gu Kang, Federica Nasr, Giacomo Sala, and Pietro Gambardella — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Momentum-space orbital texture, or orbital character of electrons, enables the orbital Hall effect (OHE), a current-induced flow of nonequilibrium orbital angular momentum in centrosymmetric systems with negligible spin-orbit coupling. This orbital current, which can be orders of magnitude larger than its spin counterpart, offers transformative potential for spin-orbitronics, yet the mechanisms of orbital relaxation remain unclear. In this work, we present temperature-dependent orbital Hanle magnetoresistance and associated orbital relaxation mechanisms in Mn thin films. The results clearly show that the orbital Hanle magnetoresistance depends on the structure of the Mn thin films and can be associated with competing Dyakonov-Perel and Elliott-Yafet orbital relaxation effects. Our study highlights the critical role of orbital relaxation in determining the magnitude of current-induced orbital effects in 3d transition metal films.

TT 14.14 Tue 13:00 H18

Tuning of spin transport properties in 2D ferromagnet VSe_2 by structural polytypes of TaS_2 electrodes — •Biplab Sanyal and Masoumeh Davoudiniya — Department of Physics & Astronomy, Ångströmlaboratoriet, Uppsala University, Box-516, 75120 Uppsala, Sweden

2D magnets and their heterostructures are promising materials for future spintronic applications. Here, we present a study of spin transport through a ferromagnetic monolayer of 1T-VSe_2 with two structural polytypes of TaS_2 electrodes stacked in van der Waals heterostructures. Using density functional theory coupled with the nonequilibrium Green function framework, we explore the impact of TaS_2 electrode polytypes on the device's quantum transport properties. We observe that devices with 1T-TaS_2 electrodes exhibit higher spin-dependent transmission compared to 2H-TaS_2 electrodes. Incorporating MoS_2 as a tunnel barrier, anisotropic tunnel magnetoresistance enhances significantly, reaching 168% for the 1T-device and 1419% for the 2H-device. Spin-transfer torque (STT) analysis shows that its magnitude is highest at 90° (−702 μeV/V for 1T and −1561 μeV/V for 2H devices) and decreases towards 180°. The 1T-device shows superior performance with lower Gilbert damping, reduced critical current density and voltage for magnetization switching, compared to the 2H-device, which requires significantly higher current and voltage. Our predictions reveal the potential of 1T-VSe_2-based heterostructures for advanced spintronic applications.

TT 15: Quantum Coherence and Quantum Information Systems (joint session TT/DY)

Time: Tuesday 9:30–13:15 Location: H31

Invited Talk TT 15.1 Tue 9:30 H31

Solving Many-Body Problems on Quantum Computers — •Benedikt Fauseweh — TU Dortmund University, Otto-Hahn-Str 4, 44227 Dortmund

In this talk, I will provide an overview on the state-of-the art in digital quantum simulations (DQS) for many-body systems [1]. Modern quantum computers present challenges due to the noisy nature of these systems. Novel quantum algorithms, especially hybrid classical-quantum algorithms [2], have been developed to fit the specifications of such devices. For DQS, the prevailing question today is: What problems are amenable to be simulated on noisy quantum computers? I will discuss recent work on simulating quantum many-body dynamics [3], algorithmic advances to detect ground state phase transitions and the potential of stabilizing exotic non-equilibrium phases of matter, e.g., discrete time crystals [4], using quantum-classical feedback.

[1] B. Fauseweh, Nat. Comm. 15, 2123 (2024).
[2] B. Fauseweh and J.-X. Zhu, Quantum 7, 1063 (2023).
[3] B. Fauseweh and J.-X. Zhu, Quantum Inf. Process. 20, 138 (2021).
[4] G. Camacho and B. Fauseweh, Phys. Rev. Res. 6, 033092 (2024).

TT 15.2 Tue 10:00 H31

Fast Initialisation of Bell States in Kerr Cat Qubits — •Miriam Resch[1], Ciprian Padurariu[1], Björn Kubala[1,2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

Schrödinger cat states play an important role for applications in continuous variable quantum information technologies. As macroscopic superpositions they are inherently protected against certain types of noise making cat qubits a promising candidate for quantum computing [1]. It has been shown recently that cat states occur naturally in driven Kerr parametric oscillators (KPOs) as degenerate ground states with even and odd parity that are adiabatically connected to the respective Fock states by switching off the drive [2]. To perform operations with several cat qubits one crucial task is to create entanglement between them. This can be done by initializing the cats from entangled Fock states or by performing operations directly in cat space. Here we show efficient transformations of multi mode cat states through adiabatic and diabatic switching between Kerr-type Hamiltonians with degenerate ground state manifolds and show how those transformations can be used to directly initialize the cat states as entangled Bell states.

[1] Réglade et al., Nature 629, 778 (2024);
[2] Puri et al., npj Quantum Inf. 3, 18 (2017).

TT 15.3 Tue 10:15 H31

Impurity models in waveguide QED — •Adrian Paul Misselwitz[1,2,3], Jacquelin Luneau[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

In this talk I will discuss photonic impurity models, which emerge from the coupling of two-level atoms to a 1D photonic waveguide in the presence of strong photon-photon interactions. Such models appear, for example, in the context of superconducting microwave circuits, where Josephson junctions give rise to strong Kerr-nonlinearities at the few-photon level. In this case, the resulting competition between photon-photon repulsion and the attractive atom-photon interaction leads to the formation of localized bound states with a well-defined photon number and, under certain conditions, the build-up of long-range, algebraically decaying correlations between the impurity sites. I will show how these strongly-correlated phases of light and matter can be simulated efficiently with the help of large-scale tensor network simulations and discuss a possible explanation of the observed long-range correlations in terms of a simpler, effective Bose-Hubbard model.

TT 15.4 Tue 10:30 H31

Voltage without current — Christina Koliofoti and •Roman-Pascal Riwar — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Superconductors famously give rise to equilibrium currents without voltages. But can the converse exist? We argue that voltage-dependent Josephson effects generically provide exactly such a classical time crystal behaviour – bringing with them known conceptual issues, such as discontinuous "brick-wall" trajectories, and ill-defined canonical quantization. With the example of quantum phase slip junctions in the presence of electro-motive forces, we resolve these lingering problems. Decoherence provokes a phase transition from a quantum Hamiltonian (non-Lagrangian) system with nonlinear Cooper-pair tunneling to a Lagrangian (non-Hamiltonian) classical time crystal. Our work illustrates that direct canonical quantization of low-energy theories may fail, and that the nonadiabaticity of brick-wall trajectories leads to a temporary break down of the classical theory even for strong decoherence.

TT 15.5 Tue 10:45 H31

Of gyrators and anyons I - Anyons — •Oleksiy Kashuba, Ram Mummadavarapu, and Roman-Pascal Riwar — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

In recent years there have emerged various ideas to create and control topological excitations in superconducting devices. Notably, nontrivial Chern bands were predicted to exist in conventional multiterminal Josephson junctions, but the Chern number is yet to be experimentally verified, and the pathway towards feasible quantum hardware applications is unclear. In this talk, we show how generic multiterminal circuits can be expressed as gyrator networks with quantized gyration conductance, giving rise to anyonic excitations carrying q/p fractional fluxes (q, p integer), measurable via a fractional Aharonov-Casher phase. We further present concepts for error correction protocols, and quantum simulations of interacting fermionic (or generally anyonic) many-body systems—notably, introducing the possibility to mimic fractional quantum Hall physics or to implement local fermionic models that explicitly break the Wigner superselection rule. The latter indicates that a full understanding of multiterminal circuits will require grappling with a virtually unexplored class of parity-breaking quantum field theories.

TT 15.6 Tue 11:00 H31

Of gyrators and anyons II - Gyrators — •Ram Mummadavarapu, Oleksiy Kashuba, and Roman-Pascal Riwar — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

In recent years, significant progress has been made in developing methods to create and control topological excitations in superconducting devices. Among these, the prediction of nontrivial Chern bands in conventional multiterminal Josephson junctions stands out as a particularly promising development. However, despite theoretical predictions, the experimental verification of the nontrivial Chern number remains an open challenge. Based on the realization that multiterminal junctions generically map on special gyrator networks hosting anyons (see also talk "Of gyrators and anyons I"), we here present circuit-specific band-engineering techniques to minimize parasitic anyon interactions. We show in particular how circular scattering in three-terminal quantum dot chains gives rise to a flat topological ground state, where disorder mitigates Chern number fluctuations and the quasiparticle continuum provides a work-around for known limitations to create nontrivial flat bands. Further band-engineering strategies are presented where the superconducting phase is scrambled either via parallelization or dissipative phase transitions.

15 min. break

TT 15.7 Tue 11:30 H31

Minimal SU(2) models for analog simulation in small-scale superconducting quantum devices — •Lucia Valor[1,2,3], Jacquelin Luneau[1,2,3], Klaus Liegener[1,2,3], Stefan Filipp[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Lattice gauge theories (LGTs) are essential tools for studying fundamental interactions in particle physics and have broad applications in condensed matter physics and quantum information. Quantum simulation of non-Abelian theories remains challenging. Recent research on the analog simulation of LGTs has focused on scalable atomic quantum platforms. In contrast, we propose minimal SU(2) LGT models for analog simulation, tailored for small-scale superconducting quantum hardware. By adopting concepts from quantum optics, our approach emphasises coarse-grained systems that capture internal degrees of freedom and relevant non-Abelian properties with just a few qubits, bypassing the scalability demands of fine-grained models. We explore unique features of these non-Abelian systems and provide a circuit design for their experimental realisation. This work advances the study of non-Abelian gauge theories and introduces a novel method for implementation of LGTs using superconducting qubits.

TT 15.8 Tue 11:45 H31

Secure squeezed state microwave quantum communication with spin ensembles (part 1) — •Florian Fesquet[1,2], Patricia Oehrl[1,2], Kedar E. Honasoge[1,2], Maria-Teresa Handschuh[1,2], Achim Marx[1], Rudolf Gross[1,2,3], Hans Huebl[1,2,3], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Quantum key distribution (QKD) holds the promise of delivering unconditionally secure distribution of classical keys between remote parties. So far, its implementation in the microwave regime, which is frequency-compatible with superconducting quantum circuits, has been missing. Here, we present the realization of a continuous-variable QKD protocol using propagating squeezed microwave states and demonstrate a finite-size security. In order to store these states for quantum memory applications, we investigate a scheme based on the excitation of high-coherence spin ensembles by microwave quantum signals. Here, we focus on a phosphorus donor electron spin ensemble hosted in isotopically engineered silicon. Our measurements indicate a successful coupling of microwave squeezed states to the spin ensemble with an estimated efficiency of 36%.

TT 15.9 Tue 12:00 H31

Secure squeezed state microwave quantum communication with spin ensembles (part 2) — •Patricia Oehrl[1,2], Florian Fesquet[1,2], Tahereh Parvini[1,2,3], Maria-Teresa Handschuh[1,2], Kedar E. Honasoge[1,2], Achim Marx[1], Nadezhda Kukharchyk[1,2,3], Rudolf Gross[1,2,3], Kirill G. Fedorov[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Solid-state spin ensembles offer exceptional coherence times at low temperatures and transition frequencies in the GHz range, which makes them ideal for interfacing with superconducting quantum circuits. Moreover, they are promising candidates for the storage of microwave quantum states, providing great potential for quantum memory and quantum sensing applications. Here, we investigate a phosphorus donor electron spin ensemble hosted in silicon. It is coupled to a superconducting microwave resonator and probed at millikelvin temperatures as well as moderate magnetic fields. We investigate the efficiency of photon absorption for coherent and squeezed microwave signals. To this end, we use continuous wave and pulsed electron spin resonance protocols. We verify our results with an input-output model of our hybrid system and discuss the storage efficiency of microwave signals.

We acknowledge financial support from the Federal Ministry of Education and Research of Germany (project number 16KISQ036).

TT 15.10 Tue 12:15 H31

Quantum thermodynamics of non-Markovian Otto cycles using the principle of minimal dissipation — •Salvatore Gatto[1], Alessandra Colla[2], Heinz-Peter Breuer[1], and Michael Thoss[1] — [1]University of Freiburg — [2]Università degli Studi di Milano

A central challenge in quantum thermodynamics revolves around establishing a consistent and universally accepted definition for work, heat, and entropy production in open quantum systems subjected to thermal reservoirs. A recently developed approach, known as principle of minimal dissipation [1,2], leads to a unique decomposition of the quantum master equation into coherent and dissipative dynamics, allowing to identify uniquely the contributions describing work and heat. In this contribution, we apply this approach to investigate the thermodynamic characteristics of the quantum Otto cycle[3] of a single-impurity Anderson model, with a particular focus on memory effects and strong system-bath couplings. The study uses the hierarchical equations of motion approach (HEOM), which allows a numerically exact simulation of nonequilibrium transport in general open quantum systems involving multiple bosonic and fermionic environments [4].

[1] A.Colla and H.-P.Breuer, Phys Rev.A 105, 052216 (2022).
[2] S.Gatto,A.Colla,H.-P.Breuer,M.Thoss,Phys.Rev.A110,032210(2024)
[3] I.A.Picatoste,A.Colla,H.-P.Breuer, Phys.Rev.Res.6,013258 (2024).
[4] J.Bätge, Y.Ke, C.Kaspar, M.Thoss, Phys.Rev.B 103, 235413 (2021).

TT 15.11 Tue 12:30 H31

Non-Hermitian dynamics close to exceptional points — •Aisel Shiralieva, Grigorii Starkov, and Björn Trauzettel — University of Würzburg, Würzburg, Germany

Exceptional points (EPs), which are degeneracies occurring in both open classical and quantum systems, play a crucial role across numerous areas of physics. This work examines the behavior of dissipative systems with N levels, with a particular emphasis on non-Hermitian qubits and qutrits. These systems are of interest due to recent experimental studies involving a driven non-Hermitian superconducting qubit embedded within a three-level structure, where the ground state serves as an "effective bath". Although significant progress have been made in understanding EPs, the precise connection between their occurrences in non-Hermitian Hamiltonians and in the Lindblad formalism remains unclear, especially if quantum jumps are treated as perturbations. Our results reveal how EPs in these two frameworks relate to each other and illustrate how perturbations can either lift the degeneracy or eliminate the EPs entirely in the Lindblad formalism.

TT 15.12 Tue 12:45 H31

Post-measurement Quantum Monte Carlo — •Kriti Baweja[1], David Luitz[1], and Samuel Garratt[2] — [1]Institute of Physics, Nussalle 12 53115, Bonn, Germany — [2]Department of Physics, University of California, Berkeley, CA 94720, USA

We study the effects of extensive measurements on many-body quantum ground and thermal states using Quantum Monte Carlo (QMC). Measurements generate density matrices composed of products of local nonunitary operators, which we expand into operator strings via a generalized stochastic series expansion (SSE). This 'post-measurement SSE' employs importance sampling of operator strings contributing to a measured thermal density matrix. Our algorithm is applied to the spin-1/2 Heisenberg antiferromagnet on a square lattice. Thermal states of this system exhibit SU(2) symmetry, which is preserved through SU(2)-symmetric measurements. We identify two classes of post-measurement states: one where correlations can be efficiently computed using determinis-

tic loop updates, and another where SU(2)-symmetric measurements induce a QMC sign problem in any site-local basis. Using this approach, we demonstrate measurement-induced phenomena, including the creation of long-range Bell pairs, symmetry-protected topological order, and enhanced antiferromagnetic correlations. This method offers a scalable way to simulate measurement-induced collective effects, providing numerical insights to complement experimental studies. Our work opens the door to exploring how measurements influence many-body quantum systems, enabling deeper understanding of their dynamics. [1] arXiv:2410.13844

TT 15.13 Tue 13:00 H31

Zero-temperature magnon-mediated long-range entanglement in Heisenberg chain with magnetic impurity — •Marius Melz and Jamal Berakdar — Martin-Luther-Universität Halle -Wittenberg

The understanding of many-body entanglement in solid-state systems is of interest both for fundamental and practical reasons. In this work, a spin-1/2 Heisenberg chain is coupled to a chiral magnetic impurity, acting as a magnon scatterer. The spatial entanglement structure of the ground state and its effect on the propagation of local magnons is characterized by the spatially resolved bipartition entropy and logarithmic negativity. The ground state exhibits an entanglement transition at a critical magnetic bias field. We find that magnon scattering generates steady-state long-range entanglement between two scattering regions. Furthermore, it is demonstrated that this effect is significantly amplified in the high-entanglement phase.

TT 16: Superconductivity: Properties and Electronic Structure II

Time: Tuesday 9:30–12:45 Location: H32

TT 16.1 Tue 9:30 H32

Layer-thickness and substrate effects on superconductivity in epitaxial FeSe films on BLG/SiC(0001) — •yongsong wang[1], haojie guo[1], ane etxebarria[2], sandra sajan[1], sara barja[1,2,3,4], and miguel moreno ugeda[1,3,4] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Department of Polymers and Advanced Materials, University of the Basque Country, San Sebastián, Spain — [3]Centro de Física de Materiales, San Sebastián, Spain — [4]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

The layered nature and simple structure of FeSe reveal this iron-based superconductor as a unique building block for the design of artificial heterostructure materials. While superconductivity develops in ultrathin films of FeSe on $SrTiO_3$ substrates, it remains unclear whether it can be developed on more chemically inert, layered materials such as graphene. Here, we report on the characterization of the structural, chemical and electronic properties of few-layer FeSe on bilayer graphene grown on SiC using low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) and X-ray photoelectron spectroscopy (XPS). STM imaging of our FeSe films with thicknesses up to three layers exhibit the tetragonal crystal structure of bulk FeSe, which is supported by XPS spectra consistent with the FeSe bulk counterpart. While our STS measurements at 340 mK reveal a metallic character for few-layer FeSe on BLG/SiC, they show an absence of superconductivity, as the low-lying electronic structure exhibits a spatially anisotropic dip-like feature robust against magnetic fields. Superconductivity in FeSe/BLG/SiC, however, emerges for thicker films with $T_c = 6$ K.

TT 16.2 Tue 9:45 H32

Lattice dynamical studies in the unconventional superconductor: LiFeAs — •Akshay Tewari[1], Sabine Wurmehl[2], Bernd Büchner[2], Andrea Piovano[3], and Markus Braden[1] — [1]II.Physics Institute, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany — [2]IFW Dresden, D-01171 Dresden, Germany — [3]ILL, 71 avenue des Martyrs, 38000 Grenoble, France

LiFeAs crystallizes in a tetragonal structure(P4/nmm) and is superconducting below T_c=18K. Unlike other iron pnictides, LiFeAs does not exhibit long-range magnetic order, but has AFM fluctuations at incommensurate positions. Studies suggest that superconductivity in LiFeAs is driven by electronic correlations but a contribution from electron phonon coupling is still debated. We have studied the phonon dispersion of LiFeAs using inelastic neutron scattering on large single crystals to search for anomalies in the dispersion which are signatures of electron phonon coupling. We could determine almost all branches along main symmetry directions by analyzing the data with force-model lattice dynamical calculations. Temperature dependencies of specific phonon modes were also examined. Our experimental results provide significant differences to the DFT calculations previously reported[1,2]. No pronounced instability was observed but strong relative energy shifts of 6% were detected for specific modes in the temperature dependent scans. The overall dispersion fits the lattice dynamical model and is also supported by more recent DFT calculations.

[1] G.Q. Huang et al. PRB 82, 014511 (2010).
[2] R.A. Jishi et al., Adv. in Cond.Mat.Phys. 804343(2010).

TT 16.3 Tue 10:00 H32

NMR evidence of pseudogap and against spin magnetism in the time-reversal symmetry breaking state of $Ba_{1-x}K_xFe_2As_2$ — •F. Bärtl[1], F. Caglieris[2,3,4], Y. Li[5], Q. Hu[5], Y. Zheng[5], C.-H. Yim[5], J. Wosnitza[1,6], R. Sarkar[2], H.-H. Klauss[2], E. Babaev[7], J. Garaud[8], H. Kühne[1], and V. Grinenko[5] — [1]HLD-EMFL, HZDR, Dresden — [2]University of Genoa — [3]CNR-SPIN, Genoa — [4]IFW, Dresden — [5]TDLI, Shanghai Jiao Tong University — [6]IFMP, TU Dresden — [7]Department of Physics, KTH, Stockholm — [8]Institut Denis Poisson, Université de Tours

Recently, we focused on the investigation of samples from the narrow doping range of $0.7 \leq x \leq 0.8$ in the hole-doped superconductor $Ba_{1-x}K_xFe_2As_2$. Here, the proximity to a Lifshitz transition results in a multiband $s+is$ superconducting state, which spontaneously breaks time-reversal symmetry (BTRS), manifested as spontaneous currents around non-magnetic impurities. This is theoretically predicted and was experimentally revealed by μ^+SR measurements, where the depolarization rate below T_c is only non-zero in the mentioned narrow doping regime. Moreover, the μ^+SR together with Nernst-effect measurements suggest the emergence of the BTRS already at a temperature $T_c^{Z_2} > T_c$, which indicates a behavior beyond mean-field approximation, described by a four-fermion order parameter, hence termed quartic metal. Here, we present ^{75}As NMR spectroscopy and relaxometry measurements of a sample with $x = 0.77$, which contradict the presence of conventional spin magnetism and hint at pseudogap behavior in the critical regime.

TT 16.4 Tue 10:15 H32

Observation of saddle point nesting driven charge order on the surface of a 122-type iron-based superconductors — •Yu Zheng — Tsung Dao Lee Institute, Shanghai Jiao Tong University, 1 Lisuo Road, Shanghai, 201210

Unconventional superconductivity is known for intertwining with other correlated states, making the exploration for new intertwined orders highly important for understanding the mechanism of unconventional superconductivity. Spin and nematic orders are widely observed in the iron-based superconductors (FeSCs). However, evidence for charge order in the phase diagrams of FeSCs is rarely found. Employing STM and DFT, here we demonstrate,through expanding the phase diagram of $Ba_{1-x}K_xFe_2As_2$ to the heavily hole doped regime by surface doping, the formation of a CDW order on the As-terminated surface of $Ba_{0.23}K_{0.77}Fe_2As_2$, whose emergence suppresses superconductivity completely, indicating direct competition between the two. Notably, the wavevector of the charge order matches with the nesting vector between the near-EF saddle points, suggesting saddle-point nesting as its driving mechanism.

TT 16.5 Tue 10:30 H32

Long-term stability of irradiation-induced defects in $YBa_2Cu_3O_{7-\delta}$ thin films — •Bernd Aichner[1], Sandra Keppert[2], Philip Rohringer[1], Marius-Aurel Bodea[2], Benedikt Müller[3], Max Karrer[3], Reinhold Kleiner[3], Edward Goldobin[3], Dieter Koelle[3], Johannes David Pedarnig[2], and Wolfgang Lang[1] — [1]Faculty of Physics, University of Vienna, Wien, Austria — [2]Institute of Applied Physics, Johannes Kepler University Linz, Linz, Austria — [3]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, University of Tübingen, Tübingen, Germany

Helium ion irradiation is the method of choice for creating sub-100 nm structures in cuprate superconductors suitable for pinning magnetic flux quanta.

In this presentation, we address the stability of irradiation-induced defects for irradiation performed in an ion implanter as well as in a helium ion microscope. Annealing experiments allow us to extract the activation energy for the diffusion of displaced oxygen atoms back to their original sites in the material's crystal structure. Additionally, a long-term study indicates that vortex-matching features caused by a regular array of irradiation-induced defect columns are still present after about six years of sample storage, a strong hint for the stability of the defects created by irradiation. These findings may be an important ingredient for future applications of helium ion irradiation in the production process of superconducting electronics.

TT 16.6 Tue 10:45 H32

Two-fluid model analysis of the terahertz conductivity of YBaCuO samples: Optimally doped, underdoped and overdoped cases — •Christelle Kadlec[1], Wen-Yen Tzeng[2], Chih-Wei Luo[3], Jiunn-Yuan Lin[3], and Michal Šindler[1] — [1]Institute of Physics, Prague, Czech Republic — [2]National Formosa University, Yunlin, Taiwan — [3]National Yang Ming Chiao Tung University, Hsinchu, Taiwan

The conductivity of a high-quality overdoped $Y_{0.7}Ca_{0.3}Ba_2Cu_3O_{7-\delta}$ film and of underdoped and optimally doped films of its parent compound $YBa_2Cu_3O_{7-\delta}$ was measured using time-domain terahertz spectroscopy. In the normal state, the frequency dependence of the complex conductivity is described by the Drude model. Below the critical temperature T_c, the two-fluid model was successfully employed to fit all the spectra, from 5 K up to T_c. The temperature behaviour of fundamental parameters such as the scattering rate $1/\tau$, the superfluid (normal) fraction f_s (f_n) and the complex conductivity σ was investigated at given frequencies. We observed that a fifth of the electrons do not condense to the superfluid fraction even at 5 K for the optimally doped and overdoped samples. The real part of the conductivity $\sigma_1(T)$ exhibits a peak for low frequencies. It can be observed for all three compounds and its exact shape depends on the quality of the sample. A further analysis shows that this peak is a consequence of the competition between the scattering time $\tau(T)$ and the superfluid fraction $f_s(T)$.

For further details, see https://arxiv.org/pdf/2309.17408

15 min. break

TT 16.7 Tue 11:15 H32

Higgs spectroscopy on the interplay of superconductivity and charge density waves — •Liwen Feng[1,2], Tim Priessnitz[2], Thales De Oliveira[3], Jan-Christoph Deinert[3], Sergey Kovalev[3], Hao Chu[4], and Stefan Kaiser[1] — [1]TUD Dresden University of Technology, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Shanghai Jiao Tong University, China

Superconductivity (SC) and charge density wave (CDW) often coexist. In the framework of Higgs Spectroscopy, we use high-field terahertz pulses to coherently drive the corresponding Higgs and CDW amplitude modes and investigate their interplay directly in the third harmonic generation (THG) signals. Our findings reveal that the interaction between CDW fluctuations and Higgs oscillations lead to a Fano resonance [1]. We will show that we can characterize the interplay by directly investigating the relative phase responses of these modes in the time-domain THG signal [1]. We will discuss competing interactions of SC with long-range CDW order in 2H-$NbSe_2$ [1] and hole-doped cuprate $La_{2-x}Sr_xCuO_4$, interaction with short-range CDW order in the electron-doped cuprate $La_{2-x}Ce_xCuO_4$, and a noninteracting scenario in the Bismuthate superconductor $Ba_{1-x}Rb_xBiO_3$.

[1] H. Chu et al., Nat Commun. 14 (2023) 1343.

TT 16.8 Tue 11:30 H32

Dynamics of non-thermal states in a cuprate superconductor revealed by mid-infrared three-pulse spectroscopy — •Angela Montanaro[1,2,3], Enrico Maria Rigoni[1,2], Giacomo Jarc[1,2], Viktor Kabanov[4], and Daniele Fausti[1,2,3] — [1]University of Trieste, 34127 Trieste, Italy — [2]Elettra Sincrotrone Trieste, 34127 Trieste, Italy — [3]University of Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Jožef Stefan Institute, 1000 Ljubljana, 25123 Brescia, Italy

Unconventional cuprate superconductors exhibit anomalous high-frequency electrodynamics compared to standard BCS systems. In BCS superconductors, spectral weight redistribution occurs only near the superconducting gap energy, but in cuprates, changes extend to energies two orders of magnitude higher. This implies that high-energy electronic excitations might influence the pairing mechanism.

In this work, we disentangle the effects of high- and low-photon energy excitations in a prototype cuprate system. We set up a technique which combines two pump pulses having substantially different photon energy: a visible pulse much more energetic than the superconducting gap and a mid-infrared pump with photon energy smaller than the gap. Our findings show that the two photoexcitations have a different effect on the condensate electrodynamics. Moreover, we found that the overall response of the system strongly depends on the time-order of the two photoexcitations. This allowed us to constrain the lifetime of photoinjected carriers and ultimately the recovery time of the condensate.

TT 16.9 Tue 11:45 H32

Hidden antiferromagnetism and pseudogap from fluctuating stripes — •Henning Schlömer[1], Annabelle Bohrdt[2], and Fabian Grusdt[1] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 — [2]University of Regensburg, Universitätsstr. 31, 93053 Regensburg

One of the central mysteries of hole-doped cuprates is the pseudogap phase, whose unusual properties are believed to be essential for understanding high-temperature superconductivity. While a broad variety of theoretical proposals have been put forward in the past decades, a unified view connecting the pseudogap to other observed phases, like antiferromagnetic (AFM) and stripe phases, has remained elusive. In this talk, I will propose a scenario in which the the AFM, stripe, and pseudogap phases all share a common origin: The spins in the material form an ordered AFM background, on top of which fluctuating domain walls exist that can obscure long-range order. I will argue that these fluctuating domain walls are at the heart of the pseudogap phase: They hide magnetic order in real space, leaving only short-range AFM correlations detectable in experiments. Furthermore, these fluctuations can give rise to a topological phase (an odd Z2 spin liquid) that supports a small Fermi surface, consistent with experimental data. At a (hidden) quantum critical point, hidden AFM order fully dissolves, restoring spin symmetry without a divergent correlation length.

TT 16.10 Tue 12:00 H32

Direct evidence of pairing up to the pseudogap energy in cuprate high-temperature superconductors — Jiasen Niu[1,2], Maialen Ortego Larrazabal[3], Thomas Gozlinski[1,2], •Yudai Sato[1,2], Koen M. Bastiaans[4], Tjerk Benschop[1], Jian-Feng Ge[1,5], Yaroslav M. Blanter[4], Genda Gu[6], Ingmar Swart[3], and Milan P. Allan[1,2] — [1]Leiden Institute of Physics, Leiden University — [2]Fakultät für Physik, Ludwig-Maximilians-Universität — [3]Debye Institute of Nanomaterials Science — [4]Kavli Institute of Nanoscience, Delft University of Technology — [5]Max Planck Institute for Chemical Physics of Solids — [6]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory

In cuprate high-temperature superconductors, a pseudogap state is observed in a specific region of the phase diagram. Since it exists between the Mott insulating and superconducting phases, the origin of the peudogap is thought to be associated with electron pairing and/or a locally ordered state. Despite extensive studies, however, a definitive explanation remains elusive. Shot-noise experiments, which can directly detect electron pairing, hold the potential to resolve this long-standing debate. In this presentation, I will report on local shot-noise measurements on the unconventional superconductor $Bi_2Sr_2Ca_2CuO_{8+\delta}$ using scanning tunneling microscopy. We found that the pseudogap energy is associated with electron pairing, with pairing energies reaching up to 70 meV. Our results exclude the possibility of the pseudogap arising solely from local orders, and instead indicate a clear relation between the pseudogap state and Cooper pair formation.

TT 16.11 Tue 12:15 H32

Spin susceptibility in a pseudogap state with spiral magnetic fluctuations — •Paulo Forni[1], Pietro M. Bonetti[1,2], Henrik Müller-Groeling[1], Demerio Villardi[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, USA

We explore the spin susceptibility in the pseudogap phase of the 2D Hubbard model by introducing spin fluctuations into a spiral magnetic state. This analysis is based on an emergent SU(2) gauge theory following the fractionalization of the electron field into a fermionic chargon, carrying charge, and a bosonic spinon, encoding its spin. Chargons are treated within the random phase approximation in a spiral state. Deep in the pseudogap phase, spin fluctuations can be captured by a gradient expansion of the spinon field, leading to a nonlinear sigma model whose stiffnesses are computed from the underlying chargon order. Our results reveal a gapped, nematic, and SU(2)-symmetric spin susceptibility with a broad spectrum of magnetic excitations. These findings align with key features of the pseudogap phenomenology in cuprates, offering a unified theoretical framework to describe its spin and charge degrees of freedom.

TT 16.12 Tue 12:30 H32

Rise and fall of the pseudogap in the Emery model: Insights for cuprates — •Mario O. Malcolms[1], Henri Menke[1,2], Yi-Tin Tseng[2], Eric Jacob[3], Karsten Held[3], Philipp Hansmann[3], and Thomas Schaefer[1] — [1]Max-Planck-Institut für Festkörperforschung — [2]University of Erlangen-Nürnberg — [3]Institute of Solid State Physics, TU Wien

The intriguing properties of layered cuprate superconductors have not lost their fascination since their discovery. The physical mechanisms behind this rich phenomenology -after almost 40 years of intense community effort- are still highly debated. The reason for the latter is deeply routed in the fact that cuprates are strongly interacting quantum many-body systems, many of whose properties cannot be explained by a simple single-particle picture: their electrons are strongly correlated in space and in time. Adding to the complexity of this material class it has been realized early on, that due to the hybridization of copper $d_{x^2-y^2}$- and oxygen $p_{x/y}$-orbitals in the relevant two-dimensional layers, the undoped parent compounds are charge-transfer, rather than (single-orbital) Mott-Hubbard insulators. The adequate minimal theoretical modellization of cuprates, hence, has to include the oxygen p-orbitals on top of the copper-d ones, enabling, among other properties, (Zhang-Rice) singlet-formation between these orbitals. In this work we make significant progress in the universal description of the cuprates' phase diagrams by extending the powerful λ-corrected dynamical vertex approximation (DΓA) to the three-band Emery model.

TT 17: Correlated Electrons: Method Development

Time: Tuesday 9:30–13:15 Location: H33

TT 17.1 Tue 9:30 H33

Accuracy of embedded impurity methods for spin-polarized systems — •Kevin Ackermann and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg, Germany

Ab-Initio embedded impurity approaches, such as DFT+DMFT, have proven to be a robust tool in understanding physical properties of materials for quite some time. Still the intersection between the employed mean field method, like Hartree-Fock or DFT, and the many-body impurity remains awkward. One of the issues can be exemplified for spin-polarised systems. For these materials spin is no longer a good quantum number in mean-field approximations and SU(2)-symmetry is explicitly broken by the usual spin-polarized mean-field methods. This automatically turns every spin-flip excitation into a *Hund's* coupling excitation, distorting the many-body spectral function in the process. Standard methods used in quantum chemistry to remedy this, such as restricted open shell Hartree-Fock/Kohn-Sham, average over the different spin potentials or densities. However, there are many flavors of realizing the needed spin averaging. To examine the impact of this choice, we compare ground state properties, such as bond lengths, as well as excitation spectra among a multitude of spin averaging schemes for a range of molecules.

TT 17.2 Tue 9:45 H33

Neural-network-supported Configuration Interaction as impurity solver for DMFT — •Alexander Kowalski[1], Philipp Hansmann[2], Giorgio Sangiovanni[1], and Adriana Pálffy[1] — [1]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Solving a strongly correlated lattice model by means of DMFT involves mapping it to interacting auxiliary Anderson impurity models (AIM) whose solution consumes the majority of computational resources. For the solution, algorithms such as QMC, NRG, DMRG or exact diagonalization can be used, where the latter in particular has the advantage of being able to compute exact results on the real frequency axis but is constrained to a small number of bath sites due to the exponential growth of the Hilbert space. Selected configuration interaction (CI) based approaches that operate in only a subspace of the total Hilbert space can greatly alleviate this problem while still including the most relevant contributions. Recently, a neural network has been shown to improve basis selection in ground state AIM calculations [1]. Here we investigate the use of a similar neural-network-supported CI solver to select the Hilbert space basis for the auxiliary AIM in DMFT.

[1] P. Bilous, L. Thirion, H. Menke, M. W. Haverkort, A. Pálffy, P. Hansmann, arXiv:2406.00151

TT 17.3 Tue 10:00 H33

Neural Quantum States as Dynamical Mean Field Theory solvers — •Jonas B. Rigo[1], Wladislaw Krinitsin[1,2], and Markus Schmitt[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control, 52425 Jülich, Germany — [2]University of Regensburg

Neural Quantum Sates (NQS) constitute a variational wave function ansatz, that can provably efficiently represent even highly entangled quantum many-body states. Beyond their representative power, NQS inherit the speed of modern neural networks (NN) and equally profit from the enormous development that NNs have recently received. In this work we show that NQS can efficiently find the ground state of quantum impurity models with large baths, allowing us to compute high quality real-frequency, zero-temperature Green's functions by means of a Krylov-like method. We demonstrate the capability of this approach and its potential as dynamical mean-field theory (DMFT) solver at the example of the Bethe lattice and other benchmarks.

TT 17.4 Tue 10:15 H33

Neural network supported Configuration Interaction calculations in quantum many-body clusters — •Louis Thirion[1], Pavlo Bilous[2], Yorick L. A. Schmerwitz[3,4], Gianluca Levi[3], Elvar Ö. Jónsson[3], Henri Menke[5], Maurits Haverkort[6], Adriana Pálffy-Buss[7], Hannes Jónsson[3], and Philipp Hansmann[1] — [1]University of Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]University of Iceland, Reykjavik — [4]Max Planck Institute for Coal Research, Mühlheim — [5]Max Planck Institute for Solid State Research, Stuttgart — [6]University of Heidelberg — [7]University of Würzburg

A novel method is presented for computing the ground state in finite-size quantum many-body systems using configuration interaction (CI) enhanced by machine learning. Our recently developed Python library Solax [1] is used for this purpose. A neural network classifier is trained to select an efficient many-body basis in an iterative procedure. It addresses the exponential growth of the Hilbert space while maintaining accuracy. Validation with the Single Impurity Anderson Model shows a basis reduction by at least an order of magnitude compared to standard truncation schemes [2]. Application to the N_2 molecule with $\leq 2 \times 10^5$ Slater determinants, gives results comparable to full CI calculations with nearly 10^{10} determinants [3]. We aim to extend this method to multi-tier embedding schemes for predicting critical energy scales in heterogeneous catalysis.

[1] L.Thirion, P.Hansmann, P.Bilous, arXiv:2408.16915v1;
[2] P.Bilous, L.Thirion *et al.*, arXiv:2406.00151;
[3] Y.L.A.Schmerwitz, L.Thirion *et al.*, arXiv:2406.08154.

TT 17.5 Tue 10:30 H33

Simulating two-dimensional fermionic systems with strong correlations using Neural Quantum States — •Hannah Lange[1,2,3], Annika Böhler[1,2], Christopher Roth[4], and Annabelle Bohrdt[5,2] — [1]LMU Munich — [2]Munich Center for QST, Munich — [3]Max-Planck-Institute for Quantum Optics, Garching — [4]Flatiron Institute, New York — [5]University of Regensburg

Simulating strongly interacting fermionic systems is crucial for understanding correlated phases like unconventional superconductivity, yet it remains a challenge for numerical and experimental methods in many cases. Here, I will discuss the efficiency and accuracy of fermionic neural quantum states (NQS), in particular hidden fermion determinant states (HFDS), for simulating doped quantum magnets. I will show results on the strongly interacting limit of the Fermi-Hubbard model across the entire doping regime. The HFDS achieve energies competitive with matrix product states (MPS) on lattices as large as 8 x 8 sites while using several orders of magnitude fewer parameters. This efficiency enables us to probe low-energy physics across the full doping range: Starting from the low-doping regime, where magnetic polarons dominate, we track their evolution with doping through spin and polaron correlations and compare them with experimental measurements. Furthermore, I will discuss different initializations of NQS, including a hybrid training scheme, which improves the training by incorporating experimental measurements. Our findings open the way for simulating large-scale fermionic systems at any particle filling.

TT 17.6 Tue 10:45 H33

Simulating Fermi Hubbard and t-J Models with Neural Quantum States — •Annika Böhler[1,2], Hannah Lange[1,2,3], Christopher Roth[4], and Annabelle Bohrdt[2,5] — [1]Department of Physics Ludwig-Maximilians-Universität München, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]Max-Planck-Institute for Quantum Optics, Munich Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [5]University of Regensburg, Germany

Simulating strongly correlated electron systems remains a major challenge in condensed matter physics. While these systems offer a rich playground for studying emergent phenomena such as high-temperature superconductivity, they remain challenging to study both experimentally and theoretically, due to the exponential growth of the Hilbert space dimension. Neural Quantum States (NQS) offer a versatile variational framework to address this complexity. In this presentation, I will discuss the application of NQS to the strong interaction limit of the Fermi-Hubbard model. I will explore results obtained using different NQS architectures tailored to encode specific symmetry constraints. Hidden fermion determinant states are employed to efficiently capture fermionic antisymmetry, while other architectures incorporate lattice symmetries to improve accuracy and efficiency. I will show how these models can be extended to study higher SU(N) generalizations of the t-J model, providing a flexible approach to investigate a wide range of strongly correlated quantum systems and their emergent phases.

TT 17.7 Tue 11:00 H33

Investigating Quantum Many-Body Systems with Neural Quantum States — •Fabian Döschl[1,2], Felix A. Palm[1,2,3], Hannah Lange[1,2,4], Fabian Grusdt[1,2], and Annabelle Bohrdt[2,5] — [1]Ludwig-Maximilians-University Munich, Theresienstr. 37, Munich D-80333, Germany — [2]Munich Center for Quantum Science and Technology, Schellingstr. 4, Munich D-80799, Germany — [3]CENOLI, Universite Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium — [4]Max-Planck-Institute for Quantum Optics, Hans-Kopfermann-Str.1, Garching D-85748, Germany — [5]University of Regensburg, Universitätsstr. 31, Regensburg D-93053, Germany

Neural Quantum States (NQS) have shown to be a reliable and efficient method for numerically simulating the ground states of two-dimensional quantum systems. Of particular interest for current research are fractional quantum Hall models and lattice gauge theories, both of which present significant challenges for state-of-the-art numerics. In this study, we demonstrate that NQS are capable of effectively simulating such complex systems. We focus on evaluating the strengths and weaknesses of this Ansatz from a physical perspective, providing deeper insights into the potential difficulties encountered during optimization.

15 min. break

TT 17.8 Tue 11:30 H33

X-ray absorption meets Matrix Product States: Application of a MPS-based band Lanczos solver to impurity models with core levels — •Coraline Letouzé[1], Sebastian Paeckel[2], Guillaume Radtke[1], and Benjamin Lenz[1] — [1]Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, 75005 Paris, France — [2]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics (ASC), Munich Center for Quantum Science and Technology (MCQST), Ludwig-Maximilians-Universität München, 80333 München, Germany

In strongly correlated materials like transition metal (TM) oxides, core-level spectroscopies such as X-ray Absorption Spectroscopy (XAS) are usually solved on a small cluster made of the valence and core states of the TM ion and its oxygen ligands. This cluster is then diagonalized exactly via the Lanczos algorithm. In the quest to extend this cluster model into an impurity model, beyond the capabilities of Exact Diagonalization, we apply the band Lanczos algorithm on Matrix Product States (MPS). Compared to standard valence-only impurity models, the inclusion of core levels leads to more interacting orbitals connected by an intricate interaction network.

In this talk I will present our results on impurity models for simple TM oxides (NiO, MnO), with a focus on the numerical stability and convergence of the MPS-based band Lanczos solver.

TT 17.9 Tue 11:45 H33

Diagonal isometric tensor product states in two dimensions — •Benjamin Sappler[1,2], Masataka Kawano[3], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Basic Science, University of Tokyo, Meguro-ku, Tokyo 153-8902, Japan

The numerical simulation of quantum many-body systems is a challenging problem due to the exponential growth of Hilbert space with system size. In one spatial dimension this challenge was answered by the Density Matrix Renormalization Group (DMRG) algorithm, which can be understood as a variational method over Matrix Product States (MPS). One of the reasons for the success of DMRG is the existence of a canonical form for MPS that simplifies and speeds up most algorithms. Isometric tensor product states (isoTPS) generalize the canonical form of MPS to tensor networks in two and higher dimensions and have shown first promising results. Here we introduce an alternative canonical form for isoTPS by rotating the lattice by $\pi/4$ and introducing auxiliary tensors. We implement the time evolving block decimation (TEBD) algorithm on this new canonical form and benchmark the method by computing ground states and the real time evolution of the transverse field Ising model in two dimensions on large square lattices.

TT 17.10 Tue 12:00 H33

Dual Fermion Approach to the Falicov-Kimball Model: a benchmarking of methods — •Akshat Mishra[1], Hugo U. R. Strand[2], and Erik G. C. P. van Loon[1] — [1]NanoLund and Division of Mathematical Physics, Department of Physics, Lund University, Lund, Sweden — [2]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

The Falicov-Kimball model is often said to be the simplest lattice model for electronic correlations. It consists of mobile electrons and immobile impurities and the competition between the kinetic and interaction energy governs the physics. As a function of interaction strength and doping, the model shows uniform metallic and insulating phases as well as charge-density waves. A numerically exact solution of the Falicov-Kimball model is possible using classical Monte Carlo. In this work, we use this as a benchmark for two approximate many-body methods, Dynamical Mean-Field Theory (DMFT) and Dual Fermion (DF). We explore the thermodynamic properties, the electronic structure and the momentum-dependent susceptibility.

TT 17.11 Tue 12:15 H33

Enabling accurate Quantum Chemistry on current and near-term Quantum Hardware with the Transcorrelated Method. — •Werner Dobrautz[1,2], Igor O. Sokolov[5], Ali Alavi[4], Martin Rahm[3], and Ivano Tavernelli[5] — [1]CASUS - HZDR, Görlitz, Germany — [2]ScaDS.AI - TU Dresden, Dresden, Germany — [3]Chalmers University, Gothenburg, Sweden — [4]MPI-FKF, Stuttgart, Germany — [5]IBM Research, Rüschlikon, Switzerland

In this talk I will present how to enable accurate and efficient quantum chemistry calculations on NISQ devices for relevant chemical and physical problems. This is achieved by the use of an exact explicitly correlated method in the form of the transcorrelated (TC) method.

TC methods provide an efficient way of partially transferring the description of electronic correlations from the ground state wavefunction directly into the underlying Hamiltonian. This reduces the necessary quantum resources twofold:

(1) The TC Hamiltonian possesses a more compact ground state wavefunction, which facilitates electronic structure calculations and thus requires shallower quantum circuits.

(2) For ab initio quantum chemistry problems the TC method reduces the required number of qubits, by allowing to obtain highly accurate results with small basis sets.

I will present results on the Hubbard model and small chemical test systems, like the hydrogen molecule and lithium hydride, where results within chemical accuracy to the complete basis set limit and experimental results are within reach with only 4 to 10 qubits.

TT 17.12 Tue 12:30 H33

Cluster extension of the DMF^{2}RG and application to the 2d Hubbard model — •Marcel Krämer[1,2], Michael Meixner[1], Kilian Fraboulet[1], Pietro Bonetti[3], Demetrio Vilardi[1], Nils Wentzell[4], Thomas Schäfer[1], Alessandro Toschi[5], and Sabine Andergassen[2,5] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Information Systems Engineering, TU Wien, Vienna, Austria — [3]Department of Physics, Harvard University, Cambdrige, USA — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [5]Institute for Solid State Physics, TU Wien, Vienna, Austria

The DMF^{2}RG has been introduced to overcome the weak-coupling limitation of the fermionic functional renormalization group (fRG). This approach builds on the idea to exploit the dynamical mean-field theory (DMFT) as starting point for the fRG flow, thus capturing **local nonperturbative** correlations via DMFT together with perturbative nonlocal correlations generated during the flow. We show how **nonlocal nonperturbative** correlations can be also incorporated in the DMF^{2}RG scheme by using cellular DMFT (CDMFT) for a 2×2 cluster instead of single-site DMFT as starting point of the flow. Both CDMFT and fRG implementations have been formulated within the single-boson exchange decomposition, which has already proven to be an insightful bosonization scheme. We illustrate the ability of this novel approach to efficiently capture nonlocal nonperturbative correlations to describe d-wave superconductivity in the 2d Hubbard model.

TT 17.13 Tue 12:45 H33

How to stay on the physical branch of self-consistent many-electron schemes — •Herbert Essl, Matthias Reitner, and Alessandro Toschi — TU Wien

We precisely determine the mathematical condition under which the physical solution of the many-electron problem, obtained by self-consistent resummations becomes unstable by increasing interaction strength. The evaluation of the proposed criterion only requires the calculation of two-particle correlation functions. The validity of our predictions has been explicitly verified by performing self-consistent calculations of basic interacting models. Our findings eventually unveil the precise connection linking the misleading convergence of the self-consistent schemes to the multivaluedness of the Luttinger-Ward functionals and to the divergences of the irreducible vertex functions. Further, our analysis explains how the misleading convergence occurs even in parameter regions without vertex divergences. More importantly, it allows us to define a general scheme for stabilizing the physical solution, when it is unstable in conventional self-consistent schemes.

TT 17.14 Tue 13:00 H33

Mapping energy functionals and external potential of V- representable charge densities of interacting quantum systems — •Calin-Andrei Pantis-Simut[1,2], Amanda Teodora Preda[1,2], and George Alexandru Nemnes[1,2] — [1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Reactorului 30, 077125 Magurele-Ilfov, Romania — [2]Faculty of Physics, University of Bucharest, Atomistilor 405, 077125 Magurele-Ilfov, Romania

Quantum systems are shaping the modern information processing technologies. Designing and analyzing these systems yields one of the most outstanding challenges in modern physics. These systems are fairly complex due to the Coulomb interaction between the particles. There are several methods for solving these problems, the most accurate providing solutions beyond mean-field approaches. Here the Exact Diagonalization is regarded as the gold standard for a system containing several particles. Recently, charge densities of such systems have been successfully mapped from randomly generated external potentials, using cGANs models. In this work, we intend to develop a machine learning based-model in order to obtain energy functionals E[n] for several classes of Hamiltonians (e.g. containing spin-orbit interaction), thus enabling the bypass of numerical intensive procedures like Exact Diagonalization. For this task, we employ CNNs to map the energy functionals from the ground state charge density. A more in depth analysis of the inverse problem is employed also in this work. Successfully mapping the external potential is not trivial since not every proposed charge density is V-representable.

TT 18: Focus Session: Strongly Correlated Quantum States in Moiré Heterostructures (joint session TT/HL/MA)

In recent years, significant progress has been made in realizing and exploring correlated quantum states in multilayer moiré heterostructures of graphene or transition metal dichalcogenides. These achievements have been made possible by the high level of control and tunability of these systems. Striking phenomena have been demonstrated experimentally, including unconventional superconductivity, fractional quantum anomalous Hall states, Mott-Wigner states and density waves, as well as kinetic ferromagnetism. Moreover, recently novel spectroscopic experimental techniques have been developed which allow for new ways to explore the dynamical response of these exotic states. This focus session will discuss recent experimental advancements as well as theoretical developments in the field of strongly correlated moiré heterostructures.

Organizers: Dmitri K. Efetov (LMU München), Michael Knap (TU München)

Time: Tuesday 9:30–13:15 Location: H36

Topical Talk TT 18.1 Tue 9:30 H36

The Thermoelectric Effect and Its Natural Heavy Fermion Explanation in Twisted Bilayer and Trilayer Graphene — Dumitru Calugaru[1], Haoyu Hu[2], Rafael Luque Merino[3], Nicolas Regnault[4], Frank Koppens[3], Dmitri K. Efetov[5], and •Bogdan Andrei Bernevig[1] — [1]Dept of Physics, Princeton University, Princeton, USA — [2]DIPC, San Sebastián, Spain — [3]ICFO, Barcelona, Spain — [4]Laboratoire de Physique de l'ENS, Paris, France — [5]LMU Munich, Munich, Germany

We study the interacting transport properties of twisted bilayer graphene (TBG) using the topological heavy-fermion (THF) model, where TBG comprises localized, correlated f-electrons and itinerant, dispersive c-electrons. The Seebeck coefficient of TBG exhibits unconventional traits: negative values with sawtooth oscillations at positive fillings, contrasting typical band-theory expectations. This behavior arises from the dichotomy between heavy (short-lived, correlated f-electrons) and light (long-lived, dispersive c-electrons), with transport dominated by c-electrons due to their stronger dispersion and longer lifetimes. At positive integer fillings, c- (f-)electron bands govern the electron (hole) doping side, resulting in an overall negative Seebeck coefficient. Sawtooth oscillations occur near each integer filling due to gap openings. Our results underscore the importance of electron correlations and lifetime asymmetry, naturally captured by the THF model, in understanding TBG transport properties. These findings align with experiments on twisted bilayer and trilayer graphene and highlight the interplay of heavy and light carriers.

Topical Talk TT 18.2 Tue 10:00 H36

Angle-Tuned Chiral Phase Transition in Twisted Bilayer Graphene — •Laura Classen[1;2], Nikolaos Parthenios[1,2], Cheng Huang[3], Xu Zhang[3], Maksim Ulybyshev[4], Fakher Assaad[3], and Zi Yang Meng[4] — [1]Max Planck Institute for Solid State Research — [2]Technical University of Munich — [3]University of Hong Kong — [4]University of Wuerzburg

The twist angle constitutes an important control knob in twisted bilayer graphene that has become accessible in-situ. It effectively tunes between weakly interacting, decoupled graphene layers and strongly correlated electrons at a magic angle of around 1.1 degree. We propose that this facilitates the realisation of a chiral phase transition of Dirac fermions at charge neutrality in twisted bilayer graphene. We argue that the transition can be described by the Gross-Neveu-Yukawa model that couples Dirac fermions and an XY order parameter field. The quantum critical behavior of this effective model is consistent with quantum Monte Carlo simulations of the continuum model for twisted bilayer graphene.

Topical Talk TT 18.3 Tue 10:30 H36

Quantum Optics of Semiconductor Moire Materials — •Atac Imamoglu — Institute of Quantum Electronics, ETH Zurich

Moire superlattices in two dimensional semiconductors have enabled the observation of a wealth of phenomena driven by strong electronic correlations, ranging from Mott-Wigner states to fractional quantum anomalous Hall effect. In this talk, I will present experiments exploring quantum optical control of strongly correlated electrons.

15 min. break

Topical Talk TT 18.4 Tue 11:15 H36

Probing the Band Structures of Multilayer Graphene Using the Quantum Twisting Microscope — •Martin Lee[1,2], Ipsita Das[1,2], János Papp[1,2], Marc Currle[1], Jiazhuo Li[1,2], Mudit Bhatt[1,2], Jonah Herzog-Arbeitman[3], Jiabin Yu[3], Zhiyuan Zhou[3], Markus Becherer[4], Philipp Altpeter[1], Christian Obermayer[1], Heribert Lorenz[1], Kenji Watanabe[5], Takashi Taniguchi[5], Bogdan Andrei Bernevig[3,6,7], and Dmitri Efetov[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Department of Physics, Princeton University, Princeton, New Jersey, USA — [4]School of Computation Information and Technology, Technical University of Munich, Germany — [5]National Institute of Material Sciences, Tsukuba, Japan — [6]Donostia International Physics Center, Donostia-San Sebastian, Spain — [7]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Understanding the band-structure is foundational in describing the behavior of electrons in crystalline systems. While the tight-binding model effectively captures the non-interacting band-structures in materials like graphene, it relies on analytically or numerically derived hopping parameters. In this talk, we present the development of a quantum twisting microscope (QTM), which allows the k-resolved tunneling spectroscopy between the electronic states at the 2D tip and the 2D sample by twisting in-situ. Our QTM measurements allow us to extract the hopping parameters that agree with theoretical predictions.

Topical Talk TT 18.5 Tue 11:45 H36

Gate-Tunable Bose-Fermi Mixture in a Strongly Correlated Moiré Bilayer Electron System — •Nathan Wilson[1], Amine Ben Mhenni[1], Wilhelm Kadow[2], Mikołaj Metelski[1], Adrian Paulus[1], Alain Dijkstra[1], Jonathan Finley[1], and Michael Knap[2] — [1]Walter Schottky Institute, TU Munich, Garching, Germany — [2]School of Natural Sciences, TU Munich, Garching, Germany

Quantum gases consisting of species with distinct quantum statistics, such as Bose-Fermi mixtures, can behave in a fundamentally different way than their unmixed constituents. This makes them an essential platform for studying emergent quantum many-body phenomena such as mediated interactions and unconventional pairing. Here, we realize an equilibrium Bose-Fermi mixture in a bilayer electron system implemented in a WS_2/WSe_2 moiré heterobilayer with strong Coulomb coupling to a nearby moiré -free WSe2 monolayer. Absent the fermionic component, the underlying bosonic phase manifests as a dipolar excitonic insulator. By injecting excess charges, we show that the bosonic phase forms a stable mixture with added electrons but abruptly collapses upon hole doping. We develop a microscopic model to explain the unusual asymmetric stability with respect to electron/hole doping. By monitoring excitonic resonances from both layers, we demonstrate stability of the phase over a wide range in the boson/fermion density phase space, in agreement with theoretical calculations. Our results further the understanding of phases stabilized in moiré bilayer electron systems and demonstrate their potential for exploring the exotic properties of equilibrium Bose-Fermi mixtures.

TT 18.6 Tue 12:15 H36

Theory for Optical Control of Correlated States in Moiré Transition Metal Dichalcogenide Heterostructures — •Haoyang Tian and Urban Friedrich Peter Seifert — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany

In recent years, moiré transition metal dichalcogenide (TMD) heterostructures have emerged as highly versatile platforms for investigating phases and phenomena of strongly correlated electrons on emergent lattice scales. However, experimental characterization of the precise nature of some interaction-driven long-range ordered states and their excitations has remained a challenge. Given strong light-matter couplings and valley selection rules in TMD materials, ultrafast optical methods may constitute a promising avenue for probing and controlling these states and their collective modes. In this work, we develop a theoretical framework to describe coherent light-matter interactions in moiré TMD heterostructures, and model the system's steady-state and non-equilibrium dynamics during and after photoexcitation with a laser pulse. Thus obtained characteristic signatures of the system's dynamics may allow for new experimental insights.

TT 18.7 Tue 12:30 H36

Single-Particle Spectral Function of Fractional Quantum Anomalous Hall States — •Fabian Pichler[1,2], Wilhelm Kadow[1,2], Clemens Kuhlenkamp[3,1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [3]Department of Physics, Harvard University, Cambridge, Massachusetts, USA

Fractional quantum Hall states are the most prominent example of states with topological order, hosting excitations with fractionalized charge. Recent experiments in twisted $MoTe_2$ and graphene-based heterostructures provide evidence of fractional quantum anomalous Hall (FQAH) states, which spontaneously break time-reversal symmetry and persist even without an external magnetic field. Understanding the unique properties of these states requires the characterization of their low-energy excitations. To that end, we construct a parton theory for the energy and momentum-resolved single-particle spectral function of FQAH states. We explicitly consider several experimentally observed filling fractions as well as a composite Fermi liquid in the half-filled Chern band. The parton description captures qualitatively our numerical exact diagonalization results. Additionally, we discuss how the finite bandwidth of the Chern band and the non-ideal quantum geometry affect the fractionalized excitations. Our work demonstrates that the energy and momentum-resolved electronic single-particle spectral function provides a valuable tool to characterize fractionalized excitations of FQAH states in moiré lattices.

TT 18.8 Tue 12:45 H36

Tuneability of Superconducting Properties in Transition Metal Dichalcogenide bilayers — •Michael Winter and Tim O. Wehling — I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg

In recent years, rising interest sustained in van der Waals materials, particularly in transition metal dichalcogenides (TMDs or TMDCs). This work explores the potential for bilayer [hetero-]structuring in TMDs, which have garnered significant attention due to the discovery and prediction of exotic quantum phases, such as superconductivity and Mott insulating behaviour.

I present predictions derived from a minimal quantum lattice model, incorporating ab initio calculations based on plane-wave density functional theory (DFT), density functional perturbation theory (DFPT), and subsequent electron-phonon interaction calculations. The resulting model allows us to investigate the effects of different material combinations (e.g., MoS_2, $MoSe_2$, WS_2, WSe_2) and electron doping on superconductivity in such [hetero-]bilayer.

TT 18.9 Tue 13:00 H36

Proximity-Induced Spin-Triplet Superconducting Correlations in Transition Metal Dichalcogenides — •Florian Kayatz, Jorge Cayao, and Annica Black-Schaffer — Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

The realization of spin-triplet Cooper pairs is a key ingredient for superconducting spintronics. One promising route to achieve this task is by exploiting the strong intrinsic spin-orbit coupling of transition metal dichalcogenides (TMDs). In this work, we consider a TMD layer coupled to a conventional spin-singlet s-wave superconductor and demonstrate the emergence of spin-triplet superconducting correlations. We find that these spin-triplet pair correlations form in the TMD as a proximity-induced effect but also appear in the superconductor as an inverse proximity effect and as a nonlocal phenomenon that exists between the TMD and superconductor. Furthermore, we relate these emergent superconducting correlations to experimentally observable features in the density of states and conductance.

TT 19: Many-body Quantum Dynamics I (joint session DY/TT)

Time: Tuesday 9:30–13:00 Location: H37

TT 19.1 Tue 9:30 H37

Controlling Many-Body Quantum Chaos — •Lukas Beringer[1], Mathias Steinhuber[1], Juan Diego Urbina[1], Klaus Richter[1], and Steven Tomsovic[1,2] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA USA

Controlling chaos is a well-established technique that leverages the exponential sensitivity of classical chaotic systems for efficient control. This concept has been generalized to single-particle quantum systems [1] and, more recently, extended to bosonic many-body quantum systems described by the Bose-Hubbard model [2]. In direct analogy to the classical paradigm, a localized quantum state can be transported along a specific trajectory to a desired target state. In the latter context, this approach reduces to time-dependent control of the chemical potentials, making it suitable for implementation in optical lattice experiments. Highlighted potential applications are rapid, customizable state preparation and stabilization of quantum many-body scars in one-, two-, and three-dimensional lattices. Recent progress includes potential applications to large time-crystal platforms and preparation protocols for entangled states, such as cat-like states.

[1] S. Tomsovic, J. D. Urbina, and Klaus Richter, Controlling Quantum Chaos: Optimal Coherent Targeting, PRL 130.2 (2023): 020201.

[2] L. Beringer, M. Steinhuber, J. D. Urbina, K. Richter, S. Tomsovic, Controlling many-body quantum chaos: Bose-Hubbard systems, New J. Phys (2024): 26 073002.

TT 19.2 Tue 9:45 H37

Exact spectral function and nonequilibrium dynamics of the strongly interacting Hubbard model — Ovidiu I. Pâțu[1], •Andreas Klümper[2], and Angela Foerster[3] — [1]Institute for Space Sciences, Bucharest-Măgurele, R 077125, Romania — [2]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [3]Instituto de Física da UFRGS, Av. Bento Gonçalves 9500, Porto Alegre, RS, Brazil

Analytical results on the correlation functions of strongly correlated many-body systems are rare in the literature and their importance cannot be overstated. We present determinant representations for the space-, time-, and temperature-dependent correlation functions of the strongly interacting one-dimensional Hubbard model in the presence of an external trapping potential. These representations are exact and valid in both equilibrium and nonequilibrium scenarios like the ones initiated by a sudden change of the confinement potential. In addition, they can be implemented numerically very easily significantly outperforming other numerical approaches. As applications of our results we investigate the single particle spectral functions of systems with harmonic trapping and show that dynamical quasicondensation occurs for both fermionic and bosonic spin-1/2 systems released from a Mott insulator state.

TT 19.3 Tue 10:00 H37

Quantum many-body scars beyond the PXP model in Rydberg simulators — Aron Kerschbaumer[1], Marko Ljubotina[1,2,3], Maksym Serbyn[1], and •Jean-Yves Desaules[1] — [1]Institute of Science and Technology Austria, Klosterneuburg, Austria — [2]Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Persistent revivals recently observed in Rydberg atom simulators have challenged our understanding of thermalization and attracted much interest to the concept of quantum many-body scars (QMBSs). QMBSs are non-thermal highly excited eigenstates that coexist with typical eigenstates in the spectrum of many-body Hamiltonians, and have since been reported in multiple theoretical models, including the so-called PXP model, approximately realized by Rydberg simulators. At the same time, questions of how common QMBSs are and in what models they are physically realized remain open.

In our work, we demonstrate that QMBSs exist in a broader family of models that includes and generalizes PXP to longer-range constraints and states with different periodicity. We show that in each model, multiple QMBS families can be found. Each of them relies on a different approximate su(2) algebra, leading to oscillatory dynamics in all cases. However, in contrast to the PXP model, their observation requires launching dynamics from weakly entangled initial states rather than from a product state. The new QMBSs we unveil may be experimentally probed using Rydberg atom simulator in the regime of longer-range Rydberg blockades.

TT 19.4 Tue 10:15 H37

Roughening dynamics of quantum interfaces — Wladislaw Krinitsin[1,2], •Niklas Tausendpfund[1,3], Matteo Rizzi[1,3], Markus Heyl[4], and Markus Schmitt[1,2] — [1]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, Jülich, Germany — [2]Faculty of Informatics and Data Science, University of Regensburg, Regensburg, Germany — [3]Institute for Theoretical Physics, University of Cologne, Köln, Germany — [4]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The roughening transition, known from three-dimensional classical spin systems, describes how fluctuations of interfaces transition from being bounded to being extensive when crossing the characteristic roughening temperature. We explore signatures of such phenomena in the dynamics of domain walls in the two dimensional quantum Ising model, where we observe pre-thermal steady states in their evolution well beyond the perturbative limit using Tree Tensor Networks. We formulate an effective model of the interface, which captures qualitative features of a roughening transition. Most notably, it exhibits a Berezinskii Kosterlitz Thouless quantum phase transition from smooth to rough interfaces, whose signatures extend to finite temperatures. These findings can be related to the observed slow thermalization in the full model, opening the way to a bet-

ter understanding of pre-thermalization effects in interface dynamics, which can be easily implemented and tested in experimental setups such as Rydberg atom experiments.

TT 19.5 Tue 10:30 H37

Semigroup Influence Functionals for the Dynamics of Quantum Impurity Models — •Michael Sonner[1], Valentin Link[2], and Dmitry Abanin[3,4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — [4]Google Research, Brandschenkestrasse 150, 8002 Zürich, Switzerland

Quantum impurity models~(QIM) consist of a local interacting impurity which is coupled to baths of free fermions. These models exhibit a range of non-trivial phenomena such as the Kondo effect. and play a central role in the dynamic mean field theory (DMFT) approach to correlated matter. However, despite their importance, computing the real time dynamics of QIM remains a challenge. Recently, approaches based on matrix product states (MPS) representation of influence functionals (IF) have been proven effective approaches to this problem. These method work by capturing the, generically non-markovian dynamical effects of the quantum environments on the local impurity in a multi time object, which then is compressed as MPS. Taking explicit advantage of time-translation invariance of the model, we find an infinite MPS or semigroup representation of the IF. I will demonstrate how these ideas can be used to predict QIM dynamics for very long times as well as give direct access to stationary non-equilibrium states.

TT 19.6 Tue 10:45 H37

Quantum Fisher information of monitored random circuits — •Arnau Lira Solanilla, Xhek Turkeshi, and Silvia Pappalardi — Universität zu Köln

We characterize the multipartite entanglement structure of monitored random quantum circuits using the quantum Fisher information. We show that, despite the known phase transition in bipartite correlations, the multipartiteness is bounded. On the other hand, we generate a phase with extensive multipartite entanglement under symmetry preserving random operations by introducing two-qubit measurements. We focus on the limit where no unitary operations are applied, but there is a competition between two noncommuting projective measurements. We exploit a map to bond percolation to precisely calculate the universal scaling of multipartite entanglement.

TT 19.7 Tue 11:00 H37

Entanglement in quantum circuits with SU(2) symmetry — •Tobias Dörstel and Michael Buchhold — Institute for Theoretical Physics, Cologne

Quantum circuits offer a robust framework for studying the out-of-equilibrium dynamics of quantum many-body systems. We investigate one-dimensional monitored quantum circuits with global SU(2) symmetry, serving as digital counterparts to the Heisenberg chain. These circuits consist of unitary qubit SWAPs and non-unitary SWAP-measurements. Entanglement in the chain is governed by the configuration of qubit singlet states, whose count is fixed by the symmetry sector. Varying the measurement rate, unitary operations, and singlet number reveals diverse entanglement behaviors, ranging from volume law to $\log^2(L)$ and $\log(L)$ scaling of half-chain entanglement. We explain these scaling regimes analytically using an SU(2)-symmetric "Page law" and a mapping to loop models with crossings.

15 min. break

TT 19.8 Tue 11:30 H37

Generalized dual-unitary circuits from biunitarity — •Michael A. Rampp, Suhail A. Rather, and Pieter W. Claeys — Max-Planck-Institut für Physik komplexer Systeme, Dresden

We present a general framework for constructing solvable lattice models of chaotic many-body quantum dynamics with multiple unitary directions using biunitary connections. We show that a network of biunitary connections on the Kagome lattice naturally defines a multi-unitary circuit, where three 'arrows of time' directly reflect the lattice symmetry. These models unify various constructions of hierarchical dual-unitary and triunitary gates and present new families of models with solvable correlations and entanglement dynamics. Using multilayer constructions of biunitary connections, we additionally introduce multilayer circuits with monoclinic symmetry and higher level hierarchical dual-unitary solvability and discuss their (non-)ergodicity. Our work demonstrates how different classes of solvable models can be understood as arising from different geometric structures in spacetime.

TT 19.9 Tue 11:45 H37

Magic spreading in doped Clifford circuits — •Jiangtian Yao and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems

We study the spreading of magic, or nonstabilizerness, in Clifford circuits with doping by non-Clifford gates. We characterize the spatial extent of magic in classes of Clifford circuits where the growth behavior of entanglement entropy and operator strings are known. The dynamics of magic spreading in such circuits is compared to that of entanglement entropy, and quantitative measures for longer-ranged magic are also explored.

TT 19.10 Tue 12:00 H37

One magnon magnetization dynamics for the kagome lattice antiferromagnet — Henrik Schlüter, •Jannis Eckseler, and Jürgen Schnack — Faculty of Physics, Bielefeld University, Bielefeld, Germany

We present aspects of the one-magnon dynamics of the antiferromagnetic kagome lattice as an example of flat-band dynamics extending the work of [1] to two dimensional systems. We illustrate how localized eigenstates also called localized magnons [2] influence the dynamics of excitations and possibly prevent the system from thermalization. To this end we introduce a $J_1 - J_2$-model for the kagome lattice which guarantees the stability of one out of three localized magnons and lets us distinguish the different flat bands.

[1] F. Johannesmann, J. Eckseler, H. Schlüter, and J. Schnack, Phys. Rev. B 108, 064304 (2023).

[2] J. Schnack, H.-J. Schmidt, J. Richter, and J. Schulenburg, Eur. Phys. J. B 24, 475 (2001).

TT 19.11 Tue 12:15 H37

Towards a Many-Body Generalization of the Wigner-Smith Time Delay — •Georg Maier[1], Carolyn Echter[2], Juan Diego Urbina[1], Caio Lewenkopf[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik Universität Regensburg, Regensburg, Germany — [2]Mathematische Fakultät Universität Regensburg, Regensburg, Germany — [3]Instituto de Física Universidade Federal Fluminense, Niterói RJ, Brazil

Many body systems with a large number of degrees of freedom are usually described by statistical physics on the theoretical side while experiments usually relay on scattering (e.g. particle physics). Is it possible to relate scattering and statistical physics, or to measure scattering-related observables which directly relate to quantities of statistical physics? At least for single particle systems a close relation exists between the well known Wigner-Smith delay time in scattering theory and the density of states of the scattering system.

I will present a novel ansatz relating a many-body version of dwell-/Wigner-Smith delay time and many body density of states based on the famous Birman-Krein-Friedel-Loyd formula connecting scattering theory and statistical observables in the many-body context. Due to the flexibility of this ansatz it can be used to investigate a wide variety of MB systems. I will discuss interesting scaling behaviors for different systems, like the harmonic trap[1] or the free particle together with the different behavior of bosons, fermions and indistinguishable particles.

[1] C. Echter et. al 2409.08696

TT 19.12 Tue 12:30 H37

Subleading logarithmic behavior in the parquet formalism — •Marcel Gievers[1,2], Richard Schmidt[3], Jan von Delft[1], and Fabian B. Kugler[4] — [1]Ludwig-Maximilians-Universität, München — [2]Max-Planck-Institut für Quantenoptik, Garching — [3]Universität Heidelberg — [4]CCQ, Flatiron Institute, New York

The Fermi-edge singularity in x-ray absorption spectra of metals is a paradigmatic case of a logarithmically divergent perturbation series. Prior work has thoroughly analyzed the leading logarithmic terms. Here, we investigate the perturbation theory beyond leading logarithms and formulate self-consistent equations to incorporate all leading and next-to-leading logarithmic terms. This parquet solution of the Fermi-edge singularity goes beyond the previous first-order parquet solution and sheds new light on the parquet formalism regarding logarithmic behavior. We present numerical results in the Matsubara formalism and discuss the characteristic power laws. We also show that, within the single-boson exchange framework, multi-boson exchange diagrams are needed already at the leading logarithmic level.

TT 19.13 Tue 12:45 H37

Ballistic transport in a disordered, boundary-driven XXZ spin chain. — •Johannes S Hofmann[1], Adam McRoberts[2], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]International Centre for Theoretical Physics, Strada Costiera 11, 34151, Trieste, Italy

Recent experiments on Google's sycamore NISQ device on spin transport realised ballistic transport in a edge-driven XXZ chain without disorder; and theoretical works on the classical variant demonstrated the survival of ballistic regime in the easy-plane upon the introduction of bond disorder. Here, we consider various generalisations of this set-up.

TT 20: 2D Materials: Electronic Structure and Exitations I (joint session O/HL/TT)

Time: Tuesday 10:30–13:00 Location: H8

TT 20.1 Tue 10:30 H8

Line-moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) — •Romana Ganser, Muthu P. T. Masilamani, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

We present angle-resolved photoemission spectroscopy (ARPES) measurements on tunable one-dimensional moiré phases of an epitaxial honeycomb monolayer AgTe/Ag(111) [1]. In this model system, the moiré structure can be tuned almost continuously in contrast to hardly controllable twist angles in bilayer van-der-Waals heterostructures [2]. We experimentally observe moiré minibands and band gaps of 120 - 170 meV suggesting sizable superlattice potentials. By comparing the experimental data to simple model calculations, we analyze the local character of the potential. This provides important information of interface hybridization effects on the band structure, which may not be limited to the system at hand but rather a broad range of moiré interfaces.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020).
[2] Lisi, S. et al. Nat. Phys. 17, 189-193 (2021).

TT 20.2 Tue 10:45 H8

Photoemission Time Scale Determination: the Effect of Crystal Dimensionality and Electronic Correlation — •Fei Guo[1], Dmitrii Usanov[2], Eduardo B. Guedes[2], Mauro Fanciulli[3], Arnaud Magrez[1], Michele Puppin[1], and Hugo Dil[1,2] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, 95031, France

Spin polarization of photoelectrons from spin-degenerate dispersive initial states originates from the interference of multiple photoemission channels, measuring the spin polarization with spin- and angle-resolved photoemission spectroscopy (SARPES) allows the estimation of the phases of the interfering channels, and hence the Eisenbud-Wigner-Smith (EWS) time delay of photoemission, which is the amount of time required by the photoelectron to evolve into a free particle final state. While not directly measurable for solid-state photoemission, this time scale has been measured for gaseous photoionization, which is generally in the attosecond (10^-18s) range.

We present investigations with multiple materials of different properties, and by comparing with previous studies, we propose a relationship between the EWS time delay, electronic correlation mechanism, and dimensionality.

TT 20.3 Tue 11:00 H8

Disorder effects in the Band Structure of Transition Metal Dichalcogenide alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W) — •Sarath Sasi[1], Aki Pulkkinen[1], Laurent Nicolaï[1], Raphaël Salazar[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

Recent advances in materials synthesis have enabled the creation of 2D TMDC alloys, which offer unique opportunities for tailoring electronic and optoelectronic properties to meet diverse application demands.[1].This study investigates the band structure evolution of $A_xB_{1-x}Se_2$ alloys (A, B = Cr, Mo, W) across varying composition fractions (x). Using the Coherent Potential Approximation (CPA)[2], which accurately models scattering in disordered systems, theoretical calculations were performed with the *SPR-KKR* package[3]. Results reveal that some of the TMDC alloys maintain their band structures without significant disorder effects. Angle-Resolved Photoemission Spectroscopy (ARPES) measurements align closely with one-step model photoemission calculations, confirming theoretical predictions. These insights provide a foundation for tailoring electronic properties, advancing their applicability in next-generation devices.

[1] Zhou, J., Lin, J., Huang, X., et al. Nature, 556, 355-359 (2018).
[2] Soven, P., Phys. Rev., 156, 809(1967).
[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

TT 20.4 Tue 11:15 H8

Unveiling Doping-Induced Electronic Modifications in Antiferromagnetic MPS_3 van der Waals Materials — •Till Willershausen[1], Jonah Elias Nitschke[1], Patrick Merisescu[2], David Janas[1], Lasse Sternemann[1], Michele Capra[1], Mira Arndt[1], Valentin Mischke[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Bath University

Antiferromagnetic van der Waals (vdW) materials, with scalability to monolayer thickness, semiconducting properties, and intrinsic antiferromagnetic ordering, hold promise for spintronic and quantum technology applications. We investigate alkali metal doping effects on the MPS_3 family (M = Mn, Ni, Co, Fe) of 2D antiferromagnetic vdW materials, revealing doping-induced changes in their electronic structure. X-ray Photoelectron Spectroscopy (XPS) shows shifts in oxidation states in $NiPS_3$, $CoPS_3$, and $FePS_3$, while $MnPS_3$ displays no significant changes, indicating distinct charge transfer. Further investigation with Angle-Resolved Photoelectron Spectroscopy (ARPES) reveals new alkali-metal induced bands appearing above the previous valence band maximum. This analysis highlights doping-induced modifications and contrasts in transition metal behavior in MPS_3, providing insights into doping mechanisms and electronic tunability.

TT 20.5 Tue 11:30 H8

Enhanced electron-phonon coupling in few-layer $MoTe_2$ from micro-ARPES — •Thomas P. van Waas[1], Julia Issing[2], Marco Gibertini[3], Christophe Berthod[2], Anna Tamai[2], Felix Baumberger[2,4], and Samuel Poncé[1,5] — [1]European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Belgium — [2]Department of Quantum Matter Physics, University of Geneva, Switzerland — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland — [5]WEL Research Institute, Belgium

Bulk orthorhombic T_d-$MoTe_2$ is a type-II Weyl semimetal with a superconducting critical temperature of T_c = 0.1 K. Transport measurements show a monotonic increase in T_c as the thickness of multilayer $MoTe_2$ is reduced, reaching T_c = 7.6 K in the monolayer. We investigate photoemission kinks in the electron pocket of exfoliated mono- bi-, and trilayer $MoTe_2$ from micro-focused angle-resolved photoemission spectroscopy. We use a custom code to quantify the electron self-energy $\Sigma_n(E)$ for a parabolic non-interacting dispersion, and obtain from $\Sigma_n(E)$ the Eliashberg spectral function $\alpha^2F_n(\omega)$ using the maximum entropy method. We find two dominant phonon modes in $\alpha^2F_n(\omega)$ for the mono- and trilayer, with a large enhancement of the lower-frequency phonon mode in the former. We also provide tentative results for the bilayer, where quantification is more challenging due to a small splitting of the electronic bands.

TT 20.6 Tue 11:45 H8

Electronic structure of V-doped WSe_2 — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics represents a promising and energy-efficient alternative to conventional electronics, with significant potential applications, e.g., in areas such as classical and quantum computing. The vanadium-doped layered transition metal dichalcogenide 2H-WSe_2 is a promising candidate to fulfill the desired properties as a room-temperature magnetic semiconductor with gating tunability. Here, we present a comprehensive electronic structure study of chemical vapor transport-grown pristine and V-doped WSe_2 by soft X-ray, VUV and 11eV-laser ARPES, highlighting the influence of a low V doping concentration on the electronic structure of WSe_2.

TT 20.7 Tue 12:00 H8

Unraveling magnetic ordering in a van der Waals correlated material — Tommaso Pincelli[1,2], •Tania Mukherjee[1,2], Lawson Lloyd[2], Shuo Dong[2,3], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], and Ralph Ernstorfer[1,2] — [1]Technische Universität Berlin, 10623 Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society, 14195 Berlin, Germany — [3]Beijing National Laboratory for Condensed Matter Physics, China

Layered van der Waals (vdW) materials offer a compelling platform to investigate various emergent quantum properties in low dimensions. Fe_3GeTe_2 (FGT), a vdW ferromagnetic metal, is well-known for exhibiting exotic phenomena, ranging from skyrmion formation to heavy fermion behavior. However, an understanding of the magnetic ordering, a key feature for spintronic applications, still remains elusive in this material. In particular, the interplay of both local magnetic moments and an itinerant mechanism in the formation of ferromagnetic ordering in FGT, a non-f-electron correlated system, remains to be clarified. Using time- and angle-resolved photoemission spectroscopy (trARPES) and first-principles calculations, we provide evidence for an ordering mechanism in FGT by observing a pronounced reduction in the Stoner exchange gap. This stands in contrast to earlier temperature-dependent ARPES studies of the electronic structure of FGT, which favored a localized excitation model over the weak-coupling itinerant picture. We also observe the impact of phononic excitations which further confirm our findings.

TT 20.8 Tue 12:15 H8

Spin structure of the unoccupied surface state at AgTe/Ag(111) — •Carolin Benfer, Marcel Holtmann, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

The AgTe/Ag(111) surface alloy has recently been investigated as a model system for the role of orbital angular momentum in the formation of spin effects in the electronic structure [1]. Two *p*-like surface states were detected in ARPES measurements, one shows a Rashba-type spin splitting, while the other one does not. This behavior is attributed to the symmetries of the orbital wave functions of the electrons. For the unoccupied states a third surface state has been predicted. Following the symmetry arguments given in [1], a Rashba-type spin splitting of the state is expected.

We use inverse photoemission (IPE) to directly study the unoccupied state of the surface alloy. Low-energy electron diffraction and scanning tunneling microscopy measurements confirm a homogeneous monolayer film of the surface alloy, which is growing in a honeycomb structure. Angle-resolved IPE measurements detect the predicted surface state with free electron-like dispersion. Spin-resolved IPE measurements reveal a Rashba-type spin structure.

[1] M. Ünzelmann *et al.*, Phys. Rev. Lett. **124**, 176401 (2020)

TT 20.9 Tue 12:30 H8

Orbital mixing as key mechanism for ferromagnetism in van der Waals CrI3 — •Alessandro De Vita[1,2], Srdjan Stavrič[3], Roberto Sant[4], Nicholas B. Brookes[4], Giancarlo Panaccione[5], Silvia Picozzi[3], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Straße des 17 Juni 135, 10623 Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [3]Consiglio Nazionale delle Ricerche CNR-SPIN, c/o Università degli Studi G. D'Annunzio, 66100 Chieti, Italy — [4]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [5]Istituto Officina dei Materiali (IOM)-CNR, Laboratorio TASC, in Area Science Park, S.S.14, km 163.5, I-34149 Trieste, Italy

Van der Waals ferromagnets constitute a versatile platform where exotic quantum states can be realized; among them, CrI3 is a prototypical and widely studied 2D ferromagnet, with promising applications in spin- and orbitronics. Despite that, key information on its electronic occupation and stabilization of the magnetic configuration are missing. By means of complementary absorption and photoemission spectroscopies, and density functional theory calculations, we give a description of the orbital character of bulk CrI3, and demonstrate that the emergence of ferromagnetism in this material is underpinned by the orbital mixing between I p and Cr eg states. Our results have clear impact on the understanding of how microscopic interactions at the orbital level stabilize ordered states in van der Waals ferromagnets.

TT 20.10 Tue 12:45 H8

Resonant Photoemission Studies of Transition Metal Sulfides and Selenides — •Yashasvi Mehra[1,2,3], Samuel Beaulieu[4], Mauro Faniculli[1,2], Olivier Heckmann[1,2], Karol Hricovini[1,2], Aki I.O. Pulkkinen[3], Jan Minar[3], and Maria Christine Richter[1,2] — [1]Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — [2]CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — [3]University of West Bohemia, NTC, Pilsen, Czech Republic — [4]Universite de Bordeaux CNRS CEA, CELIA, UMR5107, F33405 Talence, France

By performing resonant ARPES measurements and SPR-KKR photoemission calculations on Transition Metal Selenide, Sulfide and the Vanadium intercalated NbS2 systems, we study the interplay between different decay mechanisms in resonant conditions, radiation-less Raman Auger and Classical Auger emissions. Through a method proposed by Cini and Sawatzky we can determine the on-site Coulomb interaction per element in some cases. On the theoretical front the calculations are performed using the SPR-KKR method, which is based on one-step model, that incorporates the effect of all matrix elements which accounts for the photoemission process. Furthermore, we analyze calculated ARPES, XAS, element and orbital resolved band structure underlining agreement with experimental results and helping with its interpretation.

TT 21: Quantum Dots and Wires: Transport (joint session HL/TT)

Time: Tuesday 11:15–13:00 Location: H13

TT 21.1 Tue 11:15 H13

Transport properties of quantum dots for single-electron pumps — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Frank Hohls, and Hans W. Schumacher — Physikalisch-Technische Bundesanstalt, 31668 Braunschweig, Germany

A single-electron pump (SEP) is a device emitting a well-defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e, this results in a current of $I = nef$. Since the revision of the SI system, the elementary charge e hereby is an exact value, so that SEPs provide a suitable basis for a quantum current standard. The accuracy of this current is directly related to erroneous cycles, where the emitted number of electrons deviates from n. Our SEP devices are based on electrostatically defined quantum dots in GaAs/AlGaAs two-dimensional electron gases. In such devices, the tunnel barriers as well as the energy levels are controllable via gate voltages. Based on multiple quantum dot devices we here investigate relations between transport properties and SEP operation characteristics.

TT 21.2 Tue 11:30 H13

Non-Markovian higher-order electron pump: improvement of efficiency — •Lukas Litzba, Jürgen König, and Nikodem Szpak — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany

We consider an electron pump that consists of a non–interacting quantum dot and electron baths. Our pumping setup utilizes only higher–order tunneling processes, which are purely quantum mechanical and have no classical analog. In order to study higher order tunneling–mechanism and non–Markovian effects, we extend the exact Heisenberg equation and the Laplace transform technique to time–dependent Hamiltonians and apply this technique to our model. Thereby, we identify parameter ranges which lead to a significant increase of the current flowing through the quantum dot and an improvement of the energetic efficiency of these processes.

TT 21.3 Tue 11:45 H13

Fast Machine-Learning assisted characterisation of current quantisation — •Wang Ngai Wong[1], Yannic Rath[1], Nikolaos Schoinas[1], Shota Norimoto[1], Masaya Kataoka[1], Alessandro Rossi[1,2], and Ivan Runnger[1,3] — [1]National Physical Laboratory, Teddington, TW11 0LW, UK — [2]Department of Physics, SUPA, University of Strathclyde, Glasgow G4 0NG, UK — [3]Department of Computer Science, Royal Holloway, University of London, Egham, TW20 0EX, UK

Characterisation of single-electron pumps (SEPs) has long been bottlenecked by the process of fine-tuning measurement parameters to study their novel properties. This limits potential experimental parameters to those that can remain static throughout the fine-tuning process. We demonstrate a novel method assisted by machine learning which has led to an eightfold speedup in the measurement process (see Appl. Phys. Lett. 125, 124001 (2024)), and in so doing opens the door to further characterisation experiments which are impossible using conventional methods. Our method is based around an active learning cycle to navigate the information landscape of the gate voltage parameter space, while also significantly reducing the number of measurement points required. This is paired with a post-processing approach which allows us to accurately predict and characterise the small operational regimes significantly more efficiently than conventional sweeps across the parameter space. We exploit the framework to characterise the behaviour of multiplexed GaAs multi-pump devices across a range of magnetic fields.

TT 21.4 Tue 12:00 H13

Novel Mixed-Dimensional Reconfigurable Field Effect Transistors — •Sayantan Ghosh[1,2], Muhammad Bilal Khan[1], Phanish Chava[1], Kenji Watanabe[3], Takashi Taniguchi[3], Slawomir Prucnal[1], René Hübner[1], Thomas Mikolajick[2], Artur Erbe[1,2], and Yordan M Georgiev[1,4] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]National institute for Material Science, Tsukuba, Japan — [4]Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria

The limitations of CMOS downscaling drive the exploration of alternative device concepts like reconfigurable FETs (RFETs), which can dynamically switch between n- and p-polarity through electrostatic gating. This work introduces a novel mixed-dimensional RFET utilizing 1D silicon (Si) nanowires combined with 2D hexagonal boron nitride (hBN) as a dielectric and encapsulating layer. hBN*s insulating properties, chemical stability, and absence of dangling bonds make it ideal for its use as a dielectric in 1D electronics. The RFET fabrication employs electron beam lithography, reactive ion etching, and flash lamp annealing for precise silicide formation. Mechanically exfoliated hBN flakes (5-10 nm) were integrated using dry stamping transfer, with thickness characterized by microscopy techniques. Device characterization reveals improved subthreshold swing, on-current, and ION/IOFF ratio due to hBN*s 2D passivation, highlighting its potential for advanced nanowire-based RFET architectures.

TT 21.5 Tue 12:15 H13

Kondo effect for half-filling of the third shell of a quantum dot — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]1Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]2Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany

In this work, we investigate the electrical transport in the third shell [1] of a gate-defined GaAs quantum dot. The exact number of electrons in the quantum dot (N_e) is determined using a quantum point contact as a sensitive charge detector, detecting single-electrons tunneling through the system [2]. N_e is varied by changing the applied gate voltage.

The addition energy E_c for N_e = 7 - 11 shows a triangular behavior with a maximum at half-filling of the shell. This observed behavior is described analytically with Hund's rule exchange interaction. Besides, for successive numbers of electrons occupying the quantum dot N_e = 7 to 11, a Zero-bias anomaly (ZBA) characteristic for the Kondo effect is observed [3]. The width of the ZBA exhibits a triangular behavior, with a maximum at N_e = 9, similar to E_c. The broadening of the ZBA is attributed to the contribution of the Kondo resonance as well as Hund's satellite peaks, originating from the degenerate orbitals observed in the spectral function.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64, 701-736 (2001).
[2] T. Wagner, et. al., Nat. Phys.15, 330-334 (2019).
[3] J. Schmid, et. al., Phys. Rev. Lett. 84, 5824 (2000).

TT 21.6 Tue 12:30 H13

Beyond full counting statistics and Langevin theory: The quantum polyspectra approach to multi-detector measurements — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, Germany

The quantum polyspectra approach to quantum measurements has recently been shown to cover the full range between weak and strong quantum measurements [1 - 3]. It provides thus a more general approach to quantum measurements than the full counting statistics used in nano-electronics or the Langevin-approach used in spin noise spectroscopy. This approach draws its strength from comparing higher order spectra of the measurement record with model spectra calculated from quantum expressions that are calculated on the level of a Lindblad master equation. Here, we generalize the polyspectra approach to include the case of the simultaneous measurements of more than one quantity of a quantum system. The approach regards measurement induced damping, measurement backaction, and the quantum Zeno effect. We give a few examples of multi-detector polyspectra that were calculated by a multi-detector extension of our SignalSnap and QuantumCatch library [4, 5].

[1] Hägele et al., PRB 98, 205143 (2018)
[2] Sifft et al., PRR 3, 033123 (2021)
[3] Sifft et al., PRA 109, 062210 (2024)
[4] https://github.com/MarkusSifft/SignalSnap
[5] https://github.com/MarkusSifft/QuantumCatch

TT 21.7 Tue 12:45 H13

Revealing Hidden States in Quantum Dot Array Dynamics: Quantum Polyspectra Versus Waiting Time Analysis — •Markus Sifft[1], Johannes C. Bayer[2], Daniel Hägele[1], and Rolf J. Haug[2] — [1]Faculty of Physics and Astronomy, Ruhr University Bochum, GER — [2]Institute of Solid State Physics, Leibniz Universität Hannover, GER

We show how by virtue of the recently introduced quantum polyspectral analysis of transport measurements [1,2], the complex transport measurements of multi-electron QD systems can be analyzed. This method directly relates higher-order temporal correlations of a raw quantum point contact (QPC) current measurement to the Liouvillian of the measured quantum system. By applying this method to a two-electron double QD system, we uncover dynamics between singlet and triplet states, indistinguishable in the QPC current, without requiring the identification of quantum jumps or prior assumptions about the number of quantum states involved. Our findings demonstrate that system models in such cases of hidden dynamics are inherently non-unique. Furthermore, we compare our method to a traditional analysis via the waiting-time distribution. Our method achieves parameter estimates with up to 50% lower errors, while also being applicable in scenarios with low signal-to-noise, where traditional counting methods falter. Our approach challenges previous assumptions and models, offering a more nuanced understanding of QD dynamics and paving the way for the optimization of quantum devices. [1] Hägele et al., PRB 98, 205143 (2018), [2] Sifft et al., PRR 3, 033123 (2021)

TT 22: Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)

Time: Tuesday 14:00–15:30 Location: H37

TT 22.1 Tue 14:00 H37

Power-law banded random matrices as models for quantum many-body Hamiltonians — •Wouter Buijsman[1], Masudul Haque[2,1], and Ivan M. Khaymovich[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]TU Dresden, Institute of Theoretical Physics, Dresden, Germany — [3]Nordita, Stockholm, Sweden

Hamiltonians of one-dimensional, disordered single-particle sytems with long-range hoppings can naturally be modeled by power-law banded random matrices. In this picture, the phase diagram of power-law banded random matrices show an ergodic, weakly ergodic, and localized phase. Motivated by modern developments on ergodicity breaking and localization in interacting quantum many-body systems, we study many-body interpretations of such random matrices. We discuss a number of ways to label the basis states with many-body configurations, and compare the physical properties of the resulting Hamiltonians. Specifically, we study the scaling of the many-body entanglement entropy with system size for eigenstates at both the bulk and the edge of the spectra. Using a scaling analysis on the full sets of eigenstates, we subsequently provide a quantitative picture of the phase diagram. We elaborate on the physical relevance of this interpretation of random matrix models for quantum many-body systems.

TT 22.2 Tue 14:15 H37

Escaping the Krylov space during reorthogonalization — •Max Pieper, Jannis Eckseler, and Jürgen Schnack — Universität Bielefeld

Krylov complexity [1] is often used as a measure of complexity in quantum many-body-systems. During its calculation, the Lanzcos algorithm is used to construct an operator basis. Due to the poor orthogonality of the resulting basis reorthogonalization is often employed [2]. We investigate how using reorthogonalization causes the Lanczos algorithm to accumulate non-Krylov basis elements. We suspect this to negatively affect the Krylov algorithm.

[1] D. E. Parker et al. Phys. Rev. X 9, 041017 (2019)
[2] E. Rabinovici et al. JHEP 06, 062 (2021)

TT 22.3 Tue 14:30 H37

An estimate of the equilibration time based on the operator growth hypothesis — •Merlin Füllgraf, Jiaozi Wang, and Jochen Gemmer — Universität Osnabrück

We study the equilibration times T_{eq} of local observables in quantum chaotic systems by considering their auto-correlation functions. Based on the recursion method, we suggest a scheme to estimate T_{eq} from the corresponding Lanczos coefficients. We numerically find that, if an observable follows the *operator growth hypothesis*, a finite number of Lanczos coefficients is sufficient for a reasonable estimate of the equilibration time. This implies that equilibration occurs on a realistic time scale much shorter than the life of the universe. The numerical findings are further supported by analytical arguments.

TT 22.4 Tue 14:45 H37

Effects of chaos in Bose-Hubbard systems with few degrees of freedom. The smallest possible heat engine? — •Viviane Bauer, Nico Fink, and James Anglin — Physics Department and Research Center OSCAR, RPTU Kaiserslautern-Landau

Microscopic engines are a research focus in both biochemistry and nanotechnology. While other forms of engines besides heat engines are also being considered, the fully microscopic limit of a heat engine is a fundamentally important problem in physics. What happens to thermodynamics when not only the working fluid and mechanism of a heat engine, but even the hot and cold reservoirs are microscopic?

To realize such microscopic heat baths, we turn to the process of chaotic ergodization, studied in Bose-Hubbard dimers and trimers.

One realization we currently study is based on two Bose-Hubbard trimers, which allow energy and particle transport between them. The particle transport is furthermore coupled to a mass, so our engine works against a force to lift it. Moreover, we have identified a dynamic mechanism which can stabilize this lifting process. The result is a system which operates just like a heat engine, except for being fully microscopic. The structure of coupled chaotic subsystems both supports and requires an understanding of the fully microscopic heat engine in terms of open-system control.

TT 22.5 Tue 15:00 H37

Impurity coupled to the SYK bath — •Anastasia Enckell and Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

System-plus-bath models play an important role in addressing fundamental questions in condensed matter physics. One challenging aspect is modelling the bath, which is often approached using free-particle or open quantum system frameworks. Here, we explore the Sachdev-Ye-Kitaev (SYK) model as a new kind of quantum bath with unique properties, including the absence of quasiparticles, maximal chaos, and non-integrability, which make it a valuable framework for studying system-plus-bath interactions. We study the time evolution of the occupation of an impurity coupled to the SYK bath following a quench. From the Kadanoff-Baym equations for a noninteracting impurity, we see that the only relevant property for the impurity occupation is a combination of hybridisation and density of states of the bath. These parameters can be adjusted in order to model the impurity coupled to any bath of interest. Using this approach, we can study the impurity dynamics coupled to the SYK bath by making suitable changes to the hybridisation in impurity plus Fermi bath setting, which significantly simplifies the task. We observe oscillatory dynamics of the impurity at zero temperature, with the oscillations decreasing as the temperature increases. This behaviour contrasts with that of a free-particle bath and suggests interesting underlying physics.

TT 22.6 Tue 15:15 H37

Thermal-relaxation asymmetry in fluctuating hydrodynamics — •Felipe Pereira-Alves and Aljaž Godec — Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, 37077 Göttingen, Germany

It was theoretically predicted and recently experimentally confirmed that small systems, such as trapped colloidal particles quenched far from equilibrium, heat up faster than they cool down. The phenomenon was coined thermal-relaxation asymmetry. The proposed physical explanation of the asymmetry instigated intriguing questions about its existence in the thermodynamic limit. Here we investigate thermal relaxation dynamics in far-from-equilibrium temperature quenches on the level of fluctuating hydrodynamics of short- and long-range (logarithmically) interacting many-body systems. We prove the existence of a strict asymmetry for any temperature quench for both, short- and long-range interactions. Remarkably, in contrast to small systems, there is no "close-to-equilibrium" regime of quenches for which heating and cooling are symmetric. Notably, we find that relaxation is self-similar up to the relaxation time, and uncover intricate differences between short- and long-range interactions.

TT 23: Members' Assembly

Time: Tuesday 14:15–15:45 Location: H33

All members of the LT Division are heartfully invited to join!
Topics:

- **Report**
- **Outlook 2025**
- **Miscellaneous,**

TT 24: Unconventional Superconductors

Time: Wednesday 9:30–13:00 Location: H31

Invited Talk TT 24.1 Wed 9:30 H31

Possible Origin of High-Field Reentrant Superconductivity in UTe_2 — •Toni Helm — Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Due to its potentially spin-triplet-superconducting ground state, UTe_2 (fondly called Ute) has triggered a wave of enthusiasm among condensed-matter researchers since the discovery of superconductivity below 1.6 K in this anisotropic heavy-fermion paramagnet. As the quality of single crystals improved, e.g., T_c was pushed to 2.1 K, some of the fog about Ute's mysterious properties has cleared. Nevertheless, the excitement has only become stronger as Ute exhibits signatures of multiple superconducting phases with distinct order parameters stabilized by different tuning parameters such as pressure, magnetic field, or field orientation. Particularly, strong magnetic fields applied to Ute appear to not only suppress superconductivity, as expected for a textbook superconductor, but also enhance and enable additional phases in a rare and very unconventional phase diagram.

In this talk, we will look at Ute's high-field properties and review recent results concerned with the field-induced superconducting phases in this special compound. In particular, we will focus on what is known so far about the reentrant superconductivity that sets in for specific field orientations at field values beyond approximately 40 T. Latest results from experiments in fields up to 70 T have certain implication to the possible origin of the extremely field-robust reentrant superconductivity in UTe_2.

[1] T. Helm et al., Nat. Commun. 15 (2024).

TT 24.2 Wed 10:00 H31

Fermi surface studies on UTe_2 — •F. Husstedt[1,2], B. V. Schwarze[1], J. P. Brison[3], G. Knebel[3], G. Lapertot[3], M. Kimata[4], D. Aoki[4], T. Helm[1], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Centre CEA de Grenoble, France — [4]Institute for Materials Research, Tohoku University, Japan

To date, the presence of three-dimensional (3D) Fermi surfaces in the heavy-fermion superconductor UTe_2 is strongly debated. We had access to high-quality UTe_2 single crystals with $T_c = 2$ K to perform angle-dependent measurements of the magnetic torque, magnetotransport, and Hall effect. The observed quantum oscillations provide further insight into the electronic structure of UTe_2. We measured de Haas-van Alphen frequencies that show a very good agreement with previous reports. Consistent with two-dimensional Fermi-surface cylinders, we also observed a 100 T Shubnikov-de Haas (SdH) frequency for field oriented along the crystallographic *a* axis. We investigated the angular dependence of this frequency in the *a*-*b* plane as well as in the *a*-*c* plane to clarify if it may originate from a 3D Fermi surface. The temperature dependence of the 100 T SdH frequency reveals an effective mass much lower than the ones reported for the fundamental frequencies.

TT 24.3 Wed 10:15 H31

Investigating the strain dependence of the lower and upper superconducting critical fields in Sr_2RuO_4: A novel approach using elastocaloric effect measurements — •Aleksei Frolov[1], You-Sheng Li[1], Naoki Kikugawa[2], Andreas W. Rost[3], Andrew P. Mackenzie[1,3], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Institute for Materials Science, Japan. — [3]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

Elastocaloric measurements under uniaxial stress are an extremely sensitive technique that provides rich thermodynamic information. This is especially true when studying materials, such as the unconventional superconductor Sr_2RuO_4 [1]. In particular, the investigation of the elastocaloric effect in an applied magnetic field is challenging and pioneering, but highly relevant.

We have performed high resolution elastocaloric measurements on Sr_2RuO_4 in a magnetic field along the [001] axis with uniaxial stress applied in the [100] direction at low temperatures. We have studied the strain dependence of the lower and upper superconducting critical fields. Both show a dome-like shape with a maximum close to the Van Hove strain. We discuss the advantages and limitations of the elastocaloric technique compared to conventional probes such as electrical resistivity and susceptibility, highlighting its contribution to the understanding of unconventional superconductivity in Sr_2RuO_4.

[1] Y. S. Li *et al.*, Nature 607, 276 (2022).

TT 24.4 Wed 10:30 H31

Why scanning tunneling spectroscopy of Sr_2RuO_4 sometimes does not see the superconducting gap — •Adrian Valadkhani[1], Jonas Profe[1], Andreas Kreisel[2], Peter Hirschfeld[3], and Roser Valenti[1] — [1]Goethe University, Frankfurt am Main, Germany — [2]University of Copenhagen, Copenhagen, Denmark — [3]University of Florida, Gainesville, USA

Scanning tunneling spectroscopy (STS) and scanning tunneling microscopy (STM) are perhaps the most promising ways to detect the superconducting gap size and structure in the canonical unconventional superconductor Sr_2RuO_4 directly. However, in many cases, researchers have reported being unable to detect the gap at all in STM conductance measurements, while in others they were able to find the gap. Recently, an investigation of this issue on various local topographic structures on a Sr-terminated surface found that superconducting spectra appeared only in the region of small nanoscale canyons, corresponding to the removal of one RuO surface layer. In this talk, we analyze the electronic structure of various possible surface structures using ab initio density functional theory (DFT), and argue that bulk conditions, favorable for superconductivity, can be achieved, when removal of the RuO layer suppresses the RuO4 octahedral rotation locally. Our findings are supported by a paper recently published using numerical methods beyond DFT-random phase approximation (RPA) and functional renormalization group (FRG). We further propose alternative terminations to the most frequently reported Sr termination where superconductivity surfaces should be observed.

TT 24.5 Wed 10:45 H31

Complex impedance scanning tunneling microscopy as a probe for unconventional superconductors — •Amber Mozes[1], Sanghun Lee[2], Tjerk Benschop[1], Koen Bastiaans[1], and Milan Allan[1,2] — [1]Leiden University, Leiden, The Netherlands — [2]LMU, Munich, Germany

In many unconventional superconductors, the superconducting state is spatially inhomogeneous, and macroscopic superconductivity is suppressed. To understand what causes this suppression of superconductivity, we are developing a probe to measure the local complex impedance. We combine scanning tunneling microscopy (STM) with microwave microscopy. This could, in principle, allow to locally probe the impedance response and relate this to inhomogeneity in free carrier density whenever macroscopic homogeneity is suppressed. More specifically, it would be possible to measure the kinetic inductance of a superconductor, governed by the Meissner effect, as well as local resistivity from non superconducting carriers. Implementation of complex impedance measurements in STM requires a microwave impedance matching circuit to enable simultaneous DC and AC readout of the tip-sample response. I will present our recently developed chip circuits that are in situ replaceable, enabling sample specific circuit design, with the aim to impedance match for superconducting sample properties.

TT 24.6 Wed 11:00 H31

Tunneling spectroscopy on superconducting thin films of non-centrosymmetric niobium rhenium — •Marcel Strohmeier[1], Carla Cirillo[2], Andriy Smolyanyuk[3], Karsten Held[3], Carmine Attanasio[4], Angelo Di Bernardo[1,4], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]CNR-Spin, c/o University of Salerno, 84084 Fisciano (SA), Italy — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [4]Department of Physics 'E.R. Caianiello', University of Salerno, 84084 Fisciano (SA), Italy

In recent years, non-centrosymmetric superconductors have attracted increasing attention as they reveal various properties of unconventional superconductivity. With the absence of inversion symmetry and an asymmetric Rashba-type spin-orbit coupling (SOC) a mixed spin-singlet and spin-triplet pairing state is predicted in these materials. In our talk, we focus on the non-centrosymmetric compound $Nb_{0.18}Re_{0.82}$, whose superconducting order parameter remains under debate. Its favorable combination of material properties such as structural disorder, strong SOC and relatively high critical current densities makes NbRe an promising candidate for applications in superconducting single-photon detection and gate-controlled supercurrent devices. We present low-temperature scanning tunneling microscopy measurements on polycrystalline NbRe fabricated by magnetron sputtering. Using high-energy resolution N-I-S spectroscopy, we probe the local density of states in thin films of varying thickness and crystallinity to gain insights into the intrinsic pairing symmetry of the superconductor.

15 min. break

Invited Talk TT 24.7 Wed 11:30 H31

Unconventional Superconductivity in Epitaxial $KTaO_3$-Based Heterostructures — •Denis Maryenko — RIKEN Center for Emergent Matter Science, Wako, Japan

Spin-orbit coupling (SOC) is a driving force behind the emergence of novel quantum phenomena. Among these, superconductivity is particularly exciting due to its potential to form unconventional superconducting states that challenge conventional theories. The perovskite $KTaO_3$, with its inherently strong SOC, has recently gained attention as a promising material platform for exploring these phenomena. However, achieving precise control over interfacial electronic states to realize a conductive layer in $KTaO_3$ remains a significant challenge.

In this work, we present out recent progress on epitaxially grown $KTaO_3$-based heterostructures, with a focus on the $LaTiO_3$-$KTaO_3$ (110) interface[1]. Our findings reveal a systematic emergence of superconductivity in these structures. We demonstrate that the superconducting state, signaling unconventional Cooper pairing, can be tuned by electric and magnetic fields. This study sheds light on the interplay between superconductivity and SOC in low-dimensional systems, contributing to the broader understanding of quantum materials with strong spin-orbit interaction.

[1] D. Maryenko et al., APL Materials 11, 61102 (2023).

TT 24.8 Wed 12:00 H31

Topological Fermi Arcs and Surface Superconductivity in $PtBi_2$ — •Julia Besproswanny[1], Sebastian Schimmel[1], Sven Hoffmann[1], Gregory Shipunov[2], Saicharan Aswartham[2], Joaquin Puig[3], Yanina Fasano[3], Danny Baumann[2], Ricardo Vocaturo[2], Jorge I. Facio[3], Oleg Jansen[2], Jeroen van den Brink[2], Bernd Büchner[2], and Christian Hess[1] — [1]University of Wuppertal, 42119 Wuppertal, Germany — [2]IFW Dresden, 01069 Dresden, Germany — [3]Centro Atómico Bariloche, Instituto Balseiro, 8400 Bariloche, Argentina

t-$PtBi_2$ is a topological Weyl semimetal, as evidenced by band structure and quasiparticle interference (QPI) investigations [1]. It also exhibits unconventional surface superconductivity [2,3], with ARPES revealing a superconducting energy gap only on the Fermi arc states [3]. Low-temperature scanning tunneling microscopy and spectroscopy (STM/STS) reveals locally varying sample-dependent superconductivity revealed by the energy gap. In some cases the scale of the gap suggests BCS critical temperatures as high as 70-130 K. We study the temperature and magnetic field dependence of the the energy gap, demonstrating its persistence up to 50 K. Furthermore, QPI measurements in the superconducting state indicate an interplay between topological Fermi arcs and superconductivity.

[1] S. Hoffmann et. al., Adv. Phys. Res. 2400150 (2024);
[2] S. Schimmel et. al., Nat. Commun. 15, 9895 (2024);
[3] A. Kuibarov et. al., Nature 626, 294(2024).

TT 24.9 Wed 12:15 H31

Unconventional Superconductivity in Trigonal $PtBi_2$: Ginzburg–Landau Theory — Harald Waje[1], Ion Cosma Fulga[2], Jeroen van den Brink[2,3], and •Carsten Timm[1,3] — [1]TU Dresden, 01062 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden (IFW), 01069 Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Trigonal $PtBi_2$ is a Weyl semimetal that exhibits unconventional surface superconductivity carried by the Fermi arcs [1]. Recent results indicate that the superconducting gap might be nodal, i.e., exhibiting topologically protected Majorana cones. There are three possible superconducting order parameters, corresponding to the three irreducible representations A_1, A_2, and E of the noncentrosymmetric point group C_{3v}. The gap has s-wave ($l = 0$), i-wave ($l = 6$), or d-wave ($l = 2$) symmetry, respectively. We set up a Ginzburg–Landau theory for these order parameters, which also includes coupling to an applied magnetic field. Finally, we discuss some effects described by this theory, such as field-induced pair-density waves.

[1] A. Kuibarov *et al.*, Nature **626**, 294 (2024).

TT 24.10 Wed 12:30 H31

Symmetry-Preserving First-Order Superconductor-to-Superconductor Transition in Heavy-Fermion $CeRh_2As_2$ — •Fabian Jakubczyk[1,2], Julia Link[1,2], and Carsten Timm[1,2] — [1]TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Locally noncentrosymmetric materials are attracting significant attention due to the unique phenomena associated with sublattice degrees of freedom. The recently discovered heavy-fermion superconductor $CeRh_2As_2$ has emerged as a compelling example of this class, garnering widespread interest for its remarkable H-T phase diagram, which features field-induced multi-phase superconductivity with non-trivial angular dependencies and large critical fields, as well as antiferromagnetic order, and potential higher multipole orders. To investigate the complex interplay of the ordered phases in $CeRh_2As_2$ including the impact of a magnetic field, we develop a theoretical framework based on group-theoretical considerations, combined with Bogoliubov–de Gennes and Ginzburg–Landau methods. This approach enables us to propose probable symmetries of the superconducting states and elucidate their close relationship with magnetism in this material. Intriguingly, we find that the dominant first-order transition can be interpreted as a transition between coexistence phases of the same symmetry but with distinct admixtures of individual order parameters. Our approach accurately reproduces current experimental phase diagrams, both if the transition to a magnetic phase occurs below the superconducting critical temperature and if it occurs above.

TT 24.11 Wed 12:45 H31

Cause and Effect - Understanding the Fundamental Principles Determining the Gap Structure in Fluctuation Driven Superconductors — •Jonas Profe[1], Olivier Gingras[2], Antoine Georges[3,2,4,5], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA — [3]College de France, 11 place Marcelin Berthelot, 75005 Paris, France — [4]Centre de Physique Theorique, Ecole Polytechnique, CNRS, Institut Polytechnique de Paris, 91128 Palaiseau Cedex, France — [5]DQMP, Universite de Geneve, 24 quai Ernest Ansermet, CH-1211 Geneve, Suisse

Describing and understanding unconventional superconductors is one of the major challenges of modern condensed matter physics. Here, central questions are, what determines which symmetry the superconducting order will have in a material and how can we engineer specific superconducting orders? In this talk, we disentangle how the effective pairing interaction and the electronic structure influence the resulting superconducting order for attractive interactions mediated by fluctuations. For this, we analytically dissect the linearized gap equation in order to extract as much information as possible. We then exemplify how one can utilize this understanding to design models showing specific ordering tendencies in both a single and a multi-orbital setting.

TT 25: Superconductivity: Supercurrent Diode Effect

Time: Wednesday 9:30–12:30 Location: H32

TT 25.1 Wed 9:30 H32

Gate Tunable Anomalous Josephson and Supercurrent Diode Effect — •Johanna Berger[1], Simon Reinhardt[1], Christian Baumgartner[1], Lorenz Fuchs[1], Tim Ascherl[1], Andreas Costa[2], Sergei Gronin[3], Geoff Gardner[3], Tyler Lindemann[3], Michael Manfra[3], Jaroslav Fabian[2], Denis Kochan[2,4], Christoph Strunk[1], and Nicola Paradiso[1] — [1]Institut für Experimentelle und Angewandte Physik, University of Regensburg, 93040 Regensburg, Germany — [2]Institut für Theoretische Physik, University of Regensburg, 93040 Regensburg, Germany — [3]Purdue University, West Lafayette, Indiana 47907 USA — [4]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

The discovery of the supercurrent diode effect by Ando et al. [1] and its observation in a rich variety of systems caused an increasing interest in the physics of non-reciprocal superconductivity.

Here, we study Josephson junctions in hybrid Al/InGaAs/InAs structures, which harbor strong Rashba spin-orbit interaction. In combination with a Zeeman field, this gives rise to an anomalous phase shift φ_0 in the current-phase relation (CPR). The presence of high harmonics in the CPR gives rise, in addition, to the supercurrent diode effect [2,3,4]. Using an asymmetric superconducting quantum interferometer we simultaneously measure the φ_0-shift and supercurrent diode effect on a single junction [5]. By electrostatic gating of the junction, we reveal the link between the φ_0-shift and supercurrent diode effect.

TT 25.2 Wed 9:45 H32

Unconventional Josephson Supercurrent Diode Effect Induced by Chiral Spin-Orbit Coupling — •Andreas Costa[1], Osamu Kanehira[2], Hiroaki Matsueda[2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]Tohoku University, Japan

First-principles calculations have recently predicted that chiral materials lacking mirror symmetries—such as twisted van-der-Waals homobilayers—can feature unconventional radial Rashba coupling with spins aligned fully parallel (instead of tangentially) to momentum.

In this talk, we will address Josephson transport through vertical superconductor/ferromagnet/superconductor junctions hosting crossed (radial and tangential) Rashba fields at the interfaces and demonstrate that their interplay with ferromagnetic exchange can lead to supercurrent rectification even when the magnetization is collinear with the current. This so-called unconventional supercurrent diode effect (SDE) originates from spin precessions inside the ferromagnet, which imprint polarity-dependent transmission probabilities on the Cooper pairs being well-distinct from the conventional SDE, and provides a sensitive probe of chiral spin textures.

This work has been supported by DFG Grants 454646522 and 314695032 (SFB 1277).

TT 25.3 Wed 10:00 H32

Tunable Field-Free Unidirectional Diode Effect in Single-Crystal Superconducting Device — •Tobias Faeth[1], Damien Berube[2], Killian Rigaux[2], Yuqiang Fang[3], Anyuan Gao[2], Thao Dinh[2], Yufei Liu[2], Jianxiang Qiu[2], Houchen Li[2], Charles Reichhardt[4], Cynthia Reichhardt[4], Fuqiang Huang[3], and Suyang Xu[2] — [1]Max Plack Instiute for Microstructure Physics, Halle (Saale), Germany — [2]Harvard University, Cambridge, USA — [3]Bejing University, Beijing, China — [4]Los Alamos National Laboratory, Los Alamos, USA

Superconducting diodes could become critical components of multiple technologies, from energy-efficient superconducting computing to large scale effective quantum computing, memories and switches. In this talk, we report a device made out of a 2D superconductor, that exhibits field-free, tunable, and perfectly rectifying diode effect. Starting from finite field differential conductance experiments, we demonstrate diode efficiencies up to 30% at 100mT. Measuring nonlinear resistances, we characterize magnetochiral anisotropy (MCA) and calculate a MCA coefficient of $\gamma = 6.0 \times 10^8\ \mathrm{T^{-1}A^{-1}}$, the highest ever reported. Setting the field back to 0, we investigate a novel geometry, while carrying out differential conductance measurements. In the new geometry, we find $I_c^+ = 0$ while $I_c^- = 2\mu A$, a 100% diode efficiency. We hypothesize this effect is attributed to uneven vortex flow under opposite biases. We substantiate this model with computations that confirm increased diode efficiency under the novel geometry.

TT 25.4 Wed 10:15 H32

Tunable Diode effect in a Superconducting Tunnel Junction with Biharmonic Drive — •David Scheer[1], Rubén Seoane Souto[2], Fabian Hassler[1], and Jeroen Danon[3] — [1]Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [2]Instituto de Ciencia de Materiales de Madrid, Consejo Superiorde Investigaciones Científicas (ICMM-CSIC), 28049, Madrid, Spain — [3]Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

A Josephson diode is a superconducting circuit element that enables nonreciprocal transport, allowing a dissipationless supercurrent to preferentially flow in a single direction. Existing methods for achieving the required symmetry breaking mostly rely on specifically-designed materials or carefully-engineered circuits composed of multiple Josephson junctions. In this talk, we demonstrate that applying a biharmonic drive to a conventional superconducting tunnel-junction induces a diode effect through harmonic mixing processes that shift the supercurrent region. We show that, in a conventional tunnel junction, unit efficiency is achievable while maintaining a large supercurrent. Moreover, the relative phase between the two driving tones determines the directionality of the diode, which can be tuned in situ.

TT 25.5 Wed 10:30 H32

Spin-Resolved Josephson Diode Effect in Strongly Polarized SFS Junctions — •Danilo Nikolić, Niklas L. Schulz, and Matthias Eschrig — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Strasse 6, 17489 Greifswald, Germany

We present a systematic study of equal-spin Cooper pair formation at the interface between a superconductor (S) and a helical ferromagnet (F) [1]. The theory is done in the framework of the quasiclassical Green's function formalism [2-4]. However, assuming the large splitting between the spin bands in F, the standard quasiclassical approach cannot be applied directly and requires a modified description [5-8]. Applying this approach, we account for the long-ranged (equal-spin) Josephson current-phase relation (CPR) in an SFS weak link considering a helimagnetic state in F. Remarkably, the CPR takes a nontrivial form leading to both the anomalous and Josephson diode effects. These effects have clear physical interpretations based on the coupling between the superconducting phase and the adiabatic spin gauge field (geometric phase) induced by inhomogeneous magnetization of F.

[1] A. Spuri *et al.*, Phys. Rev. Res. **6**, L012046 (2024).
[2] G. Eilenberger, Z. Phys. **214**, 195 (1968).
[3] A.I.Larkin, Yu.N.Ovchinnikov, Sov. Phys. JETP **28**, 1200 (1969).
[4] A. I. Buzdin, Rev. Mod. Phys. **77**, 935 (2005).
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[6] R. Grein *et al.*, Phys. Rev. Lett. **102**, 227005 (2009).
[7] M. Eschrig, Rep. Prog. Phys. **78**, 104501 (2015).
[8] I. V. Bobkova *et al.*, Phys. Rev. B **96**, 094506 (2017).

TT 25.6 Wed 10:45 H32

Spin and Charge Josephson Diode Effect in Diffusive Superconductor-Ferromagnet Heterostructures — •Niklas L. Schulz, Danilo Nikolić, and Matthias Eschrig — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Strasse 6, 17489 Greifswald, Germany

Long-range equal-spin triplet supercurrents in the presence of a nontrivial spin texture are of fundamental importance for applications of superconducting spintronics [1]. In this work we investigate quantum geometric phases in a Josephson trilayer consisting of a strongly spin-polarized ferromagnet connected to BCS su-

perconductors by ferromagnetic insulating barriers. For non-coplanar spin textures of the device, spin-geometric phases arise, which enter the current-phase relation additionally to the superconducting phase difference [2]. In general, such spin-geometric phases are induced by gauge fields entering the transport equation [3] and in the considered case these are caused by spin-dependent U(1) gauge fields. The resulting current-phase relation in such devices allows for the observation of a Josephson diode effect in the charge current for symmetric systems and a diode effect in the spin current for asymmetric configurations. In certain cases, the device also allows to switch between fully spin-polarized supercurrents across the ferromagnet by reversing the Josephson phase.

[1] M. Eschrig, Rep. Prog. Phys. **78**, 104501 (2015)
[2] R. Grein et al., Phys. Rev. Lett. **102**, 227005 (2009)
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15 min. break

TT 25.7 Wed 11:15 H32

Josephson diode fabricated by a focused He-Ion beam in a $YBa_2Cu_3O_7$ thin film. — •Edward Goldobin, Alireza Jozani, Christoph Schmid, Reinhold Kleiner, and Dieter Koelle — Universität Tübingen, Germany

We report on the fabrication of a Josephson diode with high asymmetry and size $\approx 1\ \mu m^2$. The device is fabricated from $YBa_2Cu_3O_7$ thin films by creating nanopatterns using a focused He-ion beam (He-FIB). He-FIB irradiation of different doses allows us to "write" both Josephson barriers as well as amorphous resistive walls (circuit boundaries) on a sub-micron scale [1]. We have fabricated sub-μm Josephson junctions of in-line geometry that have rather skewed $I_c(H)$ dependences. At the optimal value of the applied magnetic field H, the ratio of positive and negative critical current I_c reaches ≈ 7. Such a high asymmetry is key for achieving good figures of merit, e.g. a wide rectification window, large stopping forces and a high rectification efficiency [2]. The rectification of an ac current into an average dc voltage $\langle V \rangle$ was investigated experimentally by measuring rectification curves $\langle V \rangle(I_{ac})$ at $T = 4.2$ K. Average dc voltages as high as 212 μV were achieved for the optimum value of the driving amplitude I_{ac}. Further, the diode was loaded, which allowed us to measure the input and the output power and, therefore, experimentally demonstrate the efficiency, which reaches 80% in some regimes [3].

[1] B. Müller et al., Phys. Rev. Applied **11**, 044082 (2019).
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TT 25.8 Wed 11:30 H32

Investigation of Josephson junctions with Weyl-Kondo semimetals — •Ronja Fischer-Süsslin[1], Roman Hartmann[1], Thành Tran[1], Diana Kirschbaum[2], Xinlin Yan[2], Andrey Prokofiev[2], Angelo Di Bernardo[1,3], Silke Paschen[2], and Elke Scheer[1] — [1]FB Physik, Universität Konstanz, Konstanz, Deutschland — [2]Institut für Festkörperphysik, TU Wien, Wien, Österreich — [3]Dipartimento di Fisica, Università di Salerno, Fisciano, Italy

A superconducting diode, i.e., a device with a polarity dependent supercurrent amplitude, would provide new functionalities for superconducting circuits. The superconducting diode effect (SDE) was observed in 2020 [1] in an artificial superlattice with inversion symmetry breaking and is now investigated in both Josephson junctions and junction-free superconductors. We have fabricated and investigated Josephson junctions composed of Nb electrodes and the Ce-based Weyl-Kondo semimetals $Ce_3Bi_4Pd_3$ [2] and $CeRu_4Sn_6$ [3] as weak links. These topologically nontrivial materials are promising candidates to investigate the SDE due to their noncentrosymmetry and strong spin-orbit coupling, which are also responsible for the purely electric-field-driven nonlinear spontaneous Hall response [2,3].

[1] F. Ando et al., Nature **584**, 373-376 (2020).
[2] S. Dzsaber et al., PNAS **118**, e2013386118 (2021).
[3] D.Kirschbaum et al., arXiv:2404.15924 (2023).

TT 25.9 Wed 11:45 H32

Cooper pair diode in Coulomb blockade Pb islands on graphene — •Stefano Trivini[1,3], Jon Ortuzar[1], Katerina Vaxevani[1], F Sebastian Bergeret[3,4], and Jose Ignacio Pascual[1,2] — [1]CICnanogune, Donostia, Spain — [2]Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [3]Centro de Física de Materiales (CFM),San Sebastián, Spain — [4]Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain

Non-reciprocity, essential for current rectification in electronics, is challenging to achieve in superconducting devices without external magnetic fields. Current methods rely on non-centrosymmetric materials or magnetochiral effects, limiting their versatility. We investigate small Pb islands on graphene where Coulomb and superconducting correlations coexist. Approaching the STM tip to Josephson regimes, we observe Resonant Cooper Pair Tunneling (RCT) peaks in the current-voltage characteristics. RCT values change with gating. We test this in a current-biased STM junction and find a CP current asymmetric with polarity. This is a realization of non-reciprocal transport of CP, tunable with a gate.

TT 25.10 Wed 12:00 H32

Magnetoelectric phenomena and radial Rashba diode effect in noncentrosymmetric superconductors — •Denis Kochan — Department of Physics, National Cheng Kung University, Tainan, Taiwan — Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia

The superconducting diode effect is a magneto-electric phenomenon where an external magnetic field imparts a non-zero center-of-mass momentum to Cooper pairs, either facilitating or hindering the flow of electric current depending on its direction. One possible mechanism leading to SDE is a lack of inversion symmetry that facilitates spin splitting of the electronic bands by the underlying spin-orbit coupling (SOC). When breaking also the time-reversal by a weak magnetic/exchange field the Cooper pairs condensate displays intriguing magneto-electric and magneto-chiral effects.

This talk will present a theoretical overview and key experimental observations, particularly supercurrent diode effect and Josephson inductance anisotropy in InAs-quantum well-based junctions [1], zero-pi-like transitions and anomalous Josephson effect in non-centrosymmetric systems [2], enhanced vortex pinning and squeezing in Rashba-based superconductors [3]. The new kid on the block is the radial Rashba SOC giving rise to a novel Radial Rashba spin-diode effect [4].

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[3] Phys. Rev. X 12, 041020 (2022).
[4] Phys. Rev. Lett. 133, 216201 (2024).

TT 25.11 Wed 12:15 H32

The Josephson diode effect with Andreev and Majorana states — •Sayan Mondal[1], Pei-Hao Fu[2], and Jorge Cayao[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden — [2]Science, Mathematics and Technology, Singapore University of Technology and Design, Singapore 487372, Singapore

We consider a Josephson junction formed by Rashba superconductors and investigate the Josephson diode effect as the system transitions from a trivial to a topological phase under an applied external Zeeman field [1]. The component of the Zeeman field parallel to the spin-orbit axis introduces asymmetry in the Andreev bound states, which in turn leads to an asymmetry in the Josephson current, giving rise to the diode effect. In this study, we analyze the forward and backward currents, which differ due to the presence of the parallel Zeeman field. We discover that the diode's efficiency as a function of the Zeeman field exhibits a rich structure strongly dependent on the Andreev bound states. This dependence reveals clear signatures of the topological phase of transition. Notably, in the topological phase, the diode efficiency develops an oscillatory pattern reflecting Majorana bound states' formation. We have also verified that the functionality of the obtained Josephson diode is robust against finite temperatures, below the superconducting gap. Our findings help us understand the realization of Josephson diodes in topological superconductors and can also be useful for identifying the emergence of Majorana bound states.

[1] S. Mondal, P. -H. Fu, and J. Cayao, In preparation.

TT 26: Correlated Magnetism – Frustrated Systems

Time: Wednesday 9:30–12:45 Location: H33

TT 26.1 Wed 9:30 H33

Temperature-magnetic field phase diagram of the honeycomb Kitaev system $Na_2Co_2TeO_6$ — •Sebastian Erdmann[1], Prashanta Mukharjee[1], Chanhyeon Lee[2], Kwang-Yong Choi[3], and Philipp Gegenwart[1] — [1]Experimental Physics VI, University of Augsburg, Germany — [2]Institute for Materials Research, Tohoku University, Japan — [3]Department of Physics, Sungkyunkwan University, Republic of Korea

Co-based honeycomb magnets have recently attracted considerable interest as promising candidates for the realization of the bond-directional Kitaev exchange [1]. $Na_2Co_2TeO_6$ belongs to this class of materials and displays antiferromagnetic order below 27 K [2]. We investigate a series of phase transitions in $Na_2Co_2TeO_6$ below 4 K, induced by the application of magnetic fields along the a- and a*-axes. The H-T phase diagram is determined by low-temperature measurements of the specific heat and magnetic Grüneisen parameter, supplemented

by literature results. We also compare the thermodynamic behavior upon field tuning to similar studies on other Kitaev materials, such as the prototype system α-$RuCl_3$.[3]

[1] H. Liu, G. Khaliullin, Phys. Rev. B 97, 014407 (2018).
[2] E. Lefrançois et al., Phys. Rev. B 94, 214416 (2016).
[3] S. Bachus et al., Phys. Rev. B B 103, 054440 (2021).

TT 26.2 Wed 9:45 H33

Anisotropic magnetetoelastic coupling in $Na_3Co_2SbO_6$ — •Prashanta K. Mukharjee[1], Lichen Wang[2], Anton Jesche[1], Julian Kaiser[1], Matthias Hepting[2], Pascal Puphal[2], Masahiko Isobe[2], Bernhard Keimer[2], Philipp Gegenwart[1], and Alexander A. Tsirlin[3] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Felix Bloch Institute for Solid-State Physics, University of Leipzig, 04103 Leipzig, Germany

Research on 3d-based Co^{2+} materials has intensified as they offer the potential to explore novel regimes of honeycomb magnets, including different versions of the extended Kitaev model. In this study, we investigate the thermodynamic properties of the Kitaev candidate $Na_3Co_2SbO_6$ using complementary thermodynamic measurements, including magnetometry, calorimetry, and high-resolution dilatometry. Our results reveal significant in-plane lattice effects both in the zero-field magnetically ordered phase and in the field-induced states, highlighting a robust anisotropic spin-lattice coupling. Notably, we observe a sign change in both thermal expansion and the structural Grüneisen parameter, which points to a quantum critical endpoint. These findings shed new light on the critical behavior and spin-lattice interactions in $Na_3Co_2SbO_6$ contributing to the understanding of its anisotropic magnetic behaviour.

TT 26.3 Wed 10:00 H33

Revisiting magnetic phases of the Kitaev quantum spin liquid $Na_3Co_2SbO_6$ — •Kranthi Kumar Bestha[1,2], Manaswini Sahoo[1,2], Niccolò Francini[3], Robert Kluge[1], Ryan Christopher Morrow[1], Andrey Maljuk[1], Sabine Wurmehl[1], Sven Luther[4], Hannes Kühne[4], Bernd Büchner[1,2], Laura Teresa Corredor Bohorquez[1], Lukas Janssen[1], and Anja U. B. Wolter[1] — [1]Institute for Solid State Research, Leibniz IFW Dresden 01069, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [3]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [4]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

The quest for the elusive Kitaev Quantum Spin Liquid phase (KQSL) in Kitaev candidates has resulted in the discovery of unexpected exotic magnetic phases due to competing Kitaev, Heisenberg and off-diagonal interactions in real materials. Honeycomb cobaltate, $Na_3Co_2SbO_6$ (NCSO) has attracted much interest due to the predictions of its proximity to the KQSL phase. Using magnetic and thermodynamic methods, we mapped out the magnetic phase diagram of high-quality NCSO single crystals for all three main crystallographic directions. We observe a $J_{eff} = \frac{1}{2}$ ground state with antiferromagnetic order (T_N = 7 K) and multiple field-induced metamagnetic transitions in three field directions. The observed anisotropy and field-induced transitions are modeled within an extended $JK\Gamma\Gamma'$ model. Our work uncovers new exotic magnetic phases both in-plane and out-of-plane field directions.

TT 26.4 Wed 10:15 H33

Magnetic-field induced phase transition crossover in the triangular lattice antiferromagnet $Ba_3CoSb_2O_9$ — •Sanjay Kumar[1], Rashi Nathawat[1], Arvind Kumar Yogi[2], and Satyapal S. Rathore[3] — [1]Functional Ceramics and Smart Materials Lab, Department of Physics, Manipal University Jaipur, Jaipur - 303007, India. — [2]UGC-DAE Consortium for Scientific Research, Indore - 452001, India. — [3]Department of Physics, Cluster University of Jammu, Jammu - 180001, India.

The effect of magnetic field on the ground state properties of triangular lattice antiferromagnet (TLAF) compound $Ba_3CoSb_2O_9$. The temperature-dependent X-ray diffraction (10 to 300 K) shows no structural changes. The temperature and field-dependent susceptibility indicate that TLAF orders antiferromagnetically below $T_N \sim 3$ K. The susceptibility follows a Curie-Weiss law (above 100 K) with q_{CW} = -133.2 K. The frustration index (f ~ 44) indicates a highly frustrated system. Magnetization curves (dM/dH) at 2 K reveal field-induced spin-flop transitions near H ~ 9 T. Magnetic susceptibility shows a broad peak at T_{max} = 5 K, becoming more pronounced with increasing field. A spin-glass signature appears near $T_g \sim 6.5$ K but vanishes at higher fields. Interestingly, the magnetic ground state in this compound shows a crossover from the various possible spin orders. A significant shoulder-like hump in heat capacity near $T_c \sim 15$ K suggests structural changes, deviating from the typical λ-anomaly. The change in magnetic properties is attributed to the interplay between antisite defects, quantum fluctuations, and geometric frustration in TLAF.

TT 26.5 Wed 10:30 H33

First-principles modeling of Ni-based honeycomb compounds — •Thore Martens and Alexander Tsirlin — Leipzig University, Germany

In recent years, there has been an increasing interest in Kitaev materials for spins higher than 1/2. Using Density functional theory (DFT), anisotropic spin couplings as well as single-ion anisotropy are calculated and compared for several Ni-based honeycomb compounds: $KNiAsO_4$, $BaNi_2(AsO_4)_2$, $BaNi_2(PO_4)_2$ and $Na_3Ni_2BiO_6$. Most of these investigated compounds share a particularly large antiferromagnetic J_3 and a weaker ferromagnetic J_1 as leading couplings giving rise to a zig-zag magnetic structure. The dependence of these couplings on U from LSDA+U as well as full calculations on the tensor elements of J_1 are performed. From this, potential Kitaev interactions are obtained for the four Ni-compounds.

TT 26.6 Wed 10:45 H33

Exploring Geometrical Frustration in Ho_3ScO_6-II: Magnetic Properties and Structural Insights — •Abanoub Hanna[1], Cintli Aguilar Maldonado[1], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik,Technische Universität Berlin, Berlin, Germany

Geometrical frustration occurs in magnetic compounds when the arrangement of magnetic ions in triangular or tetrahedral lattices leads to competing interactions, resulting in non-classical magnetic states. This study examines the cubic compound Ho_3ScO_6-II, which crystallizes in a bixbyite-type structure with a centrosymmetric cubic space group Ia3* and exhibits no magnetic ordering above 1.8 K, underscoring its geometrically frustrated nature. Unlike its polymorph Ho_3ScO_6-I, which shows long-range magnetic order at 4.4 K, Ho_3ScO_6-II lacks magnetic anisotropy and presents a Curie-Weiss temperature of approximately -20 K and an effective magnetic moment (μ_{eff}) of 9.8 μB, indicating significant antiferromagnetic interactions. Additionally, the study compares Ho_3ScO_6-II with Er_3ScO_6, which is isostructural and exhibits magnetic ordering around 2.1 K that is suppressed under external magnetic fields. This comparison highlights the contrasting behaviours of these compounds, contributing to a deeper understanding of frustrated magnetism within the RE_3ScO_6 system (RE = Ho, Er). The findings provide valuable insights into the unique structural and magnetic properties of Ho_3ScO_6-II and suggest potential applications in spintronic devices and quantum computing.

15 min. break

TT 26.7 Wed 11:15 H33

Continuous Similarity Transformations for the Easy-Axis XXZ Model on the Honeycomb Lattice — •Matthias R. Walther[1], Dag-Björn Hering[2], Vanessa Sulaiman[2], Maximilian Bayer[1], Götz S. Uhrig[2], and Kai P. Schmidt[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

Neutron scattering experiments on $YbCl_3$ show that it realizes the antiferromagnetic Heisenberg model on a honeycomb lattice [1]. While key features are captured by linear spin-wave theory (LSWT), a full dispersion cannot be reproduced. We apply continuous similarity transformations (CSTs) [2-4] to the easy-axis antiferromagnetic XXZ-model on the honeycomb lattice. This allows us to derive an effective model which takes the relevant magnon-magnon interactions beyond LSWT into account targeting a quantitative description of the single-particle properties. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with $d \leq 2$ are taken into account. The resulting quartic magnon-conserving effective Hamiltonian is analyzed in the zero-, one-, and two-magnon sector.

[1] G. Sala et al., Nat. Comm. 12, 171 (2021).
[2] M.R. Walther et al., Phys. Rev. Res., 013132 (2023).
[3] M. Powalski et al., Rev. Lett. 115, 207202 (2015).
[4] M. Powalski et al., SciPost Phys. 4, 001 (2018).

TT 26.8 Wed 11:30 H33

Magnetic Frustration and Weak Mn Magnetic Ordering in $EuMn_2P_2$ — Sarah Krebber[1], Marvin Kopp[1], Jens Müller[1], Jörg Sichelschmidt[2], Michael Baenitz[2], Kurt Kummer[3], Cornelius Krellner[1], and •Kristin Kliemt[1] — [1]Physikalische Institut, Goethe Universität Frankfurt, Deutschland — [2]Max-Planck-Insitut für Chemische Physik fester Stoffe, 01187 Dresden, Deutschland — [3]European Synchrotron Radiation Facility, 38043 Grenoble, France

$EuMn_2P_2$ is a member of the Eu-based 122-systems with a trigonal $CaAl_2Si_2$ crystal structure. The magnetic properties of the Eu ion in this compound are located in triangular layers of Eu^{2+}. Several quantaties indicated the presence of A-type antiferromagnetic Eu order at ≈ 18 K, with magnetic moments oriented in the a-a plane. Nevertheless, no magnetic order of Mn was observed [1,2]. This is intriguing, given that the analogous compounds $EuMn_2As_2$ and $EuMn_2Sb_2$ exhibit phase transitions attributed to Mn magnetic order at elevated temperatures

(T_N = 135 K, T_N = 128 K) [3,4].
In this study, we present the results of electron spin resonance (ESR), heat capacity, magnetization, nuclear magnetic resonance (NMR) and electrical resistivity measurements on $EuMn_2P_2$ single crystals, which exhibite a weak magnetic ordering attributed to Mn magnetism.
[1] A. Payne et al., J. Solid State Chem. 163, 2 (2002);
[2] T. Berry et al., J. Am. Chem. Soc. 145, 8 (2023);
[3] V. K. Anand et al., Phys. Rev. B 94, 014431 (2016);
[4] I. Schellenberg et al., ZAAC 636, 85 (2010).

TT 26.9 Wed 11:45 H33

Exploring the Anisotropic Shastry-Sutherland Model by Strain Tuning of $SrCu_2(BO_3)_2$ — •Francisco Lieberich[1,4], Pascal Puphal[2], Ekaterina Pomjakushina[3], and Elena Gati[1,4] — [1]MPI-CPfS, Dresden, Germany — [2]MPI-FKF, Stuttgart, Germany — [3]PSI, Villigen, Switzerland — [4]TUD, Dresden, Germany

The Shastry-Sutherland model is a hallmark of frustrated magnetism and is realized by $SrCu_2(BO_3)_2$, where competing intra-dimer and inter-dimer interactions J and J' stabilize a dimerized ground state. The Shastry-Sutherland model can be generalized to an anisotropic model with two sets of inequivalent couplings J_1, J_2 and J_1', J_2'. This model is predicted to host novel ground states [1] and may address the debate [2] on the nature of the plaquette phase of $SrCu_2(BO_3)_2$. Experimentally, anisotropic strains break the lattice symmetry of $SrCu_2(BO_3)_2$ and may therefore be used to tune the anisotropy in the Shastry-Sutherland model. We use the AC elastocaloric effect, a thermodynamic probe of strain-tuned quantum materials [3], to map out the entropic landscape of $SrCu_2(BO_3)_2$ under large anistropic strains. By comparing the results under [100] and [110] strain, we disentangle the effects of symmetry-breaking and symmetry-conserving strains on $SrCu_2(BO_3)_2$. Our phase diagrams reveal features consistent with hydrostatic-pressure studies [4], alongside new effects that may arise from symmetry breaking.

Supported by the DFG through SFB 1143.
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[2] Zayed et al., Nat. Phys. 13, 962 (2017);
[3] Ikeda et al., RSI 90, 083902 (2019);
[4] Guo et al., PRL 124, 206602 (2020).

TT 26.10 Wed 12:00 H33

Search for Precursors of Multi-Magnon Bound States in Li_2CuO_2 Single Crystals in Specific Heat Data — •Stefan-Ludwig Drechsler[1], Eli Zoghlin[2], Wolfram Lorenz[1], and Ulrich Roessler[1] — [1]IFW-Dresden, Dresden, Germany — [2]J. Hopkins University, Baltimore, Maryland, USA

We report specific heat c_p-data for high quality single crystals of the edge-sharing chain cuprate Li_2CuO_2 collected in a wide temperature region from 20 to 70 K well above the Ne'el transition $T_N \approx 9.2$ to 9.4 K at ambient magnetic field. The c_p is analyzed within a sensitive c_p/T^3-plot adopting and generalizing an analytical expression [1] by adding precursor multi-magnon bound state (PMMBS) of any order. This way, the problem of missing intensity around 40 K can be resolved. The obtained excitation energies of PMMBS are in accord with recent inelastic neutron scattering data for Li_2CuO_2 [2] regarding single-magnon, two-magnon and three-magnon bound states. The results are discussed within the context of a recenly proposed Bose condensation scenario of MMBS [3] at very low temperature and ambient field.
[1] S. Ebisu *et al.*, J. Phys.Chem.Sol. **59**, 1407 (1998);
[2] E. Zoghlin *et al.*, PRB **108** 064408 (2023);
[3] C.E. Agrapidis, S.-L. Drechsler, S. Nishimoto, arXiv: 2410.00734, Phys. Rev. X (submitted).

TT 26.11 Wed 12:15 H33

Anisotropic Spin Ice on a Breathing Pyrochlore Lattice — •Gloria Isbrandt[1,2], Frank Pollmann[1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Spin ice systems have long captivated researchers due to their exotic magnetic properties and emergent excitations. Recently, breathing pyrochlore compounds have been identified as a platform for studying novel phases, including fracton physics and quantum spin liquids. We explore a spin ice model on a breathing pyrochlore lattice, introducing sublattice-dependent anisotropic interactions that are potentially realizable experimentally, for example, through uniaxial strain. We theoretically uncover a rich phase diagram by varying the strain and show how these anisotropic constraints reduce the ground state degeneracy across the different phases. Our numerical simulations reveal that, at low temperatures, the models undergo a crossover into a constrained spin ice manifold, characterized by an entropy density that falls below the celebrated Pauling entropy of conventional spin ice. Moreover, we observe glassy dynamics in spin correlations when probing the out-of-equilibrium behavior, suggesting slow relaxation and memory effects. This model provides a new perspective on spin ice physics, offering a potentially robust platform for studying fracton phenomena and experimental exploration of constrained magnetism and emergent glassy dynamics.

TT 26.12 Wed 12:30 H33

Efficient Optimization and Conceptual Barriers with Projected Entangled-Pair States — •Erik Weerda[1], Daniel Alcalde[1,2], Konrad Schröder[1], and Matteo Rizzi[1,2] — [1]University of Cologne, Cologne, Germany — [2]Forschungszentrum Jülich

Finite projected entangled-pair states (PEPS) are becoming a widely used tool in the computational study of strongly correlated systems. However, no standard set of computational tools has yet emerged to exploit the power of this approach. In this work we investigate a promising approach to ground state search with PEPS based on sampling methods. Along with presenting strategies for more effi cient optimisation, we also discuss conceptual barriers associated with this approach. A benchmark illustrates the power of these tools in the study of ground states of frustrated magnetic models.

TT 27: Focus Session: Nonlinear Spectroscopy of Collective Excitations in Quantum Magnets (joint session TT/MA)

In recent years, significant progress has been made in understanding strongly correlated quantum magnets, with a particular focus on fractionalized states of matter such as quantum spin liquids. These achievements in understanding have been made possible by remarkable developments in both materials science and experimental techniques. In particular, improvements in both traditional experimental tools (e.g., inelastic neutron scattering, Raman scattering, resonant X-ray scattering, etc.) and the introduction of innovative techniques such as 2D coherent THz spectroscopy and sophisticated noise experiments have advanced studies of quantum matter to qualitatively new levels of insight. This focus session will discuss these recent advancements in nonlinear spectroscopy techniques along with theoretical inroads in describing the nonlinear spectroscopic signatures of complex quantum magnets.

Organizers: Simon Trebst (Universität zu Köln), Johannes Knolle (TU München)

Time: Wednesday 9:30–12:45 Location: H36

Topical Talk TT 27.1 Wed 9:30 H36

Detecting Anyons Using Nonlinear Pump-Probe Spectroscopy — •Max McGinley[1,2], Michele Fava[2], and Sid Parameswaran[2] — [1]Cambridge University, UK — [2]Oxford University, UK

Topologically ordered two-dimensional systems can host excitations that possess statistics that interpolate between bosonic and fermionic—so called anyons. In this talk, I will explain how the presence of such anyonic excitations can be inferred from nonlinear spectroscopic quantities. In particular, we consider pump-probe spectroscopy, where a sample is irradiated by two light pulses with an adjustable time delay between them. The relevant response coefficient exhibits a universal form that originates from the statistical phase acquired when anyons created by the first pulse braid around those created by the second. This behaviour is shown to be qualitatively unchanged by non-universal physics including non-statistical interactions and small finite temperatures. In magnetic systems, the signal of interest can be measured using currently available terahertz-domain probes, highlighting the potential usefulness of nonlinear spectroscopic techniques in the search for quantum spin liquids. I will discuss future prospects for inferring properties of collective excitations using analogous techniques.

Topical Talk TT 27.2 Wed 10:00 H36

Two-Dimensional Nonlinear Dynamic Response of Frustrated Magnets — •Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Two-dimensional nonlinear (2DNL) coherent optical spectroscopy is of great interest in order to deconvolute excitation continua in correlated magnets, potentially allowing to analyze individual quasiparticles, including those of fractionalized magnets. We discuss the relevant response functions for the coupling of spin systems to electric fields and analyze the 2DNL dynamical susceptibilities for two scenarios of frustrated magnetism, namely for a quantum spin-liquid (QSL) as well as for a case of incommensurate spiral long-range order (ICO). For the former, we consider the Kitaev magnet, which hosts a quantum spin-liquid, featuring fractionalization in terms of mobile Majorana fermions and static flux-visons. We show that the 2DNL response does not only probe characteristic features of both fractional excitations, but also allows to extract single quasiparticle lifetimes from its multi-particle continua. These properties will be discussed over a wide range of temperatures. For the case of 2DNL response from a magnet with ICO, we chose the J_1-J_3 spin-model on the square lattice. Here, some features of the 2DNL spectra are found to be remarkably similar to those of the QSL case. Going beyond a bare quasiparticle approach, we will also comment on the impact of final-state interactions.

Work done in collaboration with Olesia Krupnitska and profiting from interactions with Roser Valentí, Natalia Perkins, Marius Möller, Anna Keselman, and David Kaib.

Topical Talk TT 27.3 Wed 10:30 H36

Imaging Magnetization Dynamics and Collective Spin Excitations in Compensated Magnets on Ultrafast Timescales — •Benjamin Stadtmüller — Experimentalphysik II, Institute of Physics, Augsburg University, 86159 Augsburg, Germany

Fundamental to the advancement of spintronics and quantum technologies is the ability to encode, manipulate and store information in the spin angular momentum of electrons on ever faster timescales. In this contribution, we therefore discuss the ultrafast magnetic response of compensated magnets, which are interesting candidates for applications due to their robustness against external fields and their fast manipulation speed. We start with the ultrafast magnetization dynamics of conventional antiferromagnets (AFMs), for which the possibility of optical excitation of collective magnon modes on ps timescales has already been demonstrated. For the case of NiO, we show that these timescales can be further reduced by exploiting the strong non-equilibrium excitation with fs laser pulses. These conditions lead to a significant loss of magnetic order and to the excitation of collective magnon modes. We then turn to the ultrafast optical response of the recently discovered class of altermagnets with their d-wave-like spin split band structure. By combining theoretical calculations with ultrafast magneto-optical experiments, we demonstrate the generation of a macroscopic spin polarization in the otherwise fully compensated altermagnet RuO_2, which can additionally be controlled by the excitation geometry [1]. [1] M. Weber and S. Wust et al. arXiv: 2408.05187

15 min. break

Topical Talk TT 27.4 Wed 11:15 H36

Revealing Dynamics of Hidden Sectors with Nonlinear Spectroscopy — •Yoshito Watanabe[1], Simon Trebst[1], and Ciarán Hickey[2,3] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [3]Centre for Quantum Engineering, Science, and Technology, University College Dublin, Dublin 4, Ireland

Nonlinear spectroscopy, especially in its two-dimensional coherent spectroscopy (2DCS) form, is an emerging and promising tool for studying the dynamics of quantum materials. Unlike traditional linear probes, 2DCS employs a multi-pulse approach that reveals intricate dynamics, including the ability to resolve fractional excitation continua as sharp spinon-echo signals and to study interactions between excitations, phenomena often obscured in traditional measurements.

In this work, we focus on the potential of 2DCS to detect and characterize quadrupolar excitations in quantum magnets. Using exact diagonalization and establishing an effective Hamiltonian that reflects the dynamics of hidden sectors and higher-order excitations, we identify distinct spectroscopic features, including new signatures associated with quadrupolar excitations. These results provide a guide for the experimental detection and characterization of hidden dynamics in quantum materials.

Topical Talk TT 27.5 Wed 11:45 H36

Theory of Nonlinear Spectroscopy of Quantum Magnets — Anubhav Srivastava[1,2], •Stefan Birnkammer[1], GiBaik Sim[3], Michael Knap[1], and Johannes Knolle[1,4] — [1]Technical University of Munich, Garching, Germany — [2]Indian Institute of Science, Bengaluru, India — [3]Hanyang University, Seoul, Korea — [4]Imperial College London, London, United Kingdom

Two-dimensional coherent spectroscopy (2DCS) is an established method for probing molecules and has been proposed in the THz regime as a new tool for probing exotic excitations of quantum magnets but the precise nature of coupling between pump field and spin degrees of freedom has remained unclear. Here, we develop a general response theory of 2DCS and show how magneto-electric as well as polarization couplings contribute to 2DCS in addition to the standardly assumed magnetization. We propose experimental protocols to distill individual coupling contributions, for example from exchange-striction or spin current mechanism. We provide example calculations for the paradigmatic twisted Kitaev chain material $CoNb_2O_6$ and highlight the crucial role of contributions from cross-coupling between polarization and magnetic nonlinear susceptibilities. Our work paves the way for systematic studies of light-matter couplings in quantum magnets and for establishing 2DCS as a versatile tool for probing fractional excitations of exotic magnetic quantum phases.

TT 27.6 Wed 12:15 H36

Quantitative Prediction of the Dynamics of In-Gap States in Correlated Materials as Seen in Pump-Probe PES, XAS and RIXS Experiments: A NiO Case Study — •Sina Shokri and Maurits W. Haverkort — Universität Heidelberg, Institut für Theoretische Physik, Philosophenweg 19, Heidelberg 69120 Germany

Attosecond pump-probe experiments allow one to study and steer quantum materials on their fundamental time-scales. For atoms and small molecules one can theoretically predict the electronic and vibrational dynamics induced by ultrafast light pulses [1,2]. In solids a theoretical understanding is much harder. The coupling to many continuous degrees of freedom can result into rapid loss of coherence. Quantitative predictions how coherently driven excitations decohere is highly non-trivial. Correlated Mott- Hubbard or charge transfer insulators can show a variety of long lived excitonic excitations within the optical gap. With attosecond pump-probe spectroscopy it is possible to investigate the propagation and decay of such excitations, as recently shown by two-photon photo-emission spectroscopy of NiO. These experiments show photo-induced, long-lived in-gap states with coherent oscillations [3]. In this talk we will show, using non-linear response theory, how to quantitatively predict the dynamics of in-gap states in correlated materials after an optical excitation. We will furthermore show how this dynamics can be probed with different pump-probe experiments including photo-emission spectroscopy, x-ray absorption spectroscopy and resonant inelastic x-ray scattering.

[1] PRL 128, 153001 (2022).
[2] PRA 108, 032816 (2023).
[3] Nat. Commun. 11, 4095 (2020).

TT 27.7 Wed 12:30 H36

Higher-Order Susceptibilities in Extended Kitaev Models Computed Via Krylov-Space Based Methods — •David Kaib, Marius Möller, and Roser Valenti — Institut für theoretische Physik, Goethe-Universität Frankfurt

Recently, it was proposed that techniques measuring higher-order dynamical response, such as two-dimensional coherent spectroscopy (2DCS), could provide more distinguishable signatures in analyzing the excitations of different systems. This is particularly true when linear response reveals only a featureless continuum, which could arise from various different types of excitations, or, for example, static disorder. The numerical evaluation of nonlinear response functions can, however, be computationally very demanding. Here, we propose an efficient Lanczos-based method that computes higher-order susceptibilities directly in the frequency domain. As an application case, we consider extended Kitaev models, that are relevant to α-$RuCl_3$ and related materials. We compare the nonlinear response from our method to the one obtained within linear spin-wave theory, showcasing that nonlinear response measurements can distinguish whether an observed excitation continuum is of conventional two-magnon type or has a different origin.

TT 28: Many-body Quantum Dynamics II (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: H37

TT 28.1 Wed 9:30 H37

The Sound of Entanglement — •Benjamin Orthner[1], Clemens Wenger[5], Johannes Kofler[2], Richard Küng[2], Enar de Dios Rodríguez[3], Martin Ringbauer[4], Alexander Ploier[2], and Philipp Haslinger[1] — [1]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Vienna, Austria — [2]Johannes Kepler University Linz, Austria — [3]Internationale Forschungszentrum Kulturwissenschaften, Kunstuniversität Linz, Austria — [4]University of Innsbruck, Austria — [5]Universität für Musik und darstellende Kunst Graz, Austria

This contribution presents *The Sound of Entanglement*, a project at the intersection of quantum physics, music, and visual art. At its core lies a Bell experiment setup, where polarization-entangled photon pairs are generated through spontaneous parametric down-conversion in a β-BBO crystal. The experiment acts as a quantum conductor, utilizing the quantum correlations between the photons to coordinate and influence the choices of live musicians in real-time, creating a performance guided by principles beyond classical physics.

This work seeks to make these abstract concepts more accessible and engaging to broader audiences by transforming them into tangible, sensory experiences. By combining live music with a dynamic light show, both controlled by the experiment, this project illustrates how advancements in technology, like those shaping the second quantum revolution, can redefine artistic expression and bridge the gap between science and art.

TT 28.2 Wed 9:45 H37

A Solvable Model for Full Eigenstate Thermalization — •Felix Fritzsch and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The Full Eigenstate Thermalization Hypothesis (Full ETH) aims to characterize thermalization in many-body quantum systems in terms of the dynamics of higher-order spatiotemporal correlation functions, going beyond the current standard ETH paradigm. In this talk, we introduce a solvable random matrix model for many-body quantum dynamics in which the asymptotic dynamics of generalized out-of-time-order correlation functions can be exactly obtained in the thermodynamic limit. The dynamics of this model naturally maps to dynamics on the lattice of non-crossing partitions, combinatorial structures underlying the mathematics of Free Probability and Full ETH. We demonstrate how local observables approach asymptotic freeness at late times and explicitly characterize all relevant time scales. We confirm our analytical results with numerical simulations performed directly in the thermodynamic limit.

TT 28.3 Wed 10:00 H37

Scrutinizing the Mori memory function for transport scenarios — •Scott Daniel Linz, Jiaozi Wang, Robin Steinigeweg, and Jochen Gemmer — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

Diffusion is a phenomenological hydrodynamic transport behavior that holds over a wide range of materials. Within condensed matter physics there is the opinion that as long as the area under the current-current correlation function converges in time, one has a criterion for diffusive behavior of the corresponding spatiotemporal density dynamics. Attempts to derive this statement are notoriously challenging. We will first demonstrate that it is possible to construct correlation functions of some local density, where the area under a current-current correlation function converges, but the system is not diffusive. After this is demonstrated, we shall introduce a method based on the recursion method and the Mori memory formalism, that yields insight into whether or not a process is truly diffusive. The only disadvantage of this strategy is that one would have to know the behavior infinitely many Lanczos coefficients, whereas in practice one can only calculate a finite number of them in most cases. In the cases examined in this talk, however, the convergence or lack thereof becomes apparent to the naked eye with the finite amount of coefficients that were calculated.

TT 28.4 Wed 10:15 H37

Long-time Freeness in the Kicked Top — •Elisa Vallini and Silvia Pappalardi — University of Cologne, Köln, Germany

Recent work highlighted the importance of higher-order correlations in quantum dynamics for a deeper understanding of quantum chaos and thermalization. The full Eigenstate Thermalization Hypothesis, the framework encompassing correlations, can be formalized using the language of Free Probability theory. In this context, chaotic dynamics at long times are proposed to lead to free independence or "freeness" of observables. We investigate these issues in a paradigmatic semiclassical model - the kicked top - which exhibits a transition from integrability to chaos. Despite its simplicity, we identify several non-trivial features. By numerically studying 2n-point out-of-time-order correlators, we show that in the fully chaotic regime, long-time freeness is reached exponentially fast. These considerations lead us to introduce a large deviation theory for freeness that enables us to define and analyze the associated time scale. The numerical results confirm the existence of a hierarchy of different time scales, indicating a multifractal approach to freeness in this model. Our findings provide novel insights into the long-time behavior of chaotic dynamics and may have broader implications for the study of many-body quantum dynamics.

TT 28.5 Wed 10:30 H37

Periodically and aperiodically Thue-Morse driven long-range systems: from dynamical localization to slow dynamics — •VATSANA TIWARI — Indian Institute of Science Education and Research Bhopal, Bhopal, India

In this talk, I will discuss the impact of time-periodic and aperiodic field on power-law random banded matrix (PLRBM) model where variation in the power-law exponent yields a delocalization-to-localization phase transition. We investigate the periodically driven PLRBM model with the help of the static measures such as level spacing ratio and generalized inverse participation ratio and report the drive-induced multifractal to localization transition. The transport study of the periodically driven system demonstrates the transition from diffusive to logarithmically slow relaxation at dynamical localization point. Extending our analysis to the aperiodic Thue-Morse driving, we find that specific driving parameters leads to the *exact dynamical localization* in a disordered-free long-range model regardless of the long-range parameter. In the disordered case, the localized phase exhibits a long prethermal plateau followed by diffusion to an infinite temperature state, while the delocalized phase shows immediate diffusion. Additionally, we compare this with a quasi-periodic model that also undergoes a localization-delocalization transition, noting that, unlike the delocalized side of the disordered long-range model, it features a prolonged plateau followed by diffusion to the infinite temperature state.

TT 28.6 Wed 10:45 H37

Symmetry-Resolved Out-of-Time-Order Correlators with Projected Matrix Product Operators — •Martina Gisti, David Luitz, and Maxime Debertolis — Institute of Physics, University of Bonn, Nußallee 12, 53115 Bonn, Germany

Out-of-Time-Order Correlators (OTOCs) are key measures of quantum many-body chaos and information spreading. We systematically analyse OTOCs as a function of particle number for interacting spinless fermions in one dimension. With the concept of generalized operator charge, we develop a formalism for the time evolution of symmetry-projected matrix product operators, which we use to resolve the scrambling behaviour by particle number sector. Our results reveal a crossover from ballistic to diffusive dynamics at early times and a saturation regime at late times.

TT 28.7 Wed 11:00 H37

Revealing ultrafast phonon mediated inter-valley scattering through transient absorption and high harmonic spectroscopies — •Kevin Lively[1], Shunsuke Sato[2,3], Guillermo Albareda[2,4], Angel Rubio[2], and Aaron Kelly[2] — [1]Deutsches Zentrum für Luft- und Raumfahrt — [2]Max Planck Institute for the Structure and Dynamics of Matter — [3]University of Tsukuba — [4]Ideaded

Processes involving ultrafast laser driven electron-phonon dynamics play a fundamental role in the response of quantum systems in a growing number of situations of interest, as evinced by phenomena such as strongly driven phase transitions and light driven engineering of material properties. To show how these processes can be captured from a computational perspective, we simulate the transient absorption spectra and high-harmonic generation signals associated with valley selective excitation and intraband charge-carrier relaxation in monolayer hexagonal boron nitride. We show that the multitrajectory Ehrenfest dynamics approach, implemented in combination with real-time time-dependent density-functional theory and tight-binding models, offers a simple, accurate, and efficient method to study ultrafast electron-phonon coupled phenomena in solids under diverse pump-probe regimes which can be easily incorporated into the majority of real-time ab initio software packages.

15 min. break

TT 28.8 Wed 11:30 H37

Chiral basis for qubits and decay of spin-helix states — •Frank Göhmann — Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

In a recent cold-atom experiment by the Ketterle group at MIT one-dimensional spin-helix states could be prepared and their time evolution induced by the XXZ Hamiltonian could be observed. The experiment allows to adjust the anisotropy parameter of the latter. For the special case of the XX model we describe the spatio-temporal decay of a transversal spin helix explicitly. The helix pattern stays stable in space, but has a non-trivial time-dependent decay amplitude which is of scaling form and is governed by a universal function that can be

represented as a semi-infinite determinant related to the discrete Bessel kernel. This representation is valid for all times, is numerically utterly efficient and allows us to obtain the long-time asymptotics of the function. Our work is a rare example of a quench that has been experimentally realized and for which the full time dependence could be calculated exactly.

V. Popkov, X. Zhang, F. Göhmann and A. Klümper, *Chiral basis for qubits and spin helix decay*, Phys. Rev. Lett. **132** (2024) 220404 (5pp)

TT 28.9 Wed 11:45 H37

Towards the chaotic melting at low energies in large systems — •Mathias Steinhuber[1], Jonas Rigo[2], Juan Diego Urbina[1], Klaus Richter[1], and Markus Schmitt[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), Jülich, Germany

Thinking in a classical phase space picture, a many-body ground state should be localized around the minimum of the classical mean-field energy landscape with stable integrable features. But here, we investigate many-body ground states on chaotic features, as the phase space picture is actually fragile if we increase the system size and keep the quantum scale (the effective Plank constant $\hbar_{\text{eff}}$) fixed. With the new degrees of freedom, we disturb the energy landscape in the classical limit more and more such that classical chaos is present even for low energies. We show this phenomenon, called 'chaotic melting' [1,2], is indeed happening in the Bose-Hubbard system with disorder. By using neural quantum states we can push quantum calculations for ground states to large systems and find signatures of chaos at the ground state. An intriguing application for these large systems is that the Bose-Hubbard Hamiltonian with disorder is an effective model for transmon arrays which are a prime candidate for quantum computer hardware. Therefore we also gain access to quantum states describing a possible quantum computer with chaotic features.

[1] S.-D. Börner, et al. Phys. Rev. Research 6, 033128 (2024)
[2] J. Chávez-Carlos, et al. arXiv: 2310.17698 (2024)

TT 28.10 Wed 12:00 H37

Period n-tupling in driven two level systems — •Dhruv Deshmukh and Joachim Ankerhold — Institute for complex quantum systems, Ulm University, Germany

This talk presents the necessary and sufficient conditions for realizing period n-tupling phenomena in periodically driven two-level systems. For the specific case of a two-level system driven linearly by a sinusoidal drive, we numerically identify the drive parameters that enable period n-tupling. Experimental results verifying period doubling in an NV centre driven by a microwave drive, are given. Further, we show that period quadrupling drives yield pulses which are much faster than the standard (Rabi) $\pi/2$ and π pulses built from weak drives. These stronger and faster pulses can be utilized for qubit manipulation, enabling faster gates and more efficient pulse sequences. Moreover, they inspire a new strategy for constructing efficient pulses using a Floquet theory approach to optimal control. Furthermore, the drive parameters could also be set to achieve period-1 (stroboscopic) dynamical freezing. The fragility of such phenomena can be exploited for sensing applications, as illustrated with an example in magnetometry.

TT 28.11 Wed 12:15 H37

Efficient computation of cumulant evolution and full counting statistics: application to infinite temperature quantum spin chains — •Angelo Valli[1,2], Cătălin Pascu Moca[2,3], Miklós Antal Werner[1,4], Márton Kormos[1,2], Žiga Krajnik[5], and Tomaž Prosen[6] — [1]Budapest University of Technology and Economics, Muegyetem rkp. 3., 1111 Budapest, Hungary — [2]HUN-REN BME Quantum Dynamics and Correlations Research Group — [3]University of Oradea, 410087, Oradea, Romania — [4]HUN-REN Wigner Research Centre for Physics, P.O. Box 49, 1525 Budapest, Hungary — [5]New York University, 726 Broadway, New York, NY 10003, USA — [6]University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia

We propose a numerical method to efficiently compute quantum generating functions (QGF) for a wide class of observables in one-dimensional quantum systems at high temperature. We obtain high-accuracy estimates for the cumulants and reconstruct full counting statistics from the QGF. We demonstrate its potential on spin S=1/2 anisotropic Heisenberg chain, where we can reach time scales hitherto inaccessible to state-of-the-art classical and quantum simulations. Our results are in excellent agreement with a recent Google Quantum AI experiment [2] and challenge the conjecture of the Kardar-Parisi-Zhang universality for isotropic integrable quantum spin chains.

[1] A. Valli et al. arXiv:2409.14442 (2024)
[2] E. Rozenberg et al. Science 384, 48-53 (2024)

TT 28.12 Wed 12:30 H37

Machine learning approach to study the properties of ground and excited states in the 1D Bose-Hubbard model — •Yilun Gao[1], Alberto Rodríguez González[2,3], and Rudolf A. Römer[1] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL — [2]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain — [3]Instituto Universitario de Física Fundamental y Matemáticas (IUFFyM), Universidad de Salamanca, E-37008 Salamanca, Spain

Many-body quantum interacting systems continue to play a key role in theoretical developments of modern condensed matter physics. Various numerical techniques have been used to explore the features of these many-body systems. Exact diagonalization methods, which most results going beyond ground state properties are based on, can only deal with small system sizes $L \lesssim 15$ because the Hilbert dimensions grow exponentially in L. Recently, deep learning has emerged as a numerical technique that uses strategies of artificial intelligence to predict the physics of such systems. Here we focus on the Bose-Hubbard chain and use HubbardNet [1] to investigate the physics of ground and excited states. We show that the energies and wavefunctions predicted by HubbardNet agree well with the ones calculated by exact diagonalization over a broad range of interaction strengths. We investigate the properties of the eigenstates via their finite-size generalized fractal dimensions. [1] Ziyan Zhu, et al., HubbardNet: Efficient predictions of the Bose-Hubbard model spectrum with deep neural networks, Phys. Rev. Res., **5**, 043084 (2023)

TT 28.13 Wed 12:45 H37

Entanglement Transitions in Quantum Games through Reinforcement Learning — •Giovanni Cemin[1], Marin Bukov[1], and Markus Schmitt[2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Regensburg, Regensburg, Germany — [3]Forschungszentrum Jülich, Institute of Quantum Control, Jülich, Germany

In this research, we investigate the dynamics of entanglement in Cliord circuits by employing a reinforcement learning (RL) algorithm in competition with a random agent. The RL agent is designed to strategically place gates that decrease entanglement, while the random agent aims to increase entanglement. This interaction between the two agents results in an entanglement transition, the nature of which is induced by the level of information accessible by the RL agent. By systematically varying the information provided to the RL agent, we analyze its impact on the transition characteristics. Our findings provide new insights into the interplay between entanglement manipulation and information constraints, shedding light on the fundamental mechanisms governing quantum circuit dynamics.

TT 29: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

TT 29.1 Wed 10:30 H11

The Bell-Shaped Component in Diffraction from 2D Materials — •Birk Finke[1], Christian Brand[1], Karim Omambac[1,2], Pascal Dreher[1], Hannah Kohler[1], Frank-J. Meyer zu Heringdorf[1,3,4], and Michael Horn-von Hoegen[1,3] — [1]Universität Duisburg-Essen — [2]Polytechnique Montréal Canada — [3]Center for Nanointegration Duisburg-Essen — [4]Interdisciplinary Center for Analytics on the Nanoscale

In 2D materials, the formation of moiré superlattices with graphene or hBN on crystalline surfaces alters electronic, vibrational, and chemical properties. Here we analysed an unusual broad diffraction background observed in low energy electron diffraction from 2D material systems, which is called the bell-shaped component (BSC). Employing SPA-LEED, LEEM, and μ-LEED we propose the origin to be the inelastic scattering of the low energy electrons at the vertically polarized ZA-phonons of the weakly bound graphene and hBN layers on Ir(111) and SiC(0001). For these systems the ZA-phonon branch exhibits a parabolic dispersion with a finite phonon frequency of a few meV at the Γ point. This results in a high phonon density at low energy, but high momentum causing the strong intensity of the BSC in diffraction. In the framework of kinematic scattering theory, we performed simulations of the inelastic diffuse scattering which quantitively confirm our proposal.

TT 29.2 Wed 10:45 H11

Combining DFT and ML to Explore the Electronic Properties of Nanoporous Graphene — •Bernhard Kretz and Ivor Lončarić — Institut Ruder Bošković, Zagreb, Croatia

Nano-porous graphene (NPG) holds great potential in electronics due to its tunable electronic properties. However, establishing a comprehensive understanding of how structural parameters influence these properties remains a challenge.

This work employs density functional theory (DFT) calculations combined with machine learning (ML) to systematically investigate both static and dynamic electronic properties across a set of 460 NPG structures derived from four distinct templates.

Our DFT results reveal correlations between structural features and band gaps within subsets of our NPG structures. Notably, we identify certain NPG configurations exhibiting band gap behavior analogous to armchair graphene nanoribbons. To predict the dynamic response of our NPG structures, we train two distinct ML networks: one for predicting forces and total energies, and another one for predicting band gaps. Using the former allows us to perform temperature-dependent molecular dynamics simulations for all 460 NPG structures, while the latter enables us to predict band gap evolution under varying operating temperatures, a crucial factor for semiconductor device performance. Our findings identify several NPG structures exhibiting band gaps suitable for semiconductor applications while demonstrating sufficient thermal stability to function effectively at typical operating temperatures.

Invited Talk TT 29.3 Wed 11:00 H11

Polaritons in two-dimensional materials and hybrids probed by electron beams — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel

Polaritonic quasiparticles in two-dimensional (2D) materials have garnered significant attention in recent years, emerging as a promising platform for studying novel photon- and phonon-mediated correlations between various material excitations. In this work, we employ electron beams to investigate exciton and plasmon polaritons in diverse 2D materials, including transition-metal dichalcogenides, perovskites, hexagonal boron nitride, borophene, and hybrid systems. By comparing cathodoluminescence and photoluminescence spectroscopy, we uncover differences in the selection rules governing the excitation of quasiparticles by coherent light versus electron beams. Furthermore, leveraging a recently developed method that utilizes electron-driven photon sources inside an electron microscope for Ramsey-type spectroscopy, we examine the coherence of cathodoluminescence emitted by exciton polaritons (Nature Physics 19, 869 (2023)) and defects in hexagonal boron nitride (arXiv:2404.09879). These results provide new insights into the temporal coherence of the radiation from 2D materials excited by coherent and incoherent excitations.

TT 29.4 Wed 11:30 H11

Electron-phonon interaction in polar two-dimensional materials — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We recently developed a generally applicable ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation, which are usually neglected [1].

Incorporating effects from macroscopic electric fields into our implementation allows us to extend our calculations to the class of polar materials. In this presentation we discuss our results for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

TT 29.5 Wed 11:45 H11

Structural modulations of unidirectional charge density waves in rare earth tellurides — •Eunseo Kim[1], Sanghun Lee[1], Junho Bang[1], Hyungryul Yang[1], Jongho Park[2], Changyoung Kim[2], Dirk Wulferding[2], Doohee Cho[1], Makoto Hashimito[3], Donghui Lu[3], and Sunghun Kim[4] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea — [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Department of Physics, Ajou University, Suwon 16499, Korea

Charge density waves (CDWs) in rare earth tellurides (RTe_3) provide a unique platform for exploring the interplay between lattice deformations and electronic order. Using scanning tunneling microscopy and spectroscopy (STM/S), we investigate unique surface features in two different materials, $GdTe_3$ and $DyTe_3$, that influence the CDW behavior. In $GdTe_3$, twin domain boundaries provide a static platform for observing the spatial "melting" of unidirectional CDWs and the emergence of bidirectional CDWs. Our spatial lock-in analysis demonstrates the attenuation of CDW order parameters and the proliferation of topological defects at these boundaries, correlating with enhanced local density of states near the Fermi level. In $DyTe_3$, nanowrinkles act as topological interfaces, hosting phase-winding CDWs and confining one-dimensional metallic states. These findings emphasize the role of local structural distortions in shaping CDW phenomena, offering insights into manipulating quantum states via lattice engineering.

TT 29.6 Wed 12:00 H11

Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field — •Jan-Philip Joost and Michael Bonitz — Kiel University, Institute for Theoretical Physics and Astrophysics, 24098 Kiel, Germany

When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [1]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [2]. Further, we demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects greatly benefit from surface screening, while in free-standing systems the targeted charge excitation is restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

[1] J.-P. Joost et al., Nano Lett. **19**, 9045 (2019)
[2] J.-P. Joost et al., Phys. Rev. B **105**, 165155 (2022)

TT 29.7 Wed 12:15 H11

Two-dimensional breathing Kagome lattice of antimony atoms on a SiC substrate — •Bing Liu[1], Kyungchan Lee[1], Jonas Erhardt[1], Manish Verma[1], Stefan Enyner[1], Cedric Schmitt[1], Philipp Kessler[1], Lukas Gehrig[1], Chris Jozwiak[2], Aaron Bostwick[2], Martin Kamp[1], Eli Rotenberg[2], Jörg Schäfer[1], Simon Moser[1], Giorgio Sangiovanni[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The Kagome lattice, characterized by flat electronic bands, which represents a class of candidate materials for charge order, time-reversal symmetry-breaking and exotic superconductivity. In this work, we report the successful synthesis of a breathing Kagome lattice of Sb on SiC surface. Band mapping reveals a significant gap opening at the K point near the Fermi level, driven by different hopping parameters within the breathing Kagome lattice. Scanning tunneling microscopy measurements of this phase confirm a well-ordered 2x2 lattice reconstruction, consistent with the breathing Kagome unit cell. Furthermore, DFT calculations elucidate the role of the Sb p-orbitals. Specifically, near the Fermi level the physics is dominated by px and py orbitals, which are sensitive to hopping and possibly electron correlation, giving rise to an energy gap, and by their splitting reflect the breathing Kagome lattice situation. Our findings demonstrate a pathway for constructing two-dimensional Kagome lattices on semiconductor surfaces, and are encouraging further research into their spin and electronic properties.

TT 29.8 Wed 12:30 H11

Ultrafast lattice dynamics of monolayer ReS_2 — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Within the transition metal dichalcogenide (TMDC) material family, TMDCs containing rhenium stand out due to their low crystal symmetry. Instead of the common hexagonal structure, ReS_2 exhibits in-plane 1D chains of rhenium ions due to a Peierls-like distortion. This highly anisotropic crystal structure results in a range of material properties, such as anisotropic effective carrier masses, polarization dependent optical absorption, and extremely weak interlayer coupling.

We present femtosecond electron diffraction (FED) measurements of monolayer ReS_2. FED is a direct probe of photoexcited lattice dynamics, providing quantitative information on coherent and incoherent atomic vibrations on femtosecond timescales. In ReS_2 monolayers we observe a strong and complex lattice response to photoexcitation. In particular, we observe a rapid (<1 ps) collective response, indicative of a concerted change in ionic positions within the unit cell. We measure the fluence dependence of this response and investigate the effect of the pronounced polarization dependence of the optical excitation, which results from the material's in-plane anisotropy.

TT 30: Nanomechanical systems (joint session HL/TT)

The session covers the physics of nanomechanical systems.

Time: Wednesday 15:00–15:45 Location: H17

TT 30.1 Wed 15:00 H17

Optimizing an Integrated Photonic Racetrack Resonator for Optomechanical Synchronization — •Agnes Zinth[1] and Menno Poot[1,2,3] — [1]Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Institute for Advanced Study, Technical University of Munich, Garching, Germany

In the field of optomechanics, synchronization will be an essential tool in fields like sensing and quantum technologies. Towards this goal, we develop a photonic integrated optomechanical device consisting of a silicon nitride racetrack cavity with partly suspended waveguide that can vibrate freely. A second beam is added to improve the optomechanical coupling. The observed mechanical modes do not match in frequency, so we use a predisplaced beam instead [1]. The remaining frequency distance can be tuned by the laser power. As the light propagates in the predisplaced beam and only past the PhC beam, it shifts further than the photonic crystal one due to thermal effects. To synchronize them with optomechanical backaction, we also need to enhance the optical cavity. Therefore, we modify the transition from supported to suspended parts. Two different approaches lead to the desired improved optical quality. Currently, we are investigating their impact on the mechanics. We believe that, in the next generation of devices, we can synchronize the racetrack and photonic crystal beam.

[1] Geometric tuning of stress in predisplaced silicon nitride resonators. Nano Letters, 22(10), 4013-4019.

TT 30.2 Wed 15:15 H17

Quantum Mechanics in Two-Dimensional Dynamic Spaces — •Benjamin Schwager and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

In the study of systems with reduced dimensions one encounters quantum particles under spatial constraints. Their dynamics have to be modeled based on a configuration space that is a Riemannian manifold, in general, and the resulting quantum wave equations contain correction terms in dependence of its geometric properties. We consider particles which are confined to a flexible thin material shell by studying the Schrödinger equation on moving domains. The model assumes a static observer and couples the deformation dynamics of the material to the quantum dynamics it hosts via additional potential fields. Effects caused by the interplay of geometry and the temporal evolution of the underlying configuration space will be discussed.

TT 30.3 Wed 15:30 H17

Towards cavity optomechanics using 2D materials — •Petricia Sara Peter[1,2], Lukas Schleicher[1,2], Anne Rodriguez[1,2], Leonard Geilen[2,3], Alexander Musta[2,3], Benedict Brouwer[2,3], Alexander Holleitner[2,3], and Eva Weig[1,2] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Walter Schottky Institute, TU Munich, Germany

Two-dimensional (2D) materials, such as hexagonal boron nitride (hBN), are promising candidates for advancing cavity optomechanics due to their low mass, high mechanical strength, and unique optical properties. This work focuses on the fabrication of freely suspended hBN membranes on silicon oxide (SiO_2) and silicon nitride (Si_3N_3) substrates, utilizing a water-assisted wet transfer technique. Compared to the dry transfer method, this approach minimizes inhomogeneous stress and preserves optimal mode shapes, improving mechanical quality factors. A Michelson interferometer is used to measure the mechanical properties of the resulting drumhead resonators, including vibrational resonances, mode shapes, and quality factors. These results provide important insights into the performance and quality of the resonator, laying the groundwork for incorporating 2D materials into cavity optomechanical studies.

TT 31: Topology: Quantum Hall Systems

Time: Wednesday 15:00–16:45 Location: H31

Invited Talk TT 31.1 Wed 15:00 H31

Quantum Skyrmion Hall Effect — •Ashley Cook — MPI-PKS, Dresden, Germany

Motivated by recent discovery of additional topologically non-trivial phases of matter in lattice models beyond established classification schemes, we generalise the framework of the quantum Hall effect (QHE) to that of the quantum skyrmion Hall effect (QSkHE). This involves one key generalisation: considering particles on a two-sphere, which see a U(1) monopole, one can project to the lowest Landau level (LLL). Upon performing such a projection, the position coordinates become proportional to SU(2) generators by quenching of kinetic energy. An almost point-like LLL corresponds to matrix representation size for the SU(2) generators of N by N, with N small. The key generalisation is that such an almost point-like LLL with small orbital degeneracy can still host an intrinsically 2+1 dimensional topologically non-trivial many-body state. Equivalently, in regimes in which spin has previously been treated as a label (small N), spin encodes some finite number of spatial dimensions, in general. This many-body state can play the role, in the QSkHE, that a charged particle plays in the QHE.

TT 31.2 Wed 15:30 H31

Electric Field Induced Second-Order Anomalous Hall Transport in an Unconventional Rashba System — •Ankita Bhattacharya and Annica Black-Schaffer — Uppsala University, Sweden

Nonlinear responses in transport experiments may unveil information and generate new phenomena in materials that are not accessible at linear order due to symmetry constraints. While the linear anomalous Hall response strictly requires the absence of time-reversal symmetry, the second order, thus nonlinear, Hall response needs broken inversion symmetry. Recently, much effort has been made to obtain a second-order Hall voltage in response to a longitudinal ac driving current, both to obtain information about band geometric quantities and for its useful technological applications in rectification and frequency doubling. Typically, additional material engineering is required in noncentrosymmetric systems to obtain second-order responses since it obeys a stringent crystallographic symmetry constraint. To circumvent this, an alternative route is to apply a dc electric field. In our work, we uncover an electric field induced second-order anomalous Hall effect in an inversion-broken system possessing unconventional Rashba bands. We establish that the quantum metric, a geometrical feature of electronic wave functions providing information on non-trivial structure of Bloch bands, is responsible for providing the nonlinear Hall response. We are able to find a highly tunable electric field induced second-order anomalous Hall transport in probably the simplest system in 2D, which should be uncomplicated to verify experimentally due to multiple materials already being proposed.

TT 31.3 Wed 15:45 H31

Topological Thermal Hall Effect in the Geometrically Frustrated Magnet Gd_2PdSi_3 — •Parisa Mokhtari[1,2], Daiki Yamaguchi[1], Rinsuke Yamada[1], Akiko Kikkawa[3], Philipp Gegenwart[2], Yasujiro Taguchi[3], Yoshinori Tokura[1,3], and Max Hirschberger[1,3] — [1]Department of Applied Physics and Quantum-Phase Electronics Center, The University of Tokyo, Bunkyo-ku, Tokyo 113-8656, Japan — [2]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — [3]RIKEN Center for Emergent Matter Science, Wako, Saitama 351-0198, Japan

Geometrical frustrated Skyrmion lattices exemplify nontrivial topological states with non-zero scalar spin chirality and a finite Berry curvature in real space. In 2019, T. Kurumaji *et al.* reported a large topological Hall effect in the skyrmion phase in Gd_2PdSi_3 related to the spin chirality of the ground state [1].

In this talk, I will present the thermal Hall conductivity of the frustrated triangular-lattice magnet Gd_2PdSi_3. By entering the skyrmion lattice ground state, the field-dependent thermal Hall effect sharply increases against the adjacent incommensurate phases, similar to the electric Hall conductivity behaviour. Eventually, I will investigate the relationship of Hall entropy to the charge current and discuss the non-dissipativity of topological quantum transport in the geometrically frustrated magnet Gd_2PdSi_3.

[1] T. Kurumaji *et al.*, Science **365**, 914 (2019).

TT 31.4 Wed 16:00 H31

Orbital Magnetization of Dirac Electrons on Curved Surfaces — •Maximilian Fürst — Universität Regensburg

Orbital magnetic response of 2D, (almost) free electrons has extensively been studied in the past, starting from the discovery of Landau levels of Schrödinger [1]/(massless) Dirac [2] electrons with a linear/squareroot dispersion in the field strength B. Apart from Landau diamagnetism, this leads to De-Haas-van-Alphen type oscillations of the susceptibility, that are periodic in 1/B [3]. Confining

(massless) Dirac electrons on a curved surface predominantly leads to unusual oscillations of the susceptibility with periodicity in B. We discuss three example surfaces (Sphere, Cone, Pseudosphere) in a coaxial magnetic field.
[1] L. Landau, Z. Phys. A 64, 629 (1930).
[2] J. W. McClure, Phys. Rev. 104, 666 (1956).
[3] L. Heße, K. Richter, Phys. Rev. B 90, 205424 (2014).

TT 31.5 Wed 16:15 H31

Probing Fractional Statistics through Aharonov-Bohm Oscillations in Hanbury-Brown-Twiss Geometry — •Felix Puster, Matthias Thamm, and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 16, 04103 Leipzig, Germany

Since the theoretical prediction of anyonic excitations in the fractional quantum Hall effect, experimental evidence for their fractional statistics has been highly sought. In recent years, experiments have determined fractional braiding phases, providing clear evidence for fractional exchange phases. However, the braiding phase fixes the exchange phase of the particles only up to modulo Pi, leaving ambiguity in its exact value. Therefore, experiments capable of determining the exchange phase unambiguously are desired. To this end, we revisit the Hanbury-Brown-Twiss (HBT) geometry in the fractional quantum Hall regime. Our calculations extend previous theoretical work by incorporating an Aharonov-Bohm (AB) phase, finite temperature, and a finite distance between the tunneling points. We compute the current and current-current correlation functions and find that the anyonic exchange phase enters the AB oscillations in both quantities as an additive shift. While this shift is expected for the current-current correlations due to two-particle interference, for the current we interpret it as another example of time domain braiding of anyons – a phenomenon previously reported in geometries with tunneling of anyons across a quantum point contact.

TT 31.6 Wed 16:30 H31

Dipole Representation of Composite Fermions in Graphene's Quantum Hall Systems — •Sonja Predin — Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

The even-denominator fractional quantum Hall effect has been observed in graphene's fourth Landau level (N = 3) [1]. Motivated by recent studies [2] on pairing and the nature of the ground state in this system, we extend the dipole representation of composite fermions to adapt it to graphene's quantum Hall systems, focusing on half-filled Landau levels. We derive an effective Hamiltonian incorporating particle-hole symmetry. At the Fermi level, the energetic instability of the dipole state is driven by the interplay between topology and symmetry, pushing the system towards a critical state. While paired states are considered, our findings demonstrate that a boost-invariant state lacking well-defined pairing instabilities is energetically favorable stable state, suggesting the absence of pairing instabilities in this system.
[1] Y.Kim,A.C.Balram,T.Taniguchi,K.Watanabe,J.K.Jain, J.H.Smet, Nat. Phys. 15, 154 (2019).
[2] A.Sharma, S.Pu, A.C.Balram, J.K.Jain, PRL 130, 126201 (2023).
[3] S.Predin, A.Knežević, M.V.Milovanović, PRB 107, 155132 (2023).
[4] S. Predin, arXiv:2408.10375.

TT 32: Superconductivity: Yu-Shiba-Rusinov and Andreev Physics

Time: Wednesday 15:00–16:30 Location: H32

TT 32.1 Wed 15:00 H32

Ab-initio Investigation of YSR States of Fe Adatoms Interacting with Rashba-Split Surface States on $BiAg_2$ — •Ilias Klepetsanis[1,2], Philipp Rüssmann[1,3], and Samir Lounis[1,2] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]University of Würzburg, Germany

One of the most sought after topics in modern condensed matter physics research, has been the creation of topological superconductivity systems that are able to host Majorana states. A plethora of material configurations have been proposed to that end, with emphasis on the interplay between magnetism, SOC and superconductivity. Here, we investigate the behaviour of Fe adatoms deposited on a $BiAg_2$ surface with a superconducting Nb substrate, using the Bogoliubov-de-Gennes full-potential relativistic Korringa-Kohn-Rostoker Green function method [1]. We explore the emergence of Yu-Shiba-Rusinov (YSR) states and their dependence on the adatom deposition site and magnetic moment rotation, as well as the effect of the strong spin-orbit coupling from the substrate. We construct chains of Fe adatoms and study the YSR state behaviour with an increasing chain length and its correlation with the magnetic ground state. Finally we explore the possibility of non-trivial end-states emerging on the Fe chain.
[1] P. Rüßmann, and S. Blügel, Phys. Rev. B 105, 125143 (2022).

TT 32.2 Wed 15:15 H32

Shiba States in Magnet/Superconductor Heterostructures from First Principles — •Arnold Kole, Andrés Botello-Méndez, and Zeila Zanolli — Utrecht University, Utrecht, The Netherlands

The search for topological superconductors (TSC) with potential applications in quantum computing motivates the study of hybrid systems combining superconductivity, magnetism, and spin-orbit coupling. Previous work has shown the presence of in-gap states in these systems [1]. Of particular interest are Yu-Shiba-Rusinov (YSR) states, that arise due to interactions of magnetic impurities with a superconductor [1]. It has been proposed that these can be used to engineer topological superconductivity [1].

We demonstrate the emergence of topologically trivial in-gap YSR states in $CrCl_3$ islands on superconducting $NbSe_2$ [2]. Using Density Functional Theory (DFT), we show an increase of the Cr 3d density-of-states at the edge and an enhanced exchange interaction between the $CrCl_3$ edge and the $NbSe_2$ substrate [2]. This means that the $CrCl_3$ edge acts as a one-dimensional chain of magnetic impurities interacting with the superconducting $NbSe_2$. This can explain the emergence of the YSR states. Finally, we systematically show that these findings are robust to changes in computational details such as stacking, magnetic configuration and Hubbard U parameters [3].
[1] L. Schneider et al., Nat. Nanotechnol. 17, 384 (2022);
[2] J.P. Cuperus, A.H. Kole et al., submitted (2024);
[3] A.H. Kole et al., manuscript in preparation (2025).

TT 32.3 Wed 15:30 H32

Spin Dynamics in a Josephson Junction Between Two Superconducting Magnetic Impurity States — Fabian Ziesel[1], Björn Kubala[1,2], Joachim Ankerhold[1], and •Ciprian Padurariu[1] — [1]ICQ and IQST, Ulm University, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

We study the Josephson effect in a junction formed between two superconducting magnetic impurities. Such a junction was recently realized using a scanning tunneling microscope tip functionalized with a magnetic impurity that probes a second impurity on the sample [1]. Our work extends a recent theoretical investigation [2] by considering the mutually coupled dynamics between the impurity spins and the Josephson phase. We suggest that the Josephson effect can be exploited to manipulate the relative magnetic orientation of the impurities due to a Josephson-induced exchange interaction that arises.

Our theoretical approach treats the Josephson and spin dynamics equally. We identify a key experimental signature of spin dynamics: a small d.c. bias results in excess d.c. current due to the coupling between spins and the Josephson phase. We also discuss spin control, exemplified by inducing a spin-flip of an impurity using an adiabatic voltage pulse.
[1] H. Huang *et al.*, Phys. Rev. Res. **3**, L032008 (2021);
[2] S. Chakraborty *et al.*, Phys. Rev. B **108**, 094518 (2023).

TT 32.4 Wed 15:45 H32

Yu-Shiba-Rusinov Spectroscopy of Triple Quantum Dot Molecules — •Vladislav Pokorný[1] and Martin Žonda[2] — [1]FZU - Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 00 Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic

We study a system of three quantum dots in triangular geometry with equal distances connected to a common superconducting lead and coupled via interdot Coulomb interaction. We provide complete ground state phase diagrams for the half-filled system in various regimes and study the behavior of the in-gap Yu-Shiba-Rusinov states. We use the superconducting impurity Anderson model to describe the system and solve it using a combination of effective methods based on the superconducting atomic limit and the continuous-time hybridization expansion quantum Monte Carlo. The results can provide deep insight into experiments involving trimers made of magnetic molecules on superconducting substrates.

TT 32.5 Wed 16:00 H32

Experimental Signal of Multiple Andreev Reflexion in Spin Splitted Tunneling Junctions — •David Caldevilla-Asenjo[1], Sara Catalano[2,3], Pietro Cattaneo[4], Fernando Sebastian Bergeret[1], Maxim Ilyn[1], and Celia Rogero[1] — [1]Centro de Fisica de Materiales (CSIC-UPV/EHU),20018 Donostia San Sebastian — [2]Materials Physics Center (MPC), Paseo Manuel de Lardizabal 5,20018 Donostia, Spain. — [3]IKERBASQUE, Basque Foundation for Science,

48009 Bilbao, Basque Country, Spain. — [4]Politecnico di Milano, 20133, Milano, Italy

A ferromagnetic insulator in contact with a superconductor induces an effective exchange field, resulting in a spin splitting of the BCS density of states [1,2]. In this work, we study planar Josephson Junctions where one electrode is in contact with a thin layer of the ferromagnetic insulator europium sulfide. Samples are grown in situ by using the hard-mask technique in UHV. We characterized the junctions through DC transport measurements at a base temperature of 10mK, observing Josephson coupling and Multiple Andreev Reflection according to the transparency of the barrier. We propose a theory model to interpret the junction spectra taking into account the exchange field. Our results provide an experimental and theoretical description of ingap transport processes in superconducting junctions proximitized by a ferromagnetic insulator [3].

[1] R. Meservey and P.M. Tedrow, Phys. Rep. 238, 173 (1994);
[2] A. Hijano et al., Phys. Rev. Res. 3, 021031 (2021);
[3] B. Lu et al., Phys. Rev. B 101, 020502 (2020).

TT 32.6 Wed 16:15 H32

Nonequilibrium Josephson and Andreev Transport in Quantum Dot Junctions — •Jordi Picó-Cortés[1], Gloria Platero[2], Andrea Donarini[1], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC) 28049 Madrid, Spain

We investigate nonequilibrium transport through superconducting nanojunctions using a Liouville space approach [1]. The formalism allows us to study finite-gap effects, and to account for both quasiparticle and Cooper-pair tunneling. With focus on the weak-tunneling limit, we study the stationary dc and ac current up to second order (cotunneling) in the hybridization energy. For the particular case of a strongly interacting quantum dot sandwiched between two superconductors, we identify the characteristic virtual processes that yield the Andreev and Josephson current and obtain the dependence on the gate and bias voltage for the dc current, the critical current, and the phase-dependent dissipative current. In particular, the critical current is characterized by regions in the stability diagram in which its sign changes from positive to negative, resulting in a multitude of $0-\pi$ transitions. The latter signal the interplay between strong interactions and tunneling at finite bias.

[1] J. Picó-Cortés, G. Platero, A. Donarini, M. Grifoni, Phys. Rev. B 110, 125418 (2024).

TT 33: Correlated Magnetism – Spin Liquids

Time: Wednesday 15:00–18:15 Location: H33

TT 33.1 Wed 15:00 H33

An Atlas of Classical Pyrochlore Spin Liquids — •Daniel Lozano-Gómez[1,2], Owen Benton[3], Michel Gingras[2], and Han Yan[4] — [1]Technische Universität Dresden, Dresden, Germany — [2]University of Waterloo, Waterloo, Canada — [3]Queen Mary University of London, London, United Kingdom — [4]The University of Tokyo, Kashiwa, Japan

The pyrochlore lattice magnet has been one of the most fruitful platforms for the experimental and theoretical search for spin liquids. Besides the canonical case of spin ice, works in recent years have identified a variety of new quantum and classical spin liquids from the generic nearest-neighbor anisotropic spin Hamiltonian on the pyrochlore lattice. Despite the rich variety of SLs realized in this lattice, a general framework for the classification and characterization of these is still lacking. In this work, we develop such a theoretical framework to allocate interaction parameters stabilizing different classical SLs and derive their corresponding effective generalized emerging Gauss's laws at low-temperatures. Combining this with Monte Carlo simulations, we systematically identify all classical SLs for the general nearest-neighbor anisotropic spin Hamiltonian on the pyrochlore lattice. We uncover new SL models with exotic forms of generalized Gauss's law and multipole conservation laws. Our work serves as a treasure map for the theoretical study of classical and quantum spin liquids, as well as for the experimental search and rationalization of exotic pyrochlore lattice magnets.

TT 33.2 Wed 15:15 H33

Higher-Rank Spin Liquids and Spin Nematics from Competing Orders in Pyrochlore Magnets — •Niccolò Francini, Lukas Janssen, and Daniel Lozano-Gómez — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Pyrochlore magnets have proven to provide an excellent arena for the realization of a variety of many-body phenomena such as classical and quantum order-by-disorder, as well as spin liquid phases described by emergent gauge field theories. These phenomena arise from the competition between different symmetry-breaking magnetic orders. In this work, we consider a subspace of the most general bilinear nearest-neighbor Hamiltonian on the pyrochlore lattice, parameterized by the local interaction parameter $J_{z\pm}$, where three symmetry-breaking phases converge. We demonstrate that for small values of $|J_{z\pm}|$, a conventional $\mathbf{q} = 0$ ordered phase is selected by a thermal order-by-disorder mechanism. For $|J_{z\pm}|$ above a certain finite threshold, a novel spin-nematic phase is stabilized at low temperatures. Instead of the usual Bragg peaks, the spin-nematic phase features lines of high intensity in the spin structure factor. At intermediate temperatures above the low-temperature orders, a rank-2 U(1) classical spin liquid is realized for all $J_{z\pm} \neq 0$. We fully characterize all phases using classical Monte-Carlo simulations and a self-consistent Gaussian approximation.

TT 33.3 Wed 15:30 H33

Raman Circular Dichroism of Chiral Quantum Spin Liquids — •Eduard Koller[1,2,3], Valentin Leeb[1,3], Natalia Perkins[4], and Johannes Knolle[1,3,5] — [1]Technical University of Munich, Germany — [2]Institute for Advanced Study, TUM, Germany — [3]Munich Center for Quantum Science and Technology, Germany — [4]School of Physics and Astronomy, University of Minnesota, USA — [5]Blackett Laboratory, Imperial College London, United Kingdom

We investigate the Raman circular dichroism (RCD) of chiral Quantum spin liquids as a probe of the topological properties of fractionalised spin excitations. Starting from the Loudon Fleury formalism we show that the scattering Intensity is directly related to the light matter coupling formalism of spinon bands. We reveal that the RCD signal arises as a result of the Berry curvature and Quantum geometry contributions. We show application to different model quantum spin liquids.

TT 33.4 Wed 15:45 H33

Low-Temperature Features of the Quantum Spin Liquid Candidate PCTO Crystal Structure — •Alexander Mistonov[1], Abanoub Hanna[2], Elaheh Sadrollahi[1], Heidi Savey-Bennett[3], Martin von Zimmermann[4], Elizabeth Blackburn[5], Bella Lake[2], and Jochen Geck[1] — [1]Technische Universität Dresden — [2]Helmholtz-Zentrum Berlin — [3]The University of Manchester — [4]Deutsches Elektronen-Synchrotron DESY — [5]Lund University

$PbCuTe_2O_6$ (PCTO) is well known as a promising candidate for quantum spin liquid compounds. Magnetic ordering does not occur down to 0.02 K [1]. Additionally, diffuse continua are observed in magnetic spectra [2]. At the same time, heat capacity and dielectric response demonstrate signatures of an order-disorder ferroelectric (FE) transition at ~ 1 K [3]. According to thermal expansion measurements, this transition is believed to be accompanied by structural changes. We have performed a high-energy single-crystal X-ray diffraction experiment using a dilution refrigerator to investigate it for the first time. We have observed Bragg peaks that are forbidden for the reported high-temperature crystal structure (space group $P4_132$ [4]) and studied their evolution. In the current work, we share our findings from below and above the FE transition.

[1] P. Khuntia et al., Phys. Rev. Lett. 116, 107203 (2016).
[2] S. Chillal et al., Nat. Commun. 11, 2348 (2020).
[3] C. Thurn et. al., npj Quantum Mater. 6, 95 (2021).
[4] A. R. N. Hanna et al., Phys. Rev. Mat. 5, 113401 (2021).

TT 33.5 Wed 16:00 H33

What is carrying the heat in the thermal Hall effect of honeycomb magnets? — •Ralf Claus, Jan Bruin, Yosuke Matsumoto, Pascal Reiss, Akmal Hossain, Lichen Wang, Pascal Puphal, Bernhard Keimer, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart

The observation of a half-integer quantized thermal Hall effect in the honeycomb magnet α-$RuCl_3$ was interpreted as an experimental hallmark for Kitaev majorana fermions. However, follow-up studies only partly reproduced this result and have offered alternative explanations such as phonons or topological magnons. To narrow down the nature of the heat carrying quasiparticles, we conducted a comparative study of the longitudinal (κ_{xx}) and transversal (κ_{xy}) heat transport on α-$RuCl_3$ and $Na_3Co_2SbO_6$ (NCSO). Both share the same crystal symmetries and have comparable magnetic phase diagrams. However, one key difference is that for applied in-plane magnetic fields $B > 3$ T NCSO is in a fully spin-polarized phase convincingly excluding the presence of any majorana fermions. Remarkably, we observed a finite κ_{xy} in NCSO up to $B \approx 10$ T, which displays striking similarities in shape, angle-dependence, and magnitude to that of α-$RuCl_3$. Furthermore, the field dependences of κ_{xx} and of the thermal Hall angle (κ_{xy}/κ_{xx}) across all α-$RuCl_3$ and NCSO samples suggest a substantial phononic contribution to κ_{xy}. Ultimately, we propose that topological magnons are responsible for generating the Hall temperature gradient which in turn is significantly enhanced by phonon-magnon interaction.

TT 33.6 Wed 16:15 H33

Variational Monte Carlo Simulations of Two-dimensional Quantum Spin Liquids — •Florian Michael and Benedikt Fauseweh — TU Dortmund University, Dortmund, Germany

In this project we use state-of-the-art variational algorithms to train neural quantum states for the quantum spin liquid phase of the J1-J2 Heisenberg model on a square lattice. Specifically, this approach makes use of a hybrid architecture of a restricted Boltzmann machine and pair-product states, capturing both global and local correlations efficiently. To further increase the precision of the wave function representation as well as mitigate finite-size effects, we apply quantum number projections and impose twisted boundary conditions.

The project is implemented within the NetKet framework, leveraging the automatic differentiation and just-in-time compilation of JAX as well as GPU accelerated high-performance clusters. The goal is to further advance the application of neural quantum states in quantum many-body physics and gain new insights on properties of quantum spin liquids that are currently difficult to simulate due to their long-range entanglement and absence of magnetic order.

TT 33.7 Wed 16:30 H33

Quantum simulation of fermionic, non-Abelian lattice gauge theories in (2+1)D — •Gaia De Paciani[1,2], Lukas Homeier[1,2,3], and Fabian Grusdt[1,2] — [1]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics (ASC), Ludwig-Maximilians-Universität, München, Germany — [2]Münich Center for Quantum Science and Technology (MCQST), München, Germany — [3]University of Colorado, Boulder, Colorado

Understanding and simulating non-Abelian quantum spin-liquids and dimer models is an open challenge in the condensed matter and high energy physics landscape. Recent advancements in the field of quantum simulations have significantly expanded its potential for applications, particularly in the context of lattice gauge theories (LGTs). Nevertheless, maintaining gauge invariance throughout a simulation remains a critical challenge, especially for large-scale non-Abelian LGTs. We propose a novel approach to simulate non-Abelian U(N) LGTs with dynamical fermionic matter in (2+1) dimensions, enhancing the reliability of the simulation through the suppression of the occupation of gauge invariant sectors. We present a comprehensive framework to simulate gauge-invariant dynamics and we propose two experimental platforms – utilizing ultracold alkaline-earth-like atoms and Rydberg-dressing – to implement these models, enabling the quantum simulation of large-scale non-Abelian gauge theories in near-term experiments.

15 min. break

Invited Talk TT 33.8 Wed 17:00 H33

Emergent Dynamical Gauge Fields in Generic Kitaev Spin Liquids: From Monolayer to Multilayers — •Aprem Joy and Achim Rosch — Institute for Theoretical Physics, University of Cologne

Emergent gauge fields and fractional excitations are long sought-after in modern condensed matter physics. The Kitaev spin liquid and its potential realization in the so called “Kitaev materials" have been at the frontier of this search. The Kitaev spin liquid realizes an emergent static Z2 gauge field with vison excitations strongly interacting with Majorana fermions, by virtue of its gauge flux. While static in the idealized Kitaev model, single visons and vison pairs become dynamical degrees of freedom in the presence of perturbations. We develop a concise theory of the universal properties of single visons in weakly perturbed Kitaev models. We focus both on single-layer and multi-layer systems, motivated by the layered structure of materials. When Kitaev models are stacked on top of each other, weakly coupled by Heisenberg interaction, a rich zoo of mobile gauge excitations emerge whose dynamics is strongly constrained by topology and residual conservation laws, resulting in sub-dimensional mobilities, reminiscent of fractons. Furthermore, we show how vison dynamics in Kitaev materials can lead to novel signatures in relaxation experiments.

[1] A. Joy and A. Rosch, Phys. Rev. X 12, 041004 (2022);
[2] A. Joy and A. Rosch, npj Quantum Mater. 9, 62 (2024).

TT 33.9 Wed 17:30 H33

Pressure-dependent magnetism of the Kitaev candidate Li_2RhO_3 — •Efrain Insuasti Pazmino[1], Bin Shen[2], Ramesh Dhakal[3], Friedrich Freund[2], Philipp Gegenwart[2], Steve M. Winter[3], and Alexander A. Tsirlin[1] — [1]Leipzig University, Germany — [2]University of Augsburg, Germany — [3]Wake Forest University, USA

In the search for a Quantum Spin Liquid (QSL) state in real materials, hydrostatic pressure is employed to move honeycomb Kitaev compounds closer to or farther from a QSL state. The candidates studied so far have exhibited long-range magnetic ordering at lower temperatures. However, the candidate Li_2RhO_3 does not show a magnetic transition at low temperatures but instead exhibits spin freezing. Magnetic couplings obtained through theoretical super-exchange and Exact Diagonalization calculations evolve away from the Kitaev limit as pressure increases. Interestingly, the freezing temperature determined in our magnetization measurements remains constant under increasing pressure and does not correlate with the changes in magnetic couplings. An analysis of simulations and experiments suggests that spin freezing could arise from extrinsic factors such as stacking faults and crystal defects. Furthermore, the J_3 coupling was found to be unusually small in comparison with other Kitaev materials. Our work shows commonalities in the pressure evolution of the Kitaev iridates and rhodates where the decrease in the bond angle suppresses the Kitaev coupling while enhancing the off-diagonal anisotropy.

This work was supported by DFG via TRR360 (492547816).

TT 33.10 Wed 17:45 H33

Frustrated multipolar degrees of freedom: The quadrupolar Kitaev model — •Partha Sarker and Urban Friedrich Peter Seifert — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, D-50937 Köln

Frustrated multipolar exchange interactions between spin-S local moments ($S > 1/2$) have been suggested to possibly give rise to quantum spin liquid-like ground states featuring an emergent gauge structure and fractionalized excitations. However, only little is known about characteristic features and experimental signatures of such "multipolar spin liquids". To this end, in this work we turn to the "Quadrupolar Kitaev model" of $S = 1$ moments on a honeycomb lattice as a drosophila, for which recent numerical studies have found a deconfined ground state with topological order. As the model, similar to the spin-S generalization of the Kitaev honeycomb model, is not exactly solvable, we use a combination of mean-field theory and exact symmetry analysis to investigate competing ground states, including multipolar liquids, and their (fractionalized) excitations.

TT 33.11 Wed 18:00 H33

Phases of the Anyonic Hubbard Ladder for Fibonacci Anyons — •Nico Kirchner[1], Adam Gammon-Smith[2], and Frank Pollmann[1] — [1]Technical University of Munich, TUM School of Natural Sciences — [2]School of Physics and Astronomy, University of Nottingham

Two-dimensional systems such as quantum spin liquids may exhibit anyonic excitations that feature exchange statistics beyond the bosonic and fermionic cases. A fundamental question regarding such quasiparticles is how the richer exchange statistics influence their mutual interactions and which phases may arise in systems of anyons as a consequence. To study this topic, we consider the particular case of Fibonacci anyons subject to an anyonic Hubbard model with nearest-neighbor repulsion on a two-leg ladder. Focusing on half-filling, for low interaction strengths a metallic phase is found, whereas for strong repulsion, the anyons form a charge-density wave in real space. Within this regime, the effective interactions arising from the exchange statistics give rise to multiple distinct phases that can be distinguished using the scaling of the entanglement entropy and the spectra of matrix product state transfer matrices.

TT 34: Superconductivity: Theory

Time: Wednesday 15:00–18:30 Location: H36

TT 34.1 Wed 15:00 H36

Eliashberg theory and band-off-diagonal superconductivity — •Bernhard Putzer[1,2] and Mathias S. Scheurer[1] — [1]Institute for Theoretical Physics III, University of Stuttgart, 70550 Stuttgart, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, Innsbruck A-6020, Austria

In contrast to the mean field approximation of BCS theory, the Migdal-Eliashberg approach is a more sophisticated framework to describe phonon-mediated superconductivity. Allowing strong coupling between electronic and bosonic fields opens the door to investigate the effects of inter-band processes on the superconducting state in a controllable setting. We derive and solve the Eliashberg equations for a two-band model, inspired by twisted graphene systems, finding an entirely band-off-diagonal superconducting order parameter. By including full momentum and Matsubara fre- quency dependence, we uncover a mixing of even- and odd-frequency states induced by the band splitting. As a result, the superconductor exhibits very unconventional spectral properties for electron-phonon pairing; this includes a region with a nodal spectrum and a region with finite gap, which is, however, much smaller than the order parameter magnitude. Our findings have consequences for recent experiments on the superconducting state in twisted bilayer and trilayer graphene.

TT 34.2 Wed 15:15 H36

From charge fluctuations to pairing instabilities: Nonperturbative enhancement of the electron-phonon coupling driven by electronic correlations — •Emin Moghadas[1], Matthias Reitner[1], Alexander Kowalski[2], Giorgio Sangiovanni[2], Sergio Ciuchi[3,4], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [3]Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Coppito-L'Aquila, Italy — [4]Istituto dei Sistemi Complessi, CNR, Roma, Italy

We present a thorough investigation of the nonperturbative electronic mechanisms, which could lead to significant enhancements of the electron-phonon coupling in strongly correlated electron systems. Using dynamical mean-field theory (DMFT) for the single band Hubbard model on the square lattice, we analyze corrections to second-order electron-phonon processes arising from electronic fluctuations near the Mott metal-to-insulator transition (MIT). In this regime, the isothermal charge response becomes particularly large at small momenta, indicating tendencies towards phase-separation instabilities and enabling a substantial enhancement of the effective electron-phonon coupling. Eventually, we critically discuss the impact of our findings on observable spectral quantities as well as possible implications for the emergence of pairing instabilities.

TT 34.3 Wed 15:30 H36

Detailed analysis of the superconducting gap with Dynes pair-breaking scattering — •Anastasiya Lebedeva and František Herman — Comenius University in Bratislava

In our work, we study the energy gap behavior within the Dynes superconductor theory. This model generalizes the Bardeen-Cooper-Schrieffer (BCS) approach by including the pair-breaking disorder, introducing the tunneling in-gap states up to a Fermi level. Elaborating on the self-consistent gap equation, we obtain useful results which are also interesting from the experimental point of view. For example, the derived relations may serve to estimate the pair-breaking impurities concentration in the superconductor i.a. using only the energy gap and the critical temperature values of the material. Moreover, we offer the heuristic gap-to-temperature dependence providing up to 5%-precision in the whole temperature range. It is a more convenient tool compared to the cumbersome numerics used by now.

This work has been supported by the Slovak Research and Development Agency under the Contract no. APVV-23-0515, by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 945478.

TT 34.4 Wed 15:45 H36

Superconducting modes in the presence of Coulomb repulsion — •Joshua Althüser and Götz Uhrig — TU Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund, Deutschland

We numerically study the collective excitations present in BCS-superconductors including screened Coulomb interactions. By varying the screening strength, we analyze its impact on the system. We use a formulation of the effective phonon-mediated interaction between electrons that depends on the energy transfer between particles, rather than being a constant in a small energy shell around the Fermi edge. We compute the system's Green's functions using the iterated equations of motion (iEoM) approach, which ultimately enables a comprehensive analysis of collective excitations. For weak couplings, we identify the well-known amplitude (Higgs) mode at the quasiparticle continuum's lower edge and the phase (Anderson-Bogoliubov) mode at zero energy for a neutral system, which shifts to higher energies as the Coulomb interactions are switched on. As the phononic coupling is increased, the Higgs mode emerges from the continuum, and additional phase and amplitude modes appear, persisting even with active Coulomb interactions.

TT 34.5 Wed 16:00 H36

Obstructed pairs with zero superfluid stiffness — •Tamaghna Hazra and Jörg Schmalian — Karslruhe Institute of Technology

We present a microscopic pairing mechanism in which the kinetic energy of pairs is much lower than the kinetic energy of electrons. This results in interaction-driven localization of charge without extrinsic disorder and is characterized by a vanishing superfluid stiffness. Localized pairs gain more kinetic energy from resonating between sublattices in a bosonic compact localized state, than from delocalizing throughout the material. This is grounded in a microscopic model building on a structural motif shared by many oxide superconductors - strongly interacting localized electrons realize spin degrees of freedom on the vertices and doped charge lives on the edges of the Bravais lattice. In the strong-coupling limit, local unconventional pairs realize the bosonic analogue of flat bands supported on line graphs. We discuss the experimental implications of this pairing mechanism, with concrete falsifiability criteria, and emphasize the broad scope of this recipe in connection to diverse families of strongly correlated materials which share the key ingredients that go into it.

TT 34.6 Wed 16:15 H36

Electronic structure and superconductivity in nickelates and cuprates: Insights from DMFT and DΓA — •Eric Jacob[1], Mario Malcolms de Oliveira[2], Thomas Schäfer[2], Paul Worm[1], Liang Si[3,1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [3]School of Physics, Northwest University, Xi'an 710127, China

The infinite-layer nickelates and cuprates represent two compelling families of materials for exploring unconventional superconductivity and correlated electronic phenomena. I will discuss recent advances in understanding the electronic structure of infinite-layer nickelates, focusing on insights from dynamical mean-field theory (DMFT) and their comparison with experimental findings ([1]) from angle-resolved photoemission spectroscopy (ARPES). This helps [2] constrain possible scenarios for their electronic states. In particular, there is only one Ni orbital crossing the Fermi surface. Additionally, I will present ongoing investigations into superconductivity in both nickelates and cuprates, based on the dynamical vertex approximation ($D\Gamma A$ [3], [4]).

Funding through the FWF project I5398 is gratefully acknowledged.

[1] W. Sun et al., arXiv:2403.07344 (2024).
[2] L. Si et al., Phys. Rev. Res. 6, 043104 (2024).
[3] G. Rohringer et al., Rev. Mod. Phys. 90, 025003 (2018).
[4] M. Kitatani et al., J. Phys. Mater. 5, 034005 (2022).

TT 34.7 Wed 16:30 H36

Towards an *ab initio* theory of high-temperature superconductors: a study of multilayer cuprates. — •Benjamin Bacq-Labreuil[1,2], Benjamin Lacasse[1], André-Marie Tremblay[1], David Sénéchal[1], and Kristjan Haule[3] — [1]Institut quantique, Université de Sherbrooke, Canada — [2]IPCMS, Université de Strasbourg, France — [3]Center for Materials Theory, Rutgers University, USA

Significant progress towards a theory of high-temperature superconductivity in cuprates has been achieved via the study of effective models. Yet, material-specific predictions for high-temperature superconductors, while essential for constructing a comprehensive theory, remain out of reach. By combining cluster dynamical mean-field theory and density functional theory in a charge-self-consistent manner, here we show that the goal of material-specific predictions for high-temperature superconductors from first principles is within reach. We demonstrate the capabilities of our approach by performing an in-depth study of two representatives ($Ca_{(1+n)}Cu_nO_{2n}Cl_2$ and $HgBa_2Ca_{(n-1)}Cu_nO_{(2n+2)}$) of the still mysterious multilayer cuprates. We shed light on the microscopic origin of many salient features of multilayer cuprates, in particular the n-dependence of their superconducting properties. Our work establishes a framework for comprehensive studies of high-temperature superconducting cuprates, enables detailed comparisons with experiment, and, through its *ab initio* settings, unlocks opportunities for theoretical material design of high-temperature superconductors.

15 min. break

TT 34.8 Wed 17:00 H36

Enhanced entanglement in the pseudogap — •Frederic Bippus[1], Juraj Krsnik[1], Motoharu Kitatani[2,3], Anna Kauch[1], Gergö Roosz[4], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]Department of Material Science, University of Hyogo, Ako, Hyogo, Japan — [3]RIKEN Center for Emergent Matter Sciences (CEMS), Wako, Japan — [4]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary

We show significantly enhanced entanglement in the pseudogap regime of the Hubbard model using the dynamical vertex approximation (DGA) [1], a nonlocal extension to the dynamical mean-field theory. The pseudogap, a partially gapped electronic state, is observed near the superconducting transition in cuprates and nickelates. Leveraging DGA, we compute the quantum variance-a lower bound to the quantum Fisher information [2] from the spin susceptibility directly on the imaginary Matsubara axis. By circumventing the need for ill-controlled analytical continuation, our approach provides a robust framework for probing entanglement depth. The results show good agreement with experimental data [3]. Additionally, Ornstein-Zernike fits provide analytical insights.

This work is supported by the SFB Q-M&S (FWF project ID F86).

[1] Rohringer et al., Rev. Mod. Phys., 90, 025003 (2018);
[2] Frérot et al., Phys. Rev. B, 94, 075121 (2016);
[3] Chan et al., Nat. Commun., 7, 10819 (2016).

TT 34.9 Wed 17:15 H36

Time evolution of surface state wave packets in nodal noncentrosymmetric superconductors — •Clara Johanna Lapp[1,2], Julia Link[1,2], and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Nodal noncentrosymmetric superconductors can host zero-energy flat bands of Majorana surface states within the projection of the nodal lines onto the surface Brillouin zone. Thus, these systems can have stationary, localized Majorana wave packets on certain surfaces, which may be a promising platfrom for quan-

tum computation. However, for such applications it is important to find ways to manipulate the wave packets in order to move them without destroying their localization or coherence. As the surface states have a nontrivial spin polarization, applying an exchange field, e.g., by introducing a magnetic insulator at the surface, makes the previously flat band slightly dispersive. We aim to use an adiabatic change of the exchange field to move wave packets on the surface. We therefore investigate the time evolution of a maximally localized wave packet under the influence of such an exchange field employing exact diagonalization as well as quasiclassical approximations.

TT 34.10 Wed 17:30 H36

Interplay of superconductivity and altermagnetism: A symmetry perspective — •Kirill Parshukov[1], Niclas Heinsdorf[1,2], Benjamin T. Zhou[2], Marcel Franz[2], and Andreas P. Schnyder[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]The University of British Columbia, Vancouver BC, Canada

The interplay between altermagnetism and superconductivity gives rise to several interesting phenomena, including unconventional Josephson effects, diode effects, Cooper pair splitting, and topological superconductivity. In this talk, I investigate how altermagnetic symmetries can lead to new superconducting states with interesting topological properties. Since the superconducting gap functions must transform as irreducible co-representations of the spin-point groups, I first construct all possible superconducting basis functions. Importantly, because the spin-point group symmetries act simultaneously on the spin and the lattice, the spin and spatial parts of the basis functions are coupled in an intricate manner. I illustrate this by considering several examples in two dimensions, including the superconducting states of an altermagnet with four Dirac points [1].

[1] K. Parshukov, R. Wiedmann, A. P. Schnyder, arXiv:2403.09520.

TT 34.11 Wed 17:45 H36

Emergence of a condensate with finite-energy Cooper pairing in hybrid exciton/superconductor systems — •Viktoriia Kornich — University of Würzburg, Würzburg, Germany

I will consider a setup consisting of excitons formed in two valleys, with proximity-induced Cooper pairing, different in the conduction and valence bands. Due to the combination of a Coulomb interaction within excitons and superconducting proximity effects, Cooper pairing between electrons from valence and conduction bands from different valleys is formed. Thus, the gap between these electrons can be much larger than the usual superconducting pairing energies. This Cooper pairing has both even- and odd-frequency contributions. I will show that there is a phase transition into the formation of a robust macroscopic condensate of such Cooper pairs and then will suggest a detection scheme of it via Higgs modes.

TT 34.12 Wed 18:00 H36

Third-harmonic generation currents in pair-density wave superconductor — •Pascal Derendorf[1], Peayush Choubey[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany — [2]Indian Institute of Technology-Roorkee, Roorkee, India

We investigate the signatures of a unidirectional pair-density wave (PDW) state in the third harmonic generation (THG) using an effective microscopic model, developed previously in Refs. [1,2]. The system possesses a unidirectional PDW state with d-wave symmetry in thermodynamic equilibrium ground state without extra need for an additional perturbation such as external Zeeman field or leading charge density wave order. We extend this model under the non-equilibrium by including a periodic driving in the form of external ac-field. The signatures of the emerging massive modes on the THG are derived via a gauge-invariant effective action approach. We discuss the emerging signatures in the third harmonic generation and their origin.

[1] F. Loder et al., Phys. Rev. B 81 (2010).
[2] J. Wårdh and M. Granath., Phys. Rev. B 96 (2017).

TT 34.13 Wed 18:15 H36

Describing superconductivity through interpretable artificial intelligence — •Herzain I. Rivera-Arrieta, Lucas Foppa, and Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Superconductivity is governed by an intricate interplay among electronic structure, lattice vibrations, and pressure effects, among many other phenomena [1]. Thus, a (single) physical model might not be enough to describe superconductivity. Interpretable artificial intelligence (AI) can provide valuable insights into the underlying mechanisms driving superconductivity, e.g., in conventional superconductors. Herein, we compile a dataset containing approximately 1,000 materials [2] and a diverse range of compositional, structural, electronic, and phonon-related properties. Then, we employ the symbolic-regression SISSO and subgroup discovery AI approaches [3, 4], to identify the few, key physicochemical parameters correlated with a superconductor's critical temperature. This approach is a step towards identifying the "materials genes" [5] of superconductivity.

[1] X. Gui, B. Lv, and W. Xie, *Chem. Rev.*, **121**, 2966 (2021).
[2] K. Choudhary, and K. Garrity, *Npj. Comut. Mater.*, **8**, 244 (2022).
[3] R. Ouyang, *et al.*, *Phys. Rev. Mat.*, **2**, 083802 (2018).
[4] S. Wrobel, *1st Europ. Symp. on Princ. of Data Min. and Knowl. Discov.*, **19**, 78 (1997).
[5] L. Foppa, *et al.*, *MRS bulletin*, **46**, 1016 (2021).

TT 35: Topology: Poster

Time: Wednesday 15:00–18:00 Location: P3

TT 35.1 Wed 15:00 P3

Conductive surface states in single-crystalline FeSi — •Philip Schröder, Gilles Gödecke, Julius Grefe, Stefan Süllow, and Dirk Menzel — Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

The small-gap semiconductor FeSi exhibits an insulating ground state over a wide temperature range [1]. Notably, electric resistivity measurements imply the opening of a metallic transport channel at lowest temperatures, which historically has been attributed to conductivity among impurity levels [2]. However, recent transport studies on high-quality flux-grown FeSi single crystals discuss the conductive behavior in terms of metallic [3] and magnetic [4] surface states. We present (magneto-)resistance measurements on tri-arc Czochralski-grown FeSi single crystals in dependence of the sample thickness. The controlled manipulation of the surface-to-volume ratio by successive grinding of the specimen under investigation allows for separation of the bulk resistivity and the superimposed contribution of the surface channels. An effective two-channel model has been applied to approximate the upper limit of the surface conductivity.

[1] V. Jaccarino et al., Phys. Rev. 160, 476 (1967).
[2] S. Paschen et al., Phys. Rev. B 56, 12916 (1997).
[3] Y. Fang et al., Proc. Natl. Acad. Sci. U.S.A. 115, 8558 (2018).
[4] K. E. Avers et al., Phys. Rev. B 110, 134416 (2024).

TT 35.2 Wed 15:00 P3

Fabrication and characterization of topological insulator-based SET — •Omargeldi Atanov, Junya Feng, and Yoichi Ando — Physics Institute II, University of Cologne, Cologne, Germany

When a topological insulator (TI) Josephson junction is driven through a topological phase transition, the ground-state parity of the system is expected to change, potentially due to the fusion of Majorana bound state (MBS) pairs. Measuring the individual parity of MBS pairs is a critical step in understanding the mechanisms behind these parity changes and for more complex braiding operations. We present the fabrication and characterization of single-electron transistors (SETs) based on bulk-insulating BiSbTeSe2 flakes, which also serve as the material for TI Josephson junctions. This approach simplifies the process flow of the devices and improves fabrication yield. Initial characterization of devices demonstrates well-formed Coulomb diamonds that confirms the robust charge quantization and SET performance. These results pave the way for integrating SETs with TI Josephson junctions and measuring MBS parity in the near future.

TT 35.3 Wed 15:00 P3

Bulk and surface electron scattering in disordered Bi_2Te_3 probed by quasiparticle interference — •Vladislav Nagorkin[1,2], Sebastian Schimmel[1,2], Paul Gebauer[3], Anna Isaeva[1,4,5,6], Danny Baumann[1], Andreas Koitzsch[1], Bernd Büchner[1,3], and Christian Hess[1,2] — [1]IFW Dresden, Germany — [2]Bergische Universität Wuppertal, Germany — [3]TU Dresden, Germany — [4]University of Amsterdam, The Netherlands — [5]TU Dortmund, Germany — [6]Research Center "Future Energy Materials and Systems", UA Ruhr, Germany

We present low temperature scanning tunneling microscopy and spectroscopy studies of the electronic properties of the topological insulator Bi_2Te_3. The high-resolution differential conductance maps were measured in a relatively large energy range and allowed to reveal the quasiparticle interference in this material. We interpret our experimental data by comparing them with the modeled quasiparticle interference patterns with the use of the spin-selective joint density of states approach including the intricate three-dimensional spin texture of this material. Based on that, the topological properties are clearly demonstrated by the linear energy dispersion of the dominant scattering vector and the absence of the backscattering. In addition, non-dispersive scattering modes were detected and interpreted by scattering involving both surface and bulk states. This allowed us

to approximate the bulk energy gap range in our samples. Finally, we show that the abovementioned findings are robust against the external magnetic field of magnitude up to 15 T.

TT 35.4 Wed 15:00 P3

Planar Hall and Anomalous Planar Hall Effects up to Room Temperature in t-$PtBi_2$ — •Ankit Kumar — IFW Dresden

In topological semimetals, Hall measurements provide an important charge transport footprint of the non-trivial geometric properties of the electronic wavefunctions. In Weyl semimetals, the planar Hall effect (PHE) – the appearance of a transverse voltage when coplanar electric and magnetic fields are applied – is a direct consequence of the longitudinal linear magnetoconductance associated with the chiral anomaly of Weyl fermions, and is quantified by the large Berry curvature of Weyl nodes. The anomalous Hall effect is fully determined only by the location in the Brillouin zone and topological charge of the Weyl nodes. Time-reversal invariance prohibits any anomalous Hall signal in the large class of non-magnetic Weyl semimetals thereby leaving the PHE as the only Hall diagnostic tool of Weyl physics, at least in the linear regime. This complicates the identification of non-magnetic topological semimetals by charge transport experiments.

TT 35.5 Wed 15:00 P3

Instabilities driven by electron-electron interactions — •Eva López Rojo, Julia Link, and Carsten Timm — TU Dresen, Germany

We develop a formalism to study the effect of strong electron-electron interactions in a Weyl semimetal. In this poster, we present the findings for the case of two doped Weyl cones with opposite chirality. For this purpose, we employ a path integral formalism to study different instabilities that could take place. Instead of the charge density wave proposed in the literature, the leading instability for strong inter-valley interactions is found to be a spin density wave, which still has the potential to host axion physics.

TT 35.6 Wed 15:00 P3

The Effect of Interface Disorder on the Tunnel Conductance Across Weyl Semimetal Interfaces — •Haoyang Tian[1], Vatsal Dwivedi[2], Adam Yanis Chaou[2], and Maxim Breitkreiz[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

The chiral anomaly in Weyl semimetals is responsible for various anomalous transport phenomena. In tunnel junctions between Weyl semimetals with staggered Weyl node projections, the chiral anomaly leads to a magnetic-field activated magnetotransport. In this work, we discuss the effect of interface disorder on the magnetotransport across such a tunnel junction employing a semiclassical Boltzmann approach. Our results show that, compared to conventional transport channels, the topological connectivity of interface Fermi arcs ensures that anomalous magnetotransport exhibits stronger robustness against disorder. Additionally, interface disorder enhances magnetic breakdown, a quantum tunneling effect, between the Fermi arcs.

TT 35.7 Wed 15:00 P3

Impact of decoherence on the Kitaev honeycomb model — •Alexander Sattler and Maria Daghofer — Universität Stuttgart, 70550 Stuttgart, Germany

Quantum spin liquids (QSL) are phases of matter with unique properties, including quantum fluctuations, frustration, entanglement, fractionalized excitations, and the absence of long-range order. A rare example of an exactly solvable, strongly interacting two-dimensional model with a QSL ground state is the Kitaev honeycomb model (KHM). This model describes spin-1/2 particles on a honeycomb lattice with direction-dependent Ising-like interactions. The KHM with open boundaries supports edge-localized Majorana zero modes that are robust to certain types of disorder. Quantum systems are inherently coupled to their environment, necessitating the study of the KHM properties in open systems, where environmental interactions, such as decoherence, can influence their features. To study this, we analyze the KHM in a cylindrical geometry while modeling environmental coupling using the Lindblad master equation to simulate decoherence. By examining changes in the dispersion relation, entropy, fidelity, purity and spectral gap over time, we evaluate how environmental interactions affect the properties of the KHM.

TT 35.8 Wed 15:00 P3

Andreev reflection and interferometry of fractional quantum Hall edge states — •Tom Menei, Daniele Di Miceli, and Thomas L. Schmidt — Department of Physics and Materials Science, University of Luxembourg

Recent experimental work has demonstrated that it is possible to couple superconductors (SCs) to quantum Hall (QH) systems, both at integer and fractional filling fractions. Due to the strong required magnetic fields and the presence of disorder and Abrikosov vortices in the SC, the theoretical modeling of such QH/SC interfaces is not trivial, especially in the case of fractional QH states. In our work, we use the Laughlin edge state theory and realistic models of the superconductor to derive the coupling mechanism at QH/SC interfaces. We explore the effects on normal and Andreev reflection and discuss possible experimental implications.

TT 35.9 Wed 15:00 P3

Variational Trial States for Fractional Chern Insulators — •Giacomo Amadore — LMU, Munich, Germany

Early on, Laughlin's wave functions and other variational trial states provided deep physical insights into the nature of fractional quantum Hall (FQH) systems. One particularly fruitful approach in motivating such trial states is based on the composite fermion description of the FQH problem in the continuum. In contrast, variational states describing fractional Chern insulators in lattice systems remained scarce. While existing methods can construct lattice analogs of familiar FQH states, these states are not generally expected to be the ground state of simple discretized FQH Hamiltonians, but instead a parent Hamiltonian is only constructed a posteriori. To address this limitation, we propose a conceptually different approach motivated by the possibility to study FQH physics in optical lattice experiments realizing the Hofstadter-Bose-Hubbard model. We derive trial states for the ground state of this specific Hamiltonian by turning hard-core bosons into composite fermions through the attachment of a single flux quantum and deriving an effective Hamiltonian for the composite fermions coupled to a dynamical gauge field. To benchmark our findings, we compare the variational energies of different ansätze to (quasi-)exact numerical results. We anticipate that our preliminary results provide a promising starting point for further variational studies and investigations of lattice analogs of FQH systems.

TT 36: Nanotubes, BEC, Cryocoolers: Poster

Time: Wednesday 15:00–18:00 Location: P3

TT 36.1 Wed 15:00 P3

Quantum Dot Spectroscopy in Suspended MoS_2 Nanotubes — •Stefan B. Obloh[1], Robin T. K. Schock[1], Jonathan Neuwald[1], Matthias Kronseder[1], Matjaž Malok[2], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Institute Jožef Stefan,1000 Ljubljana, Slovenia

MoS_2 as a semiconductor has attracted a lot of attention due to its 2D nature, strong spin-orbin coupling, broken inversion symmetry, and spin-split bands. By tuning the carrier density in MoS_2 with ionic liquid gating, intrinsic superconuctivity has been achieved [1]. Recent works were able to demonstrate single level transport in planar [2,3] and nanotube-based [4] devices. A remaining challenge lies in reducing the effects of substrate inhomogenity and surface charges, resulting in disordered quantum dots. To mitigate this, one can suspend the tubes above the substrate or shield them from the amorphous SiO_2. We show quantum dot transport measurements of suspended nanotubes as well as insights into fabrication challenges regarding this approach.

[1] J. T. Ye *et al.*, Science **338**, 1193 (2012).
[2] R. Krishnan *et al.*, Nano Lett. **23**, 6171 (2023).
[3] P.Kumar *et al.*, Nanoscale **15**, 18023 (2023).
[4] R. T. K. Schock *et al.*, Adv. Mat. **35**, 13 (2023).

TT 36.2 Wed 15:00 P3

MoS_2 Nanotubes as 1D Superconductors? — •Konstantin D. Schneider[1], Robin T. K. Schock[1], Stefan Obloh[1], Matthias Kronseder[1], Matjaz Malok[2], Maja Remskar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Institute Jožef Stefan, 1000 Ljubljana, Slovenia

Due to its intrinsic two dimensional nature, planar MoS_2 is at the center of manifold research efforts. Previous work has shown that MoS_2 exhibits superconducting properties in single and multi layer flakes when increasing its charge density by heavily doping the MoS_2 surface using a liquid-ion gate [1-3].

Clean and defect-free MoS_2 nanotubes, as grown via chemical transport reaction [4,5], should provide an even better test bed for the interplay of a tubular geometry and Ising superconductivity. In addition, with ionic doping mostly affecting the outermost shell of a multi-wall nanotube, the material system lends itself intrinsically for core-shell semiconductor/superconductor hybrid structures

at strong spin-orbin interaction. Here, we present our ongoing work towards this objective [6,7].

[1] T. Ye *et al.*, Science 338, 1193 (2012).
[2] Costanzo *et al.*, Nat. Nano. 11, 339 (2016).
[3] C. Shen *et al.*, Nature 593, 211.
[4] M. Remskar *et al.*, Appl. Phys. Lett. 69, 351 (1996).
[5] M. Remskar *et al.*, Isr. J. Chemistry 62, e202100100 (2022).
[6] T. K. Schock *et al.*, Advanced Materials 35(13) (2023).
[7] Reinhardt *et al.*, pssRRL 13, 1900251 (2019).

TT 36.3 Wed 15:00 P3

Simulations to enhance the conductivity of graphene-based macromaterials — •Florian Fuchs[1,2,3], Fabian Teichert[1,2,3], and Jörg Schuster[1,2,3] — [1]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [2]Center for Microtechnologies,Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Materials, Architecture and Integration of Nanomembranes (MAIN), TU Chemnitz, Germany

Our aim is to enhance the conductivity of graphene-based macromaterials. These materials consist of many graphene flakes, which are arranged layerwise. A twofold strategy is pursued to improve the material: 1) optimizing the flake properties and the size of the macromaterial, and 2) intercalating molecules in-between the graphene layers.

A network model enables us to estimate the conductivity of the macromaterial for large model systems consisting of thousands of flakes. Particular emphasis will be given in our contribution on the variation of the layer numbers, which is of relevance for printed graphene paths.

To study the impact of intercalants, we perform density functional theory calculations. We concentrate on different fluorides and chlorides, where we vary the cation type and the anion number. The charge carrier density after intercalation is studied and related to more fundamental physical properties such as orbital overlaps and charge transfer.

TT 36.4 Wed 15:00 P3

Quantum Solvation of Flexible Molecules at Low Temperatures from Path Integral Simulations — •Katharina Leitmann[1], Harald Forbert[1,2], and Dominik Marx[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Center for Solvation Science ZEMOS, Ruhr-Universität Bochum, 44780 Bochum, Germany

Protonated methane (CH_5^+) is a fluxional molecule whose sensitivity to its environment makes it an excellent probe for studying molecular interactions at low temperatures. We investigated CH_5^+ microsolvation in *para*-hydrogen clusters $(pH_2)_n$ subject to bosonic exchange at 1 K using a hybrid simulation approach that combines Path Integral Molecular Dynamics (PIMD) for CH_5^+ and bosonic Path Integral Monte Carlo (PIMC) to establish Bose-Einstein statistics of the $(pH_2)_n$ quantum solvation environment.

Our simulations, based on highly accurate High-dimensional Neural Network Potentials parametrised using coupled cluster theory (CCSD(T)), demonstrate stable solvation of CH_5^+ at least up to $n = 12$ pH_2 molecules, which we found to build the first solvation shell. We revealed, that the structure of CH_5^+ is not significantly perturbed by the solvation with pH_2. But we revealed significant fluctuations in the large amplitude motion of CH_5^+ associated to the phenomenon of partial hydrogen scrambling as a function of cluster size n. Further, we investigated the superfluid properties of pH_2 clusters. Analysing the superfluid fraction and bosonic permutation patterns, indicates the manifestation of superfluidity.

TT 36.5 Wed 15:00 P3

Generating a photonic Bose-Einstein condensate in a waveguide — •Lukas Schamriss[1,2,3], Louis Garbe[1,2,3], and Peter Rabl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

We aim to propose a superconducting device designed to generate a photonic Bose-Einstein condensate (BEC). The core component is a coupler that induces a pure three-wave mixing interaction linking a waveguide which hosts the condensate to a LC-mode for dissipating energy from the waveguide. This interaction induces an incoherent photon-number conserving thermalization process in the waveguide. Generally, this system is a minimal example for generating a thermalization mechanism for microwave photons which is a key ingredient for the preparation of finite-temperature equilibrium states on superconducting hardware for analog quantum simulations.

TT 36.6 Wed 15:00 P3

Loop current states and their stability in small fractal lattices of Bose-Einstein condensates — •Georg Koch and Anna Posazhennikova — Institut für Physik, Universität Greifswald, 17487 Greifswald , Germany

We consider a model of interacting Bose-Einstein condensates on small Sierpinski gaskets. We study eigenstates which are characterised by cyclic supercurrents per each triangular plaquette ("loop" states). For noninteracting systems we find at least three classes of loop eigenmodes: standard; chaotic and periodic. Standard modes are those inherited from the basic three-site ring of condensates with phase differences locked to $2\pi/3$. Standard modes become unstable in the interacting system but only when the interaction exceeds a certain critical value u_c. Chaotic modes are characterised by very different circular currents per plaquette, so that the usual symmetry of loop currents is broken. Circular supercurrents associated with chaotic modes become chaotic for any finite interaction, signalling the loss of coherence between the condensates. Periodic modes are described by alternating populations and two different phase differences. The modes are self-similar and are present in all generations of Sierpinski gasket. When the interaction is included, the circular current of such a mode becomes periodic in time with the amplitude growing linearly with the interaction. Above a critical interaction the amplitude saturates signalling a transition to a macroscopic self-trapping state originally known from a usual Bose Josephson junction. We perform a systematic analysis of this rich physics.

TT 36.7 Wed 15:00 P3

Sub-50 mK Adiabatic Demagnetization Refrigeration with Frustrated Yb-Oxide Magnets in the PPMS — •Anna Klinger, Jorginho Villar Guerrero, Marvin Klinger, Tim Treu, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

Accessing temperatures in the millikelvin (mK) regime is a prerequisite for quantum-matter research and quantum technologies. Adiabatic demagnetization refrigeration (ADR) is a simple and sustainable alternative to ^{3}He/^{4}He dilution refrigeration. We have shown recently, that geometrically frustrated Yb-oxides feature important advantages compared to the traditionally utilized hydrated paramagnetic salts for mK-ADR [1,2]. We report the development of Yb-oxide-based customized ADR cooling platforms for the use in the Quantum Design Physical Property Measurement System (PPMS) ®. Temperatures below 50 mK and hold times of several hours are demonstrated. Our ADR insert offers multiple experimental capabilities, including electrical transport, stress/strain and heat capacity measurements.

[1] Y. Tokiwa et al., Commun. Mater. 2 (2021) 42.
[2] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025).

TT 36.8 Wed 15:00 P3

Experimental and Numerical Investigations of the Temperature and Mass Flow Behaviour in the Cold Heat Exchanger of a Single Stage GM-type Puls Tube Cooler — •Elias Eisenschmidt[1,3], Jack-Andre Schmidt[2,3], Bernd Schmidt[2,3], Hardy Weisweiler[1,3], and Andre Schirmeisen[2,3] — [1]Technische Hochschule Mittelhessen, Giessen, Germany — [2]Justus-Liebig-University, Giessen, Germany — [3]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany

GM-type PTCs play an important role in cooling sensitive electronics. Especially due to the recent developments in quantum computing, low vibration regenerative cooling is needed more than ever. [1]

The refrigeration power is usually calculated using a sinusoidal approximation of the mass flow, temperature and pressure of the working fluid inside a pulse tube cooler. However, several measurements have been carried out to gain insight into the actual time-dependent gas properties. It has been shown that the temperature and pressure curve differ significantly from a sinusoidal assumption. [2]

The goal of this work is to measure the time dependent mass flow and temperature behaviour of the helium gas in the cold end of the cooler, using a RTD and a CTA probe.

[1] Y. Zhai et al., IEEE Trans. Appl. Supercond. 34, May 2024
[2] P. P. Steijaert, Thermodynamical aspects of pulse-tube refrigerators, Technische Universiteit Eindhoven, 1999

TT 36.9 Wed 15:00 P3

Optimisation of Rotary Valve Size and Timing for High Massflow GM-Type Pulse Tube Cryocoolers — •Xaver Herrmann[1], Jack-André Schmidt[1,2], Bernd Schmidt[1,2], Jens Falter[2], and André Schirmeisen[1,2] — [1]Instiute of Applied Physics, Justus-Liebig University, Giessen, Germany — [2]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany

Closed-cycle cryocoolers have become a reliable and important tool for low temperature scientific research, such as IR astronomy, SNSPDs or surface science[1]. Here we focus on Gifford-McMahon (GM) type pulse tube cryocoolers (PTC), which offer low maintenance and long measurement periods[2]. A crucial component of a GM type PTC is the rotary valve. Losses in the rotary valve are a sizable fraction of overall losses in a GM type PTC [3,4]. This poster will focus on the effects of valve size and timing for a two stage high input power system(11 kW). Both valve size and timing show a strong effect on cooling performance of the first cooling stage. An increase of up to 90

[1] R. Güsten et al., Nature 568 (2019) 357.
[2] R. Radebaugh, J. Phys.: Condens. Matter 21 (2009) 164219.
[3] D. Liu et al., Cryogenics 81 (2017) 100.
[4] L.M. Qiu et al., Cryogenics 42 (2002) 327.

TT 37: Correlated Electrons: Poster

Time: Wednesday 15:00–18:00 Location: P4

TT 37.1 Wed 15:00 P4

Unveiling the Origin of Magnetic Anisotropy in $CeSb_2$ — •Jan T. Weber[1,2], Kristin Kliemt[1], Sergey L. Bud'ko[2,3], Paul C. Canfield[2,3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt am Main, Germany — [2]Ames National Laboratory, U.S. DOE, Ames, Iowa 50011, USA — [3]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

$CeSb_2$ is a well-established Kondo-lattice system, crystallizing in the orthorhombic $SmSb_2$ structure (space group 64) [1] and forming plate-like crystals. Extensive past studies have revealed a rich magnetic phase diagram for fields within the plane and a strong suppression of magnetization out of plane [2-5]. However, the in-plane magnetization anisotropy remains poorly understood. Nearly identical lattice parameters present challenges in aligning the crystals within the plane, and unexpected magnetization curves - seemingly inconsistent with symmetry arguments - pose additional questions.

In this contribution, we present rotational magnetization measurements together with magnetic measurements as a function of field, temperature and orientation, providing new insights into the in-plane anisotropy addressing these open questions.

[1] R. Wang et. al., Inorg. Chem. 6, 1685 (1967).
[2] S. L. Bud'ko et. al., Phys. Rev. B 57, 13624 (1998).
[3] Y. Zhang et al., Chin. Phys. B 26, 067102 (2017).
[4] B. Liu et al., J. Phys.: Condens. Matter 32, 405605 (2020).
[5] C. Trainer et al., Phys. Rev. B 104, 205134 (2021).

TT 37.2 Wed 15:00 P4

Single Crystal Growth and Characterisation of $EuMn_2Si_2$ and $EuMn_2Ge_2$ — •Janina Strahl, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe University, Frankfurt (Main), Germany

$EuMn_2Si_2$ exhibits a thermally driven valence transition at around 530 K of the europium ions from Eu^{3+} at low temperatures to $Eu^{\sim 2.5+}$ at high temperatures [1]. The isoelectronic and isostructural substitution of silicon with germanium leads to a stabilization of the divalent state of Eu in $EuMn_2Ge_2$ with reported ferromagnetic Eu ordering below 13 K [2]. Both rare earth intermetallic 122 compounds crystallize in the tetragonal $ThCr_2Si_2$ structure type and show antiferromagnetic ordering of the manganese sublattices above room temperature. In literature [1,2], additional Mn spin-reorientation transitions in polycrystalline $EuMn_2Si_2$ samples at low temperatures were observed. In this contribution, we present the single crystal growth and magnetic properties of both compounds. We found antiferromagnetic ordering of the Eu ions in single crystalline $EuMn_2Ge_2$ below 8.5 K and evidence that previously reported Mn reorientation transitions are absent in pure $EuMn_2Si_2$ single crystals.

[1] M. Hofmann et al., Phys. Rev. B 69, 174432 (2004)
[2] I. Nowik et al., Phys. Rev. B 55, 3033 (1997)

TT 37.3 Wed 15:00 P4

Single Crystal Growth and Characterization of a New Yb-based Heavy Fermion Compound — •Fabian Fiedler[1], Florian Stoll[1], Kristin Kliemt[1], Manuel Brando[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]MPI CPfS, 01187 Dresden, Germany

A system near a quantum-critical point usually shows anomalous thermodynamic and transport properties at low temperatures [1,2].

Presently there are only rare cases of such systems with a ferromagnetic ground state together with pronounced Kondo interactions. Especially Yb-based intermetallic compounds with their possible unstable 4f-shell are of interest due to their low magnetic ordering temperatures.

We found a candidate system for Yb-based ferromagnetic quantum criticality with a large and diverging Sommerfeld coefficient below 10 K. We used substitution in order to manipulate the ground state. Here we report on the single crystal growth as well as the structural and physical characterization of these systems.

[1] Steppke et al., Science 331, 933 (2013);
[2] Shen et al., Nature 579, 51 (2020).

TT 37.4 Wed 15:00 P4

Negative Pressure Studies on $CeRh_2As_2$ with La Substitution — •Sushma Lakshmi Ravi Sankar[1,2], Arushi Yadav[1], Manual Brando[1], Joachim Wosnitza[2], and Seunghyun Khim[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden Germany

$CeRh_2As_2$ is a Kondo-lattice system with novel phase diagrams involving a superconducting and an unknown ordered state appearing below T_c and T_0, respectively. Recent observations of a suppression of T_c and T_0 under external pressure [1] motivated an investigation of a negative pressure study, which can be achieved by a La substitution with Ce. We have succeeded in growing single crystals of ($Ce_{1-x}La_xRh_2As_2$) up to x ~ 0.1. We found a negative pressure effect as the La substitution leads to an increase in the a- and c- lattice parameters (unit cell volume increase by ~ 0.15% with x = 0.1) while maintaining the $CaBe_2Ge_2$-type crystal structure. Resistivity measurements showed that both T_c and T_0 decrease with the La substitution to be almost suppressed at x ~ 0.08, while the resistivity maximum is slightly shifted to a lower temperature. At the same time, the residual resistivity ratio decreases from 2.24 at x = 0 to 1.46 at x = 0.1, indicating additional disorder introduced by the La substitution. This suggests that both the negative pressure effect and the increased disorder should be considered in understanding the evolution of T_c and T_0 with the La substitution.

[1] M. Pfeiffer et al., Phys. Rev. Lett. 133, 126506 (2024).

TT 37.5 Wed 15:00 P4

Terahertz Time-domain Spectroscopy on the Topological Kondo Insulator SmB_6 — •Zekai Chen, Debankit Priyadarshi, Erik de Vos, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

We present a terahertz time-domain spectroscopy (THz-TDS) measurement on the topological Kondo insulator samarium hexaboride (SmB_6). These results are aimed at providing insight into the co-existence of a topologically conductive surface state and the opening of a bandgap below the Kondo temperature. Previous work on Kondo insulators has shown that the Kondo quasiparticles disintegrate near a quantum critical point (QCP) in response to THz radiation, leading to a delayed echo-pulse-like response in the time domain [1]. In contrast to these materials, SmB_6 exhibits an additional in-gap state that could be related to its topological surface conductivity. In the presented experiment, this in-gap state is resonantly probed with THz radiation. Our measurement concentrates on studying the emergence of the in-gap state through correlated electron interaction.

[1] Nat. Phys. 14, 1103 (2018).

TT 37.6 Wed 15:00 P4

Cyclotron Resonance on SmB_6 Probed by Superconducting Coplanar Microwave Resonators — •Anastasia Bauernfeind and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Samarium hexaboride (SmB_6) is a homogeneously mixed-valent, narrow-gap semiconductor typically classified as a topological Kondo insulator. Its resistivity increases sharply as the temperature decreases, showing activated behavior that saturates below approximately 5 K. Experimental evidence suggests that topological surface states dominate low-temperature transport. Two notable studies on quantum oscillations in SmB_6 have sparked intense debate about their origin: one observes behavior consistent with a two-dimensional (2D) Fermi surface attributed to surface states, while the other reports a three-dimensional (3D) bulk Fermi surface, despite the insulating nature of the bulk at low temperatures. In our research, we perform cyclotron resonance experiments on SmB_6 using superconducting coplanar waveguides, a powerful method for investigating the Fermi surface of various materials. By tracing the evolution of the cyclotron frequency (up to 20 GHz) as a function of magnetic field, we can determine the type of charge carriers, the effective mass, and the properties of the associated electronic bands. Combined with temperature-dependent measurements (down to 20 mK) and power-dependent studies, this approach provides valuable insights into the electronic structure of the strongly correlated material SmB_6.

TT 37.7 Wed 15:00 P4

Bonding in UO_2^{2+} Dumbbell Structures: The Influence of a Non-Orthogonal Atomic Basis Set and the U 5f, 6d, 7s, and 6p Orbitals — •Henrik Hahn, Michelangelo Tagliavini, Kevin Ackermann, Sarah L. Goerlitz, Johann Collard, Ruth Kaiser, and Maurits W. Haverkort — Institute for Theoretical Physics (ITP), Heidelberg University, Philosophenweg 19, 69120, Heidelberg, Germany

Actinide compounds exhibit a wide range of complex properties, making their theoretical description a significant challenge. This complexity arises primarily from the open 5f shell, which introduces strong electronic correlations, as well as the close proximity of multiple subshells with different angular momentum (l) values due to the large principal quantum numbers (n) of actinides. In this study, we investigate the U-O bond in UO_2^{2+}, a well-known coordination structure of U^{2+} ($5f^0$). Notably, the stronger σ bond derived from the 5f z^3 orbital lies higher in energy than the weaker π bonds formed by the 5f xz^2 and yz^2 orbitals - an unusual ordering. Through a detailed analysis of the underlying LDA Hamiltonian in a non-orthogonal basis, we provide an explanation for this behavior. Our findings demonstrate that fully understanding the bonding and properties of actinides requires a many-orbital model that transcends the conventional assumption that the low-energy physics is governed solely by the 5f shell. This broader perspective is essential for capturing the intricate electronic structure and bonding characteristics of these materials.

TT 37.8 Wed 15:00 P4

Quantum-Spin Impurities Coupled to a Chern Insulator: Topological Remnants — •David Alan Krüger[1] and Michael Potthoff[1,2] — [1]University of Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Treating quantum-spin impurities as classical vectors is a frequently used approximation to study the impact of local magnetic impurities on the formation of subgap bound states in insulators. Recently, the classical-spin approximation has been exploited for a "local" topological characterization of the ground-state bundle over the manifold of impurity-spin configurations, as opposed to the bundle over the Brillouin zone. This has been achieved by computing spin-Chern numbers $C^{(S)}$ as the corresponding topological invariants.

Here, we numerically solve a system with a single or two quantum spin-$\frac{1}{2}$ locally exchange coupled to a Chern insulator given by the QWZ model. Via Lanczos tridiagonalization, the system is mapped onto a gapped Kondo-impurity model. Local ground-state properties and local single-particle as well as magnetic excitations spectra are obtained by means of an adaptive natural-orbital configuration-interaction technique.

We study the interplay of possible remnants of the classical-spin topology, the intrinsic QWZ topology, and the finite-size Kondo effect. To this end we trace subgap excitations as a function of the local exchange-coupling strength and the mass parameter.

TT 37.9 Wed 15:00 P4

Chiral Kondo Lattice Analyzed via Variational Cluster Approach — •Benjamin Heinrich and Maria Daghofer — Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

Moiré systems composed of van der Waals heterostructures provide an experimentally accessible platform to realize a wide range of strongly correlated electron phenomena. Using transition metal dichalcogenide materials, such as an AB-stacked $MoTe_2/WSe_2$ bilayer, gives rise to an effective multi-orbital Hubbard model on the honeycomb lattice, which can be tuned via doping and the introduction of charge transfer energy through external voltages. Including strong Ising spin-orbit coupling leads to chiral Kondo exchange between localized and itinerant electrons in different layers near half-filling.[1]

To gain a better understanding of experimentally observed phenomena, including magnetic ordering, numerical modeling is performed using the variational cluster approach. This methodology, closely related to cluster dynamical mean-field theory, has been proven effective for studying analogous systems exhibiting Kondo lattice behavior.

[1] Guerci et al., Sci. Adv. 9, eade7701 (2023).

TT 37.10 Wed 15:00 P4

Influence of Band Mixing on FCI and CDW — •Marco Schönleber and Maria Daghofer — Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Fractional quantum hall physics with vanishing magnetic fields has become an increasingly important research topic in recent years due to new findings in the field of moiré materials. Experimental signatures of these phases are often observed in combination with signatures of charge ordered or other symmetry broken phases. This indicates that band mixing might play an elementary role in the complete description of this phase of matter. For this purpose, an extended Hubbard model on a triangular lattice with $\nu = 1/3$ and $\nu = 2/3$ is considered. This allows the formation of bands of non-trivial topology as well as the formation of commensurate charge density waves. The analysis is carried out by exact diagonalisation. By varying the band gap, it can be shown that the stability of the charge order depends on this, whereby the degree of filling plays a decisive role.

TT 37.11 Wed 15:00 P4

Quantum Monte Carlo simulations of generalized Dicke-Ising models — •Anja Langheld, Max Hörmann, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Recently, we introduced a wormhole algorithm for the paradigmatic Dicke-Ising model to gain quantitative insights on effects of light-matter interactions on correlated quantum matter [1]. This method enabled us to determine the quantum phase diagram for ferro- and antiferromagnetic interactions on the chain and square lattice alongside the criticality of its second order quantum phase transitions. The continuous superradiant phase transitions are in the same universality class as the Dicke model, leading to a well-known peculiar finite-size scaling which can be understood in terms of scaling above the upper critical dimension.

Going one step further we now introduce new ingredients to the matter Hamiltonian like geometric frustration, long-range interactions and disorder to study the interplay between a variety of correlated matter phenomena and light-matter interactions.

[1] A. Langheld et al., arXiv:2409.15082

TT 37.12 Wed 15:00 P4

Chiral quantum phase transition in moiré Dirac materials — •Ana García-Page[1] and Laura Classen[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart 70569, Germany — [2]Department of Physics, Technical University of Munich, Garching 85749, Germany

Strong enough interactions induce a semimetal-to-insulator transition in Dirac materials, which can be viewed as the solid-state analogue of the chiral phase transition in quantum chromodynamics1-4. Moiré Dirac materials such as twisted bilayer graphene offer a new opportunity to study this transition because they facilitate tuning the effective interaction via a twist angle5-6. Motivated by this, we explore the quantum phase transition of a 2D Dirac material which spontaneously develops a gap that breaks an Ising symmetry7. We model it via an effective Gross-Neveu-Yukawa theory and employ the functional renormalization group method to map out the phase diagram. We analyze the quantum critical behavior at the transition and investigate the effect of a chemical potential which introduces a finite charge density.

TT 37.13 Wed 15:00 P4

NMR in Pulsed Magnetic Fields - Recent Developments — •Hannes Kühne[1] and Yoshihiko Ihara[2] — [1]HLD-HZDR, Dresden — [2]Department of Physics, Hokkaido University

NMR measurements in the highest pulsed magnetic fields have been developed at dedicated large-scale research facilities for some time and are becoming increasingly available for user experiments. On the poster, I will give an overview of the current developments, possibilities and peculiarities of NMR experiments in pulsed magnetic fields. In particular, the implementation of NMR experiments with dynamically controlled flat-top field pulses has recently been reported, enabling the measurement of broadband NMR spectra and relaxation times up to the ms range [1]. Furthermore, through several examples on low-dimensional spin systems, I will present opportunities to work on scientific questions that can be uniquely addressed using this technique [2].

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TT 37.14 Wed 15:00 P4

Magnetic Anisotropy and Low-Energy Spin Dynamics in van der Waals Magnets $M_2P_2S_6$ Probed by Electron Spin Resonance — Joyal J. Abraham[1,2], Yurii Senyk[1,2], Yuliia Shemerliuk[1], Sebastian Selter[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2,3], Vladislav Kataev[1], and •Alexey Alfonsov[1,3] — [1]Leibniz IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden, Germany

In the past recent years magnetic van der Waals (vdW) materials have become increasingly attractive for the fundamental investigations since they provide immense possibility to study intrinsic magnetism in a low-dimensional limit. The weak vdW forces hold together the atomic monolayers in vdW crystals, which results in a poor interlayer coupling, and therefore renders these materials intrinsically two dimensional. That makes them particularly attractive for probing the low-dimensional physics while investigating bulk crystals. On the other hand, a remarkable success in exfoliation of this class of materials due to the lack of significant interlayer chemical bonds unlocks vast potential for applications in the fields of advanced electronics, optoelectronics, and spintronics. In this work we present the results of the electron spin resonance investigation of such magnetic vdW materials $M_2P_2S_6$ (M = Mn, Ni, Cu, Cr) performed in the broad range of temperatures, magnetic fields and excitation frequencies, and discuss their low-energy spin dynamics as well as magnetic anisotropy responsible for the stabilization of the magnetic order.

TT 37.15 Wed 15:00 P4

Magnetic Properties of a Trillium Lattice Compound $Li_2NiGe_3O_8$ — •Annarose Jose Palliyan[1,2], Nazmul Islam[2], Ralf Feyerherm[2], and Bella Lake[2,1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Frustrated magnets are interesting materials that exhibit exotic properties due to the competing localized spins [1]. Certain lattices are intrinsically predisposed to show frustration due to the arrangement of their magnetic ions and one such lattice is the trillium lattice [2]. The trillium lattice is composed of a three-dimensional chiral network of corner sharing equilateral triangles. $Li_2NiGe_3O_8$ is a trillium lattice candidate where each Ni^{2+} ion is shared between three equilateral triangles. Polycrystalline samples of $Li_2NiGe_3O_8$ were synthesized by solid - state reaction method. The magnetic properties of this complex spinel oxide were studied by magnetization, susceptibility and heat capacity measurements down to He-3 temperatures. Our studies shows the presence of weak antiferromagnetic interactions in this material with no long-range order. A three-level schottky anomaly was observed in this material because of the splitting of the S = 1 triplet state.

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TT 37.16 Wed 15:00 P4

Geometric Magnetic Frustration in $Mn_3Al_2Si_3O_{12}$ — •Marwa Abouelela[1,2], Nazmul Isalam[2], Ralf Feyerherm[2], and Bella Lake[1,2] — [1]Institut für Festkörperphysik, Technische Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Geometric magnetic frustration in triangular lattices has garnered significant interest in recent research [1]. $Mn_3Al_2Si_3O_{12}$ exhibits geometrical frustration, where Mn^{2+} ($3d^5$) ions form a hyperkagomé structure [2]. In this study, the spessartine was synthesized at high temperatures, and its magnetic susceptibilities and heat capacities were investigated at low temperatures. Temperature-dependent magnetic susceptibility measurements revealed an antiferromagnetic ordering of the Mn^{2+} ions below T_N=6.5K, with a Curie-Weiss temperature of -26.7K. The high ratio of Curie-Weiss temperature to Néel temperature suggests strong frustration in the system.

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TT 37.17 Wed 15:00 P4

Static and Dynamic Properties of Quantum Magnets: Results from Numerical Linked Cluster Expansion — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

We consider static and dynamic properties of two-dimensional frustrated quantum antiferromagnets utilizing the numerical linked cluster expansion (NLCE). In particular, we are interested in spin-$^1/_2$ models showing quantum phase transitions versus internal parameters, e.g., the J_1-J_2 model on the square lattice or the triangular lattice XXZ model in external magnetic fields.

For the NLCE, we employ a single-site representation focussing on three topics: First, we present results for thermodynamic quantities, namely the internal energy and the specific heat at finite temperature. Second, we study the ground-state energy per site as a function of competing exchange coupling constants focussing on its second derivative. Finally, we investigate the dynamics of the system following a quantum quench.

TT 37.18 Wed 15:00 P4

Magnetism in i-Tb-Cd Quasicrystals — •Andreas Kreyssig[1,2], P. Das[2], G. S. Tucker[2], A. Podlesnyak[3], Feng Ye[3], Masaaki Matsuda[3], T. Kong[2], S. L. Bud'ko[2], P. C. Canfield[2], R Flint[2], P. P. Orth[2,4], T. Yamada[5], and A. I. Goldman[2] — [1]Experimental Physics IV, Ruhr University Bochum, Bochum, Germany — [2]Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, USA — [3]Neutron Scattering Division, Oak Ridge National Laboratory, USA — [4]Department of Physics, Harvard University, Cambridge, USA — [5]Department of Applied Physics, Tokyo University of Science, Tokyo, Japan

i-Tb-Cd orders as icoshedral quasicrystal with the magnetic Tb^{3+} ions arranged in Tsai-type clusters. We studied the magnetic correlations and excitations by elastic and inelastic neutron scattering on single-grain isotopically enriched samples. The measurements of the crystalline electric field excitations demonstrated that the Tb^{3+} moments are directed along the local fivefold axes of the Tsai-type clusters. We calculated the magnetic diffuse scattering for the low-energy configurations using an Ising-type model for the moment arrangements on a single Tb^{3+} icosahedron. By comparison with our diffuse neutron scattering signals, we identified the most likely moment configuration in a single cluster. We further studied the role of intercluster interactions for magnetic frustration and the magnetic scattering.

This work was supported by the U. S. DOE, BES, DMSE, Contract DE-AC02-07CH11358, and resources at HFIR and SNS, U. S. DOE.

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TT 37.19 Wed 15:00 P4

Chiral spin liquid in external magnetic field: Phase diagram of the decorated-honeycomb Kitaev model — •Sabastian Granberg Cauchi and Matthias Vojta — TU Dresden, Germany

Studies of Kitaev models on different lattices have shown signatures of topological phase transitions as a function of external magnetic field direction and magnitude. These transitions are often accompanied by a change in the statistics of the low-energy anyonic excitations. In particular, the antiferromagnetic Kitaev system yields a field-induced spin liquid, of arguably gapless U(1) or Abelian character. The existence of field-induced spin liquids on different lattices has consequently been intensely investigated. Here, we determine the phase diagram of the decorated-honeycomb Kitaev model for different inter- and intra-triangle coupling ratios and magnetic fields using a mean-field theory derived from Kitaev's Majorana parton decomposition.

TT 37.20 Wed 15:00 P4

Low-energy description of the SU(3) Hubbard model on the triangular lattice — •Linus Hein — Ludwig-Maximilians-Universität München

It has been a longstanding goal to better understand strongly correlated fermionic systems. Extensive studies have been conducted on these systems, particularly on the square lattice Hubbard model. To find out which of the results are artefacts of this fine-tuned model, it is sensible to analyze slightly modified models with for instance enlarged symmetry. We consider an SU(3) antiferromagnet on a tripartite triangular lattice near one third filling. Previous works explored a non-linear sigma model and its emerging Goldstone modes. Building on these results, we derive a linear spin-wave description of the low-energy excitations. Furthermore, we consider the hole-doped system and derive an effective Hamiltonian to describe the emergent magnetic polarons. Thereby, we broaden our understanding of strongly correlated fermionic systems, in a setting that can be experimentally explored using e.g. ultracold atom experiments.

TT 37.21 Wed 15:00 P4

Temperature Dependent Infrared Spectroscopy on the Frustrated Spin-Ladder System $BiCu_2PO_6$ — •Johanna Strauss[1], Renjith Mathew Roy[1], Maxim Wenzel[1], Haidong Zhou[2], Martin Dressel[1], and Komalavalli Thirunavukkuarasu[3] — [1]1. Physikalisches Institute, University of Stuttgart, Germany — [2]Department of Physics, University of Tennessee Knoxville, Knoxville, USA — [3]3. Department of Physics, Florida A and M University, Tallahassee, USA

Spin systems with frustrated geometries are of significant interest due to their potential to exhibit quantum spin liquid behaviour. This study focuses on $BiCu_2PO_6$ which exhibits no magnetic ordering down to 0.1 K. Various experimental studies on this zig-zag spin-ladder compound reveal that the magnetism in this material arise from complex exchange coupling mechanisms that are not completely understood yet. However, it is clear that the magneto-structural correlations play a major role. Here, we present our attempt to employ infrared spectroscopy to determine the optical conductivity and phonons along planes parallel and perpendicular to the spin-ladders at temperatures ranging from 300 K to 10 K and look for signatures on the nature of spin-phonon coupling.

TT 37.22 Wed 15:00 P4

Magnetic Phase Diagrams of the Frustrated Langbeinite Material $Tl_2Mn_2(SO_4)_3$ — •Manuel Tönnissen[1], Alexander Bäder[1], Ladislav Bohatý[2], Petra Becker-Bohatý[2], Oliver Breunig[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Antiferromagnetic Heisenberg spins on the so-called trillium lattice form a highly frustrated 3-dimensional spin system [1]. This theoretical model can be realizied in cubic, low-symmetry space group $P2_13$ materials. One family of materials that partially crystallizes in this space group are langbeinites. Recent studies report that the langbeinite $K_2Ni_2(SO_4)_3$ with S=1 Ni^{2+} ions show close proximity to a field-driven quantum spin-liquid behavior, although there is magnetic order in zero field [2] [3]. Here we focus on the different magnetic phases of the related langbeinite $Tl_2Mn_2(SO_4)_3$ with S=5/2 Mn^{2+} ions. By conducting specific-heat, magnetocaloric-effect, and magnetization measurements, we derive B-T phase diagrams for different orientations of the magnetic field. Our data reveal the presence of at least 3 magnetic phases below a temperature of about 1.5 K for the magnetic field along the [1 1 1] direction and even 4 magnetic phases for fields applied along the [1 1 0] or [0 0 1] directions.

This work is supported through CRC1238 (projects A02 and B01).

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[2] M. G. Gonzalez et al., Nat. Commun. **15**, 7191 (2024);
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TT 37.23 Wed 15:00 P4

Magnetic Order in the Low-Dimensional Quantum Magnet $Cu_2(OH)_3Br$ — •S. Luther[1], Z. Wang[2], A. Reinold[2], Z. Zhao[3], J. Wosnitza[1,4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]Fakultät Physik, TU Dortmund — [3]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences — [4]Institut für Festkörper- und Materialphysik, TU Dresden

Low-dimensional quantum magnets, such as the quasi-two-dimensional spin system $Cu_2(OH)_3Br$, can host exotic phenomena and ground states. We will present results of high-field magnetization and nuclear magnetic resonance (NMR) spectroscopy that probe the microscopic details of the magnetic structure at finite magnetic fields. In $Cu_2(OH)_3Br$, the Cu^{2+} ions in the distorted crystal structure form alternating ferromagnetic and antiferromagnetic spin-1/2 chains with finite interchain coupling, leading to a Néel temperature of 9.3 K at zero field. Here, we investigate the phase diagram for $H||b$, where a splitting of the NMR spectral lines below T_N and elevated fields reveals a commensurate long-range antiferromagnetic order. Maxima in the temperature-dependent spin-lattice relaxation rate $1/T_1$ at different magnetic fields indicate the transition temperature to the ordered phase. An anomaly in the high-field magnetization at low temperatures and around 16 T suggests the suppression of the magnetically ordered phase.

TT 37.24 Wed 15:00 P4

ESR Investigations of $AgCrSe_2$, $AgCrS_2$ and Cr_3Se_4 — •Jörg Sichelschmidt, Pierre Chailloleau, Michael Baenitz, Seo-Jin Kim, Helge Rosner, Vicky Hasse, and Marcus Schmidt — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We investigated the Electron Spin Resonance (ESR) of Cr in the layered triangular lattice systems $AgCrSe_2$, $AgCrS_2$ and the structurally related Cr_3Se_4. These materials display a variety of interesting physical properties such as unconventional magnetic ordering [1], a spin-polarized surface state [2], an unconventional anomalous Hall effect [3] in $AgCrSe_2$ or multiferroic behavior in $AgCrS_2$, or directional Kondo transport [4]. At low temperatures, all these materials show a divergent ESR spin relaxation, which is typical for low-dimensional spin systems and indicates an increasing importance of Cr^{3+} spin correlations. This also leads to the formation of internal fields, as evidenced by the marked decrease in the resonance field. The relatively narrow Cr^{3+} ESR spectra allow to determine an ESR intensity which reflects the static susceptibility probed locally at the site of the Cr spins.

[1] M. Baenitz *et al.*, Phys. Rev. B **104**, 134410 (2021);
[2] G.-R. Siemann *et al.*, npj Quantum Mater. **8**, 61 (2023);
[3] S.-J. Kim *et al.*, Adv. Sci. **11**, 2307306 (2024);
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TT 37.25 Wed 15:00 P4

Electronic Structures of $AgCrS_2$, $AgCrSe_2$, and Cr_3Se_4 — •Seo-Jin Kim, Jörg Sichelschmidt, Michael Baenitz, Marcus Schmidt, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We study the electronic structures of triangular lattice systems $AgCrS_2$, $AgCrSe_2$, and the related compound Cr_3Se_4 using density functional theory (DFT). Although $AgCrSe_2$ and $AgCrS_2$ are isostrucural, they exhibit different physical properties. $AgCrSe_2$ is a self-doped p-type semiconductor characterized by spin-polarized surface states[1], the cycloidal magnetic ordering[2], and the unconventional anomalous Hall effect[3] and directional Kondo transport[4]. In contrast, $AgCrS_2$ is an insulator that undergoes symmetry lowering to a monoclinic phase and exhibits a collinear double-stripe antiferromagnetic ground state below $T_N = 42$ K. This study aims to present a comprehensive analysis of the electronic structures of these compounds. Additionally, we extend our investigation to the structurally related compound Cr_3Se_4.

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[3] S.-J. Kim et al., Adv. Sci. 11, 2307306 (2024);
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TT 37.26 Wed 15:00 P4

Synthesis and Physical Properties of 2D van der Waals Magnets $Fe_{1-x}TM_xPX_3$ (TM: Transition Metals) — •Masoumeh Rahimkhani, Saicharan Aswartham, Andreas Kreyssig, and Anna Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

Transition-metal phosphochalcogenides ($TMPX_3$) belong to the family of layered van-der-Waals materials in which TM is a transition-metal and X is a chalcogenide. These materials exhibit various electric, optical, and magnetic properties. $FePSe_3$ belongs to this family of $TMPX_3$ with interesting magnetic and electronic properties. Here, we describe the preparation of $FePSe_3$ and its substitution series with different transition metals through solid-state synthesis and CVT. The samples are characterized by X-ray diffraction and scanning electron microscope for structural and phase analysis. Further on, the magnetic and electronic properties will be investigated.

TT 37.27 Wed 15:00 P4

Single-Crystal Study of Kagome Magnets CrRhAs and CrNiAs — •Franziska Breitner, Bin Shen, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

CrRhAs and CrNiAs are metals with distorted kagome lattice of magnetic Cr atoms [1]. While CrRhAs is an antiferromagnet with a reported Néel temperature of 165 K for polycristalline samples, CrNiAs is ferromagnetic with T_C=170 K. More recently, interesting properties such as anomalous Hall effect were predicted for CrRhAs [2].

We report the first growth of CrRhAs and CrNiAs single crystals utilizing the flux method and present their specific heat, magnetic susceptibility and electrical transport. Magnetoresistance and Hall effect for CrRhAs indicate no anomalous behaviors. For CrNiAs we also investigate the influences of hydrostatic pressure as well as partial substitution of As with P on the ferromagnetic transition.

Supported by DFG-TRR 360*492547816 and the Alexander von Humboldt Foundation.

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[2] Y. N. Huang et al., npj Quantum Mater. 8, 32 (2023).

TT 37.28 Wed 15:00 P4

Inelastic Scattering in Anisotropic Heisenberg Models on Square and Honeycomb Lattice Via Continuous Similarity Transformations — •Vanessa Sulaiman[1], Dag-Björn Hering[1], Matthias R. Walther[2], Kai P. Schmidt[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

We apply a continuous similarity transformation (CST) [1,2] with a magnon-conserving generator to the antiferromagnetic anisotropic XXZ model. For the square lattice, the resulting effective Hamiltonian has already been analyzed [3]. We extend the approach by applying the CST to observables as well. Using the continuous fraction representation, we calculate spectral densities for these observables on the square and honeycomb lattice. These are then compared to experimental data from RIXS measurements [4], for example with single-layered $Ca_2CuO_2Cl_2$.

[1] M. Powalski et al., Phys. Rev. Lett. **115**, 207202 (2015);
[2] M. Powalski et al., SciPost Phys. **4**, 001 (2018);
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[4] K.-J. Zhou et al., J. Synchrotron Rad. **29**, 563 (2022).

TT 37.29 Wed 15:00 P4

Stochastic Simulation of Spin Transport — •Franz Pöschl[1,4], Xin Zhang[1,2,3], Aristo Kevin Ardyaneira P[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [4]Ludwig-Maximilians Universität München, Fakultät für Physik, Geschwister-Scholl-Platz 1, 80539 München

Simulating out of equilibrium steady states of large systems is a hard task. It is therefore necessary to develop novel approaches permitting to simulate the dynamics of those systems efficiently. In our work, we use the Discrete Truncated Wigner Approximation which is a semiclassical approach mapping hamiltonians and dissipative processes into a classical phase space. This mapping allows to compute stochastic trajectories and to evaluate the evolution of the system. In this poster I will present this method and show how it can be employed to study the out-of-equilibrium phases of the XXZ spin model and to derive its transport properties.

TT 37.30 Wed 15:00 P4

Anisotropic Magnetoresistance and Hall Effect of $Sr_4Ru_3O_{10}$ — •Simone Seipel[1], Lara Pätzold[1], Zahra Ghazinezhad[1], Augustus A. Nugroho[2], Markus Braden[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Bandung Institute of Technology, Indonesia

The layered transition-metal oxide $Sr_4Ru_3O_{10}$ is a member of the Ruddlesden-Popper series with a layered orthorhombic crystal structure. It is a ferromagnetic metal with $T \simeq 105$ K and shows an additional metamagnetic transition below 50 K, of which a deeper understanding is still missing. Here, we present a single-crystal study of the anisotropic magnetization and electrical transport properties. For in-plane electric currents ($j||ab$) and $B||c$, we present normal and anomalous Hall effect data. The latter shows a non-monotonic temperature dependence and a characteristic sign change at low temperature which similarly occurs in the magnetoresistance $\rho_{xx}(B||c)$. Such a behavior is known from the sister compound $SrRuO_3$ and associated with Weyl points in the band structure [1]. In addition, we studied the out-of-plane resistivity that is highly anisotropic ($\rho_c >> \rho_{ab}$) due to the layered crystal structure and strongly changes at the metamagnetic transition. Based on magnetoresistance data $\rho_c(B||ab)$ we derive the magnetic-field induced metamagnetic transition at low temperatures and discuss the angular dependence of the transition fields and the magnetoresistance for in-plane magnetic fields.

Funded by the DFG via CRC 1238 Projects A02, B01 and B04

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TT 37.31 Wed 15:00 P4

Thermal Transport in Swedenborgite $CaBaCo_4O_7$ — •Reza Firouzmandi[1], Matthias Gillig[1], Yasujiro Taguchi[2], Yoshinori Tokura[2], Yusuke Tokunaga[2], Vilmos Kocsis[1], and Bernd Büchner[1] — [1]IFW-Dresden, Dresden, Germany — [2]RIKEN-CEMS, Wako, Japan

The interplay between electronic, magnetic, and lattice degrees of freedom in multiferroic materials gives rise to novel transport phenomena, including the thermal Hall effect (THE), thermal analog of the Hall effect, where heat flow is deflected under an external magnetic field. Here, we investigate the thermal transport properties of the multiferroic Swedenborgite $CaBaCo_4O_7$, a compound featuring alternating Kagome and triangular layers of edge-sharing CoO_4 tetrahedra in a mixed valence state. The longitudinal thermal conductivity exhibits anomalies associated with magnetic ordering, while the transverse thermal conductivity (κ_{xy}) reveals an anomalous thermal Hall effect that vanishes at low temperatures, resembling the magnon thermal Hall effect. These results provide

insight into the role of spin-lattice coupling in the thermal transport of frustrated magnetic systems.

TT 37.32 Wed 15:00 P4

Strain dependance of the antiferromagnetic transition of $Ca_{1-x}Sr_xCo_2As_2$ with a substitution induced structural collapse — •Michael Paul, Maik Golombiewski, Teslin R. Thomas, N.S. Sangeetha, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

The tetragonal structure of $SrCo_2As_2$ undergoes a gradual collapse with the substitution of Sr by Ca atoms. This collapse is accompanied by the emergence of antiferromagnetic order with a transition temperature T_N of up to 55 K [1]. It has been shown that T_N can be tuned with biaxial strain that is created by cooling a thin $Ca_{1-x}Sr_xCo_2As_2$ sample that is glued to a quartz substrate [2].
A more controlled application of uniaxial force to the sample can be achieved with the use of the cryogenic stress cell Razorbill FC100. The modification of the antiferromagnetic transition of $Ca_{1-x}Sr_xCo_2As_2$ is investigated by applying uniaxial stress to the sample with this device.
We acknowledge the support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).
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[2] T. R. Thomas et al., in preparation

TT 37.33 Wed 15:00 P4

Single crystal synthesis of $FeSb_2$ and investigation of its electronic transport properties — •Maximilian van de Loo, Maik Golombiewski, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

$FeSb_2$ is a diamagnetic narrow band gap semiconductor with interesting electronic transport properties [1]. Huge thermoelectric power factor and a paramagnetic crossover have been reported at low temperatures [1, 2] and attempts to influence and understand these properties by doping have been made [3]. A metal-semiconductor crossover along the b axis can be observed under certain growth conditions. We have synthesized single crystals of $FeSb_2$ via self-flux growth and successfully realized substitutions $(Fe_{1-x}TM_x)Sb_2$ with different transition metals (*TM*). The samples were characterized with electron microscopy, energy-dispersive x-ray spectroscopy, powder x-ray diffraction and Laue diffraction measurements, as well as electrical resistivity measurement. The appearance of the metal-semiconductor crossover has been investigated by varying the growth conditions.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).
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TT 37.34 Wed 15:00 P4

Feshbach resonance in a strongly repulsive ladder of mixed dimensionality: a possible scenario for bilayer nickelate superconductors — •Hannah Lange[1,2,3], Lukas Homeier[1,3], Eugene Demler[4], Fabian Grusdt[1,3], and Annabelle Bohrdt[3,5] — [1]LMU Munich — [2]Max-Planck-Institute for Quantum Optics, Garching — [3]Munich Center for QST, Munich — [4]ETH Zurich — [5]University of Regensburg

Since the discovery of superconductivity in cuprate materials, the minimal ingredients for high-Tc superconductivity have been an outstanding puzzle. Motivated by the recently discovered nickelate bilayer superconductor LNO under pressure, we study a minimal bilayer model, in which, as in LNO, inter- and intralayer magnetic interactions but no interlayer hopping are present: a mixed-dimensional (mixD) t-J model. The single and coupled mixD ladders we study feature a crossover from tightly bound pairs of holes (closed channel) at small repulsion, to more spatially extended, correlated pairs of individual holes (open channel) at large repulsion. We derive an effective model for the latter, in which the attraction is mediated by the closed channel, in analogy to atomic Feshbach resonances. Using density matrix renormalization group (DMRG) simulations we reveal a dome of large binding energies at around 30% doping, accompanied by a change of the Fermi surface volume. Our work provides a microscopic theory of pairing in the doped mixD system with dominant repulsion and our predictions can be tested in state-of-the-art quantum simulators.

TT 37.35 Wed 15:00 P4

Fluctuation Spectroscopy on $La_2NiO_{4+\delta}$ RRAM devices — •Demian Ranftl[1], Yingxin Li[2], Tristan Stadler[1], Eszter Piros[2], Aleksandra Koroleva[3], Lambert Alff[2], Mónica Burriel[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University, Frankfurt am Main, Germany — [2]Institute of Materials Science, TU Darmstadt, Darmstadt, Germany — [3]Laboratory in Materials Science and Physical Engineering, Université Grenoble Alpes, Grenoble, France

Memristive devices, whose resistance is programmable and retainable, are considered to be most promising for the next generation of non-volatile memory. Low-frequency current noise spectroscopy is a non-invasive investigative tool for probing the effect of defects on resistive switching [1, 2]. Annealing $La_2NiO_{4+\delta}$ films under inert (Ar) or oxidising (O_2) atmospheres results in devices with filamentary and interfacial-type resistive switching respectively [3]. In this work we explore the effect of the switching mechanism, readout voltage and area dependency on the noise characteristics of LNO-based RRAM.
[1] E. Piros, M. Lonsky *et al.* Phys. Rev. Appl. **14** (2020)
[2] T. Thyzel, M. Kopp *et al.* Meas. Sci. Technol. **36** (2025)
[3] A. Koroleva *et al.* Adv. Electron. Mater. 2400096 (2024)

TT 37.36 Wed 15:00 P4

Resistance Fluctuation (Noise) Spectroscopy in EuS and $LiCu_3O_3$ — •Philipp Swoboda[1], Demian Ranftl[1], Nazia Kaya[1], Katharina Zoch[1], Kristin Kliemt[1], Simon Moser[2], Cornelius Krellner[1], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]Institute of Physics, University Würzburg, Würzburg, Germany

Noise spectroscopy gives insights into the low-frequency dynamics of charge carriers in condensed-matter systems, which is energy-resolved information that can't be obtained from mean values alone. Here the interest lies in $1/f^{\alpha}$-noise, which can be described as a superposition of independent two-level processes. For instance it has been used to identify energy scales of thermally-activated switching processes like fluctuating polar nanoregions (PNR) in the past [1, 2]. In general the processes observed by resistance fluctuation are sensitive to slow dynamics. Examples are the slowing down of charge carriers in the vicinity of a metal insulator transition and the freezing of PNR at the onset of glassy dynamics. This work aims to use noise spectroscopy as a function of temperature and magnetic field in order to investigate how magnetic polarons influence the colossal magnetoresistance in the ferromagnetic semiconductor EuS, as well as to investigate the exotic electron glass phase in $LiCu_3O_3$.
[1] npj Spintronics 2, 24 (2024).
[2] Meas. Sci. Technol. 36 (2025) 015501.

TT 37.37 Wed 15:00 P4

Single spin-flip dynamics in the Ising model — •Luca Cervellera and Björn Sothmann — Faculty of Physics and CENIDE, University Duisburg- Essen, 47057 Duisburg

The surface of Si(001) consists of buckled Si dimers with alternating orientation in the ground state. At around 190 K, the system undergoes an order-disorder phase transition which can be described in terms of an antiferromagnetic 2D Ising model with anisotropic couplings [1]. Here, we aim at understanding the switching dynamics of a single Ising spin by means of Monte Carlo simulations of the temperature-dependent dynamics using different algorithms which allow us to analyze the waiting-time distribution and full counting statistics of spin flips.
[1] C. Brand et al., Phys. Rev. Lett. 130, 126203 (2023).

TT 37.38 Wed 15:00 P4

Quantum Monte-Carlo study of the bond- and site-diluted transverse-field Ising model — •Calvin Krämer, Max Hörmann, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik V, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We study the transverse-field Ising model on a square lattice with bond- and site-dilution at $T = 0$ by quantum Monte Carlo simulations. By tuning the transverse field h and the dilution p, the phase diagram of both models is explored. Finite-size scaling of the order parameter and averaged Binder ratios is employed to determine the positions of critical points and the critical exponents β and ν along the critical lines and at the multi-critical point. Dynamical properties in the vicinity of the quantum critical point are analyzed through the local susceptibility. We complement these findings by stochastic analytical continuation [1] of imaginary-time Green's functions, providing momentum-resolved insights into the behavior of excitations. [1] Anders W. Sandvik, Phys. Rev. B 57, 10287

TT 37.39 Wed 15:00 P4

Typical medium theory for disordered electronic systems on simple lattices with Cauchy distribution of on-site potentials — Andreas Ostlin[1], Hanna Terletska[2], Dylan Jones[1], and •Liviu Chioncel[1,3] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Middle Tennessee State University, Murfreesboro, Tennessee, USA — [3]ACIT, University of Augsburg, Augsburg, Germany

Effective medium approaches using single-site averaging procedures of various kinds contributed substantially in understanding the density of states of electronically disordered systems in models and materials. The nature and the conditions for appearance of single-particle (Anderson) localization seems to be qualitatively understood, yet discussions concerning special applied methods and quantitative results for the critical conditions are still ongoing. Here we present results using the typical medium theory for the one-particle and two-particle Green's function (conductivities) for the special case of Cauchy-distribution.

TT 37.40 Wed 15:00 P4

Excitations and Their Decay: Calculating the Non-Lorentzian Line Shape of Excited States at the Ti $L_{2,3}$ edge in $SrTiO_3$ — •Sarah L. Görlitz[1], Sina Shokri[1], Widad Louafi[2], Martin Brass[1,3], Marc Merstorf[1], Jonas Hoecht[1], Michelangelo Tagliavini[1], Kevin Ackermann[1], and Maurits W. Haverkort[1] — [1]Institut for Theoretical Physics, Heidelberg University, 69120 Heidelberg — [2]Laboratory of Theoretical Physics, Faculty of Exact Sciences, University of Bejaia, 06000 Bejaia, Algeria — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Understanding electron dynamics in real materials following photon excitations is a challenging task. Ultrafast pump-probe and multi-color experiments require precise control, while strong electron correlations in excited states complicate the theoretical description. Accurate calculations must reproduce absorption line shapes for single-photon absorption, often non-Lorentzian due to multi-channel decay processes.

In this work, we calculate the line shape of Ti 2p → 3d core excitations in $SrTiO_3$. While crystal-field models predict seven delta-function peaks, the real spectrum reveals distinct line widths and non-Lorentzian line shapes. Incorporating Auger-Meitner decay, fluorescence decay, and coupling to the valence-conduction bath continuum, we establish a framework to explain these broadenings. This approach is critical for predicting higher-order response functions, essential for modeling resonant inelastic X-ray scattering (RIXS) and ultrafast spectroscopies, providing insights into the interplay of decay processes and electron dynamics.

TT 37.41 Wed 15:00 P4

Role of interlayer coupling and anisotropy in 1T-TaS_2 studied by ellipsometry — •Achyut Tiwari[1], Renjith M. Roy[1], Christian Prange[1], Yuan Yan[2], Bruno Gompf[1], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]School of Physics, Nankai University, Tianjin, 300071 China

The layered transition metal dichalcogenide 1T-TaS_2 has attracted considerable attention due to its rich electronic phase diagram, characterized by multiple charge density wave (CDW) phases. With decreasing temperature, the material transitions from a metallic incommensurate phase to a metallic nearly commensurate phase and finally to an insulating commensurate phase featuring the star-of-David lattice distortion. The metal-insulator transition (MIT) is a first-order phase transition that exhibits hysteresis during cooling and heating, with an additional intermediate phase in the 215 K-280 K range upon heating. Here, temperature-dependent ellipsometry revealed pronounced anisotropy between in-plane and out-of-plane responses, attributable to significant interlayer interactions. The temperature-dependent out-of-plane dielectric constant exhibited marked changes across the MIT, highlighting the role of interlayer coupling. Furthermore, the effective medium approximation confirmed the existence of the intermediate phase during heating, providing a microscopic description. These findings underscore the importance of interlayer coupling in layered materials and elucidate on the previously unexplored intermediate phase of 1T-TaS_2.

TT 37.42 Wed 15:00 P4

The Interplay Between Diagonal and Off-Diagonal Electron-Phonon Coupling in two-dimensional systems — •jadson lucas portela e silva[1,2], gabriel rein[2], sebastião a. s. júnior[1], willdauany c. f. da silva[1], fakher f. assaad[2], and natanael c. costa[1] — [1]instituto de física universidade federal do rio de janeiro, rio de janeiro, brasil — [2]institut für theoretische physik und astrophysik, universität würzburg, würzburg, germany

The interplay between diagonal and off-diagonal electron-phonon coupling in two-dimensional systems is explored using the Holstein-Su-Schrieffer-Heeger (HSSH) model through non-perturbative Monte Carlo simulations on a square lattice at half-filling. Electron-phonon coupling is crucial in determining exotic phases like charge-density waves (CDW), valence bond solids (VBS), and superconductivity. The HSSH model uniquely combines features of the Holstein and SSH models, where the former modulates the on-site potential energy, and the latter modifies the electron's kinetic energy through lattice displacements. The study constructs phase diagrams by analyzing charge-charge, bond-bond, and pairing correlation functions. Key findings include a competition between CDW and VBS phases, similar to one-dimensional systems. However, unlike the 1D case, no metallic phase is observed between these states, likely due to perfect nesting and van Hove singularities in the density of states, which destabilize the Fermi liquid state. Further exploration beyond half-filling shows that melting of CDW and VBS phases leads to superconductivity.

TT 37.43 Wed 15:00 P4

Picosecond periodic oscillation modulated by Higgs amplitude mode in a superconductor-metal hybrid metasurface — •Siyu Duan[1,2], Jingbo Wu[1], Caihong Zhang[1], Kebin Fan[1], Biaobing Jin[1], and Zhe Wang[2] — [1]School of Electronic Science and Engineering, Nanjing University, Nanjing, China — [2]Department of Physics, TU Dortmund University, Dortmund, Germany

We report on a time-resolved terahertz spectroscopic study of a superconductor-metal hybrid metasurface that is fabricated by introducing superconducting microbridges into metallic resonators. By exploiting the nonlinear response of the superconducting NbN microbridges to a multicycle narrowband terahertz excitation pulse, we observe a picosecond periodic oscillation of terahertz transmission spectra. This oscillation contains components of the fundamental frequency of the narrowband excitation pulse and its second harmonic, which we ascribe tentatively to an excited Higgs mode oscillation. Furthermore, we can modulate the amplitude and duration of periodic oscillations by changing the field strength of the terahertz excitation pulse and the sample temperature.

TT 37.44 Wed 15:00 P4

Density Functional Theory-based Multiplet Ligand Field Theory Calculations of Ultrafast Pump-Probe Electron Dynamics in Correlated Materials — •Ruth Kaiser, Sina Shokri, and Maurits W. Haverkort — Heidelberg University, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Ultrafast pump-probe spectroscopy allows one to study and steer quantum materials on their fundamental time-scales. In correlated molecules and solids a theoretical understanding is challenging and quantitative predictions how coherently driven excitations decohere is highly non-trivial. We have developed a recipe for quantitatively predicting pump-probe spectra, starting with a Hamiltonian on a basis of local Wannier orbitals derived from density-functional calculations, describing the charge-transfer in the system and, on top of that, we include the full local Coulomb repulsion [1]. Using non-linear response theory, we then calculate the time-resolved spectra, such as photo-emission spectroscopy, x-ray absorption spectroscopy and resonant inelastic x-ray scattering, which captures the pump-probe dynamics. Our routine can be used for different types of correlated materials, such as Mott-Hubbard and Charge-Transfer insulators as well as molecules [2, 3]. Furthermore, we show examples where we implemented our method for real materials like NiO and SF_6 and compare our results with experiments.

[1] PRB 85, 165113 (2012);
[2] PRL 128, 153001 (2022);
[3] PRA 108, 032816 (2023).

TT 37.45 Wed 15:00 P4

Understanding Resonant Inelastic X-ray Spectroscopy Using Dynamical Mean-Field Theory and Model Hamiltonians — •Lukas Hellmann, Aleksandrs Zacinskis, Sina Shokri, Michelangelo Tagliavini, Kevin Ackermann, and Maurits W. Haverkort — Universität Heidelberg, Institut für Theoretische Physik, Philosophenweg 19, Heidelberg 69120 Germany

Using model Hamiltonians with local Coulomb interactions, we demonstrate how resonant inelastic X-ray scattering spectra (RIXS) can be interpreted within the framework of the dynamical mean-field approximation. Our approach incorporates both valence correlations and core-valence Coulomb repulsion, enabling a detailed examination of spectral features across the metal-insulator transition. The calculated RIXS spectra reveal two distinct types of excitations: (1) locally excited excitons exhibiting a resonant enhancement at constant energy loss, and (2) a fluorescence regime characterized by resonant intensity enhancement at constant emitted energy. We analyze the transition in intensity between these two excitation regimes and discuss its implications for understanding electronic dynamics. All calculations are performed directly on the real frequency axis using the software package Quanty (www.quanty.org). This methodology not only provides accurate predictions for RIXS spectra but also offers a versatile framework for studying the dynamics of other correlated systems.

TT 37.46 Wed 15:00 P4

Material Specific Real Frequency LDA+DMFT Calculations of Transition Metals — •Johann Collard, Michelangelo Tagliavini, Kevin Ackermann, Sina Shokri, Aleksanders Zacinskis, Lukas Hellmann, and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120, Heidelberg, Germany

3d transition metals exhibit a wide range of intriguing properties. At the same time their accurate theoretical description is challenging task due to the presence of correlated electrons in their open d-shells. Ab-initio approaches, such as LDA+DMFT (Local Density Approximation + Dynamical Mean-Field Theory), have proven successful in capturing many material-specific properties and electron correlation effects. Most existing DMFT algorithms rely on Quantum Monte Carlo simulations, which operate on imaginary frequencies. While effective for static property calculations, these methods require analytical continuation to compute spectral functions, a process that is ill-posed and thus computationally challenging. In this work, we demonstrate how real-frequency DMFT, as implemented in Quanty, can directly compute spectral functions within the LDA+DMFT framework for real materials. This approach avoids the complications of analytical continuation, providing a more straightforward and reliable means of exploring the spectral properties of 3d transition metals.

TT 37.47 Wed 15:00 P4

An Accessible Implementation and Detailed Test of Real-Frequency Dynamical Mean-Field Theory — •Aleksandrs Zacinskis, Sina Shokri, Kevin Ackermann, Michelangelo Tagliavini, and Maurits W. Haverkort — Heidelberg University, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Dynamical Mean-Field Theory (DMFT) has become a powerful tool for studying materials with correlated electrons. However, most DMFT solvers operate on imaginary Matsubara frequencies, making the extraction of accurate spectral functions challenging due to the need for analytical continuation.

Here, we perform DMFT calculations using a real-frequency solver implemented in Quanty [1]. This implementation utilizes a one-particle basis of natural impurity orbitals [2] to investigate several correlated model systems with local interactions. We systematically examine critical metal-insulator transition interaction strengths and the chemical potential as a function of filling, comparing different bath discretization schemes and numerical cut-offs to manage Hilbert space size.

Our results demonstrate robust and satisfactory convergence at moderate computational costs, validating the reliability of this approach. All calculations were performed using the open-source quantum many-body code *Quanty* (www.quanty.org), emphasizing its accessibility for broader applications in correlated electron systems.

[1] Phys. Rev. B 85, 165113 (2012);
[2] Phys. Rev. B 90, 085102 (2014).

TT 37.48 Wed 15:00 P4

Engineering Correlated Electrons in Adatom Lattices on Semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project we explore other promising material candidates on SiC and other substrates that might realize (one-, two-, and three-band) Hubbard models at different fillings and a potential impact of spin-orbit coupling. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field.

[1] H.Menke, N.Enderlein *et al.*, arXiv:2410.17165.

TT 37.49 Wed 15:00 P4

Calculating Moments for Many-Electrons Systems — •Elaheh Adibi and Erik Koch — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a combinatorial approach to calculate the M^{th} moment of an N-electron system, defined as $\langle E^M \rangle = \mathrm{Tr}\, H^M$. Working in the basis of Slater determinants $|\boldsymbol{\alpha}\rangle = \prod c^\dagger_{\alpha_i}|0\rangle$, matrix elements $\langle\boldsymbol{\alpha}|H^M|\boldsymbol{\alpha}\rangle$ may only be non-zero for terms where the orbital indices of the creation operators in H^M are permutations of the orbital indices of the annihilators. The trace for a given permutation can then be evaluated combinatorially, without having to deal with the many-body Hilbert space explicitly. Since all permutations related by cyclic rotations give the same contribution, we classify them into groups and evaluate the trace only for a single group member. For the special case of all orbitals in the permutation being different, the calculation simplifies further, as in this irreducible case all permutations written in terms of cycles with a given number of descents give the same contribution to the moment. Relating the groups of permutations for the irreducible and the reducible terms allows us to efficiently evaluate the moments.

TT 37.50 Wed 15:00 P4

Exact t^1_{2g} Superexchange Hamiltonians for Complex Orbital Ordering — •Amit Chauhan, Xue-Jing Zhang, and Eva Pavarini — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

We derive exact superexchange interactions for t^1_{2g} systems with spin-orbit coupling. To this end we extend the formalism developed in [1], which we have successfully used in [2,3] to study the origin of orbital ordering. As first application we consider the case of cubic and tetragonal lattices and study the stability of complex orbital ordering in the presence of spin-orbit interaction and crystal-field splitting.

[1] X.-J.Zhang, E.Koch, E.Pavarini, Phys.Rev. B **105**, 115104 (2022);
[2] X.-J.Zhang, E.Koch, E.Pavarini, Phys.Rev. B **102**, 035113 (2020);
[3] X.-J.Zhang, E. Koch, E.Pavarini, Phys.Rev. B **106**, 115110 (2022).

TT 37.51 Wed 15:00 P4

Scaling and convergence behaviour of linked-cluster expansions — •Harald Leiser, Max Hörmann, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We derive effective block-diagonal Hamiltonians $H_{\mathrm{eff}} = T^\dagger H T$ using the projective-cluster additive transformation (PCAT) [1]. Numerical linked-cluster expansions (NLCEs) are employed to study the (anti)ferromagnetic transverse-field Ising model (TFIM) on diverse lattice geometries such as chains and various ladders. By calculating energy gaps, we compare the scaling behavior with other methods such as deepCUT [2]. A key challenge arises from the presence of avoided-level crossings (ALCs) [3] which complicates convergence. To probe this issue, we analyze ALCs in the simplified setting of the XXZ model on a chain. A key property of PCAT is the cluster additivity of both H_{eff} and the generator $S = \log(T)$. This allows transforming larger systems via a cluster expansion in S. Using S from clusters up to size N, we compute $\exp(-S)H\exp(S)$ in the thermodynamic limit and compare it with standard NLCE and CUT methods [4]. Notably, S for local clusters generates higher-order terms, mitigating some scaling challenges in traditional cluster expansions.

[1] M. Hörmann et al., SciPost Phys. 15 (2023) 097.
[2] H. Krull et al., Phys. Rev. B 86.
[3] K. Coester et al., EPL, 110(2):20006.
[4] C. Knetter et al., EPJ B 13:209.

TT 37.52 Wed 15:00 P4

Computing Excited States in Quantum Many-Body Clusters with Neural Network Support — •Max Kroesbergen[1], Louis Thirion[1], Gianluca Levi[3], Pavlo Bilous[2], Paul Fadler[1], Yorick Schmerwitz[3,4], Elvar Ö. Jónsson[3], Hannes Jónsson[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]University of Iceland, Reykjavik — [4]Max Planck Institute for Coal Research, Mühlheim

In this study, we used SOLAX [1], our newly developed Python library for configuration interaction (CI) calculations of fermionic quantum systems, to compute the energies of ground and excited states for various quantum clusters. SOLAX can leverage the power of a neural network (NN) classifier to perform selective CI which mitigates the exponential growth of the many-body Hilbert space. Our benchmarks indicate a significant boost in computational efficiency while maintaining high accuracy. We validate our method for the (discrete) Single Impurity Anderson Model [2] as well as molecular systems, such as N_2 and H_2 [3]. For the latter, we study the dissociation curves of ground- and excited states and their dependence on the underlying single-particle basis, including Hartree-Fock orbitals optimized for excited states. Additionally, SOLAX enables us to simulate spectral functions defined by a transition operator, providing deeper insights into the excitation dynamics of these systems.

[1] L. Thirion, P. Hansmann, P. Bilous, arXiv:2408.16915v1.
[2] P. Bilous *et al.*, arXiv:2406.00151.
[3] Y. L. A. Schmerwitz *et al.*, arXiv:2406.08154.

TT 37.53 Wed 15:00 P4

Using the Anderson Impurity Model to Look for Particles Beyond the Standard Model — •Vera Butz and Maurits W. Haverkort — Universität Heidelberg, Institut für theoretische Physik, Philosophenweg 19, 69120 Heidelberg

High-precision comparisons between experimental measurements and numerical simulations [1] not only test the accuracy of computational methods but also offer deeper insights into fundamental physics. In this work, we investigate the interaction of charged ions with multiple electrons and continuum states, presenting a generalized Anderson impurity model. The continuum states considered include photons, free electrons, or as-yet-unobserved particles, such as axions. These interactions can be described through the self-energy or hybridization function [2]. The real part of the self-energy induces energy shifts in atomic multiplets, such as the Lamb shift, while the imaginary part results in finite lifetimes for excited states, leading to phenomena like fluorescence or Auger-Meitner decay. When applied to highly charged heavy ions, whether in laboratory settings or astrophysical environments such as the Sun, these enhanced electron-photon (or other particle) interactions provide a platform to probe the Standard Model. Additionally, they may reveal evidence of new physics, including the potential detection of axions, a leading dark matter candidate that could also address the strong CP problem.

[1] Nat. Phys. 20, 921 (2024).
[2] arXiv:2307.13812v1.

TT 37.54 Wed 15:00 P4

Properties of the Density Matrix for Metavalent Materials — •Niklas Penner[1,2], Lucia Reining[1], Matteo Gatti[1], and Matthias Wuttig[2] — [1]ETSF, LSI, CNRS, CEA/DRF/IRAMIS, Ecole Polytechnique, Institut Polytechnique de Paris, France — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

In the experimental investigation of phase change materials and their unique properties, peculiarities in the bonding character were determined. A corresponding classification of these metavalent materials has so far been carried out on the basis of shared and transferred electrons. The corresponding values were determined using density functional theory (DFT) calculations. Density functional theory has become one of the most universal methods in condensed matter physics and material science to determine and investigate properties of materials. The longer-term goal of the present work is to investigate to which extent the spatial extension of the density matrix is characteristic for metavalent materials, and whether numerical calculations based on the Kohn-Sham formulation of density functional theory can capture this aspect.

TT 37.55 Wed 15:00 P4

Traces of powers of many-body Hamiltonians — •Marcus Kollar — Theoretische Physik III, University of Augsburg

The high-temperature expansion of the partition function for a many-body system of fermions or bosons involves Fock space traces of powers of the Hamiltonian. Here we use algebraic means to evaluate such moments for a fixed number of non-interacting particles with arbitrary discrete spectrum and express them as polynomials of power sums of the single-particle energies. In the fermionic case our expressions agree with those obtained by combinatorial considerations [1]. We discuss possible applications and generalizations of our results.

[1] E. Adibi and E. Koch, Verhandl. DPG, Berlin TT 80.44 (2024).

TT 37.56 Wed 15:00 P4

Ising model on a sphere — •Grigorios Makris[1], Fabian Hassler[2], Stefan Wessel[1], and Ion Cosma Fulga[3,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Institute for Quantum Information, RWTH Aachen University, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany

The study of the Ising models is of primary interest in the theory of phase transitions. The models have been extensively studied in flat space and analytical solutions exist in two dimensions. Their scaling behavior is known to substantial precision and confirms the theory of finite-size scaling.

Here, we study Ising models on the surface of a sphere. As it is generally not possible to place a regular lattice on a sphere, for arbitrary number of points, we implement the Fibonacci lattice. The lattice is tested to have a reasonably uniform distribution of points. In order to establish the expected $SO(3)$ symmetry, we first solve the free-particle problem as a tight-binding model and then utilize the hopping coefficients as interaction terms on the Ising model. This is shown to yield better, approximate, $SO(3)$ degeneracies on the low energy levels of the transverse-field Ising model. Having set up the Hamiltonian, we further investigate the critical point of the expected phase transition.

TT 37.57 Wed 15:00 P4

Two site entanglement in the two dimensional Hubbard model — Anna Kauch[1], •Gergo Roosz[2], Frederic Bippus[1], Daniel Wieser[1], Fakher Assaad[3,4], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]HUN-REN Wigner RCP, Budapest — [3]Universitat Wurzburg, 97074 Wurzburg, Germany — [4]Wurzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Wurzburg, Germany

We calculate the reduced density matrix of two sites in the two-dimensional Hubbard model using the D Gamma A method. We calculate the density matrix by calculating the expectation value of a complete set of hermitian operators in the subspace of the two sites. We can express these eigenvalues with the one- and two-particle Greens functions, and the imaginary time derivatives of these functions. The derivatives are calculated in Matsubara representation. To test convergence we compare our results for the second Renyi entropy with quantum Monte Carlo data. To investigate the entanglement and correlations of the Hubbard model we calculate the mutual information and the entanglement negativity between the two sites.

TT 37.58 Wed 15:00 P4

Thouless time in a spin-1/2 XX ladder — •Kadir Çeven[1], Lukas Peinemann[1], Rohit Patil[2], Marcos Rigol[2], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Pennsylvania State University, University Park, USA

The eigenstate thermalization hypothesis (ETH) offers a powerful framework for understanding many properties of thermalization dynamics in non-equilibrium quantum many-body systems. Here, determining the time scales associated with thermalization is a key focus in the research of nonequilibrium dynamics of such systems. In this study, we investigate a spin-1/2 XX ladder, an experimentally realizable model exhibiting diffusive dynamics, to explore the connections among ETH, transport properties, and measures purely based on its energy spectrum. Specifically, we analyze the spectral form factor and the smooth spectral function, each of which provides a characteristic relaxation time scale potentially linked to the Thouless time–the longest relaxation time defined in terms of the diffusion constant. Using various numerical methods, we compare the time scales obtained from these different measures to identify potential discrepancies and similarities.

We acknowledge funding from the Deutsche Forschungsgemeinschaft (German Research Foundation) within the Research Unit FOR5522 (Project No. 499180199).

TT 37.59 Wed 15:00 P4

Nonequilibrium Phenomena in Strongly Correlated Systems under Structured Fields — •Sajad Mirmohammadi and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg Karl-Freiherr-von-Fritsch-Str. 3 06120 Halle/Saale

Strongly correlated systems provide a rich platform for exploring quantum phenomena and understanding nonequilibrium many-body dynamics. A central challenge lies in unraveling the interplay of various interactions that govern the emergence of exotic quantum states. Here, we investigate how phase- and polarization-structured electromagnetic fields interact with strongly correlated materials modeled by the extended Peierls Hubbard Hamiltonian. Using exact diagonalization with the Lanczos algorithm, we demonstrate how structured fields imprint their characteristics onto excitation dynamics, including charge and spin density waves.

TT 37.60 Wed 15:00 P4

Application of the TraSPI Method to Aharonov-Bohm Interferometry with Interacting Quantum Dots — •Alexander Hahn, Jürgen König, and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Utilizing the *Transfer-matrix Summation of Path Integrals* (TraSPI) approach, we extend the method's application to the study of quantum transport in an Aharonov-Bohm interferometer housing two parallel quantum dots. Here the usage of TraSPI allows the calculation of the current influenced by the enclosed magnetic flux, in presence of Coulomb interaction. The numerical accuracy and efficiency of the TraSPI method allow for a detailed exploration of the interplay between quantum coherence and dot interactions.

TT 37.61 Wed 15:00 P4

Metastability in Correlated Electron Systems — •Lara Bremer[1], Martin Eckstein[1], Hugo Strand[2], and Tim Wehling[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [2]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

The objective of this study is to describe metastable states in correlated electron systems, with a particular focus on numerically accessing unstable solutions within coexistence regions of first-order phase transitions. Our work is based on the well-established phenomenon observed in the Mott transition of the single-orbital Hubbard model, where a coexistence region between a metallic phase and an insulating phase, accompanied by a third unstable solution, has been demonstrated within the framework of Dynamical Mean Field Theory. A Phase Space Extension algorithm is employed to effectively identify and analyse these solutions. By accessing this unstable solution, the double occupancy on this branch can be calculated, thus enabling the Landau free energy to be calculated via a thermodynamic route, as opposed to fitting a Landau free energy functional.

TT 37.62 Wed 15:00 P4

Simulating nonequilibrium systems in the steady-state: GW+EDMFT — •Fabian Künzel — University of Hamburg, 20355 Hamburg, Germany

The Keldysh formalism for nonequilibrium Green's functions provides a versatile theoretical framework for analyzing the dynamics and structure of correlated many-body systems. To address the intrinsic cubic scaling of computational time in the Kadanoff-Baym equations (KBE) for nonequilibrium Green's functions, a truncation of the underlying memory kernel can be incorporated into the time-stepping algorithm of the NESSi simulation package. This reduces the computational cost to linear scaling with respect to the maximum simulation time. For systems where long-time dynamics extend beyond the capabilities of state-of-the-art methods, the KBE can be formulated within the Keldysh steady-state formalism. The resulting equations are then solved using a Fourier transform, enabling the description of systems with exponentially separated timescales. We aim to introduce new methods that extend the reach of the existing NESSi package and present a steady-state study of a Mott insulator, incorporating non-local correlations through a steady-state GW+EDMFT formalism.

TT 38: Superconducting Electronics: SQUIDs, Qubits, Circuit QED I

Time: Wednesday 16:45–18:30 Location: H32

TT 38.1 Wed 16:45 H32

Microwave characterization of planar Josephson junction arrays — •Alexander Kirchner[1], Johanna Berger[1], Simon Feyrer[1], Narges Momeni[1], Matthias Kronseder[1], Michael Prager[1], Dieter Schuh[1], Dominique Bougeard[1], Nicola Paradiso[1], Christoph Strunk[1], and Leandro Tosi[2,1] — [1]Institut für Experimentelle und Angewandte Physik, University of Regensburg, 93040 Regensburg, Germany — [2]Centro Atómico Bariloche and Insitituto Balseiro, CNEA, CONICET, San Charlos de Bariloche, Río Negro 8400, Argentina

We present microwave characterization measurements of Josephson junction arrays (JJAs) based on a proximitized Al-InAs quantum well heterostructure. JJAs can be used to achieve high inductances, suitable for the implementation of quantum circuits. They also provide an excellent test-bed for studying the microscopic excitations of hybrid superconductor-semiconductor devices associated to the presence of Andreev states. By probing the low-energy plasmon modes of these devices, we have been able to derive the Josephson inductance and to demonstrate its tunability in out-of-plane magnetic field, following the Fraunhofer diffraction pattern of planar Josephson junctions. Furthermore, the temperature dependence of the inductance provides information about the induced superconducting gap in the two-dimensional electron gas.

TT 38.2 Wed 17:00 H32

Niobium-trilayer based Dimer Josephson Junction Array Amplifiers — •Bhoomika R Bhat, Asen L Georgiev, Fabian Kaap, Victor Gaydamachenko, Christoph Kissling, Judith Felgner, Mark Bieler, and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Qubit readout and other quantum technologies using microwave signals at low powers of a few fW benefit from amplification with the least possible added noise. Josephson parametric amplifiers are a well-established class of devices meeting this condition. We design a Dimer Josephson Junction Array Amplifier (DJJAA) [1], which has several pairs of modes, so-called dimers, in the 4 GHz to 12 GHz range. In principle, each of these dimers can be used to achieve non-degenerate amplification using the four-wave mixing regime. Our devices, consisting of arrays with 600-1200 dc-SQUIDs, are fabricated in Nb/Al-AlOx/Nb trilayer technology. We present finite element simulations of our design as well as the fabrication process and the first experimental results of our devices.

[1] P. Winkel et al., Phys. Rev. Appl. 13, 024015 (2020).

TT 38.3 Wed 17:15 H32

Towards a traveling-wave parametric amplifier with two-octave bandwidth — •Christoph Kissling, Victor Gaydamachenko, and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Traveling-Wave Parametric Amplifiers (TWPAs) are among the leading technologies for amplifying weak microwave signals. They provide a gain of 15-20 dB over a bandwidth of more than 1 GHz while keeping the added noise close to the quantum limit. Although TWPAs are widely used in quantum computing, certain applications in fields like radio astronomy require amplifiers with broader bandwidth, ranging from e.g. 4 to 12 GHz. In this work, we present a TWPA consisting of ca. 2400 rf-SQUIDs, which operates in the three-wave mixing regime and achieves a 3-dB bandwidth of 3.6 to 8.3 GHz. Our device provides a gain of 20 dB and has a saturation power of around -90 dBm. By incorporating this TWPA as the first amplifier in our readout chain, we attain a total system noise of 2-3 photons across the entire bandwidth. Finally, we discuss strategies to extend the bandwidth to two octaves and improve the flatness of the gain profile.

TT 38.4 Wed 17:30 H32

Mitigating phase velocity mismatch in flux-pumped Josephson traveling wave parametric amplifiers — •Daniil Bazulin[1,2], Lars Aaron Anhalt[1,2], Kevin Kiener[1,2], Matthias Grammer[1,2], Niklas Bruckmoser[1,2], Leon Koch[1,2], Matthias Althammer[1,2], Stephan Geprägs[1,2], Stefan Filipp[1,2,3], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Josephson traveling wave parametric amplifiers (JTWPAs) play a key role in enabling fast readout of multiple qubits in scalable superconducting quantum processors. These amplifiers utilize wave-mixing processes in extended nonlinear media, to achieve broadband amplification with noise performance close to the standard quantum limit. Flux-pumped JTWPAs, employing the SNAIL-based nonlinear media, are particularly interesting due to their potential to eliminate the problem of pump depletion and mitigate upconversion losses. However, these devices exhibit a phase velocity mismatch between pump and signal modes, which suppresses a maximum achievable amplification gain. This issue can be addressed by using materials with high dielectric constant or kinetic inductance, like $SrTiO_3$ and NbTiN, respectively. Here, we present our progress in millikelvin characterization of these materials and their prospects in the flux-pumped JTWPAs.

TT 38.5 Wed 17:45 H32

Towards superconducting quantum-accurate arbitrary waveform generators for microwave frequencies — •Michael Haas, Abdulrahman Widaa, Oliver Kieler, Shekhar Priyadarshi, Marco Kraus, Ralf Behr, Johannes Kohlmann, and Mark Bieler — Physikalisch Technische Bundesanstalt, Braunschweig, Germany

The Josephson Arbitrary Waveform Synthesizer (JAWS) consists of an array of Josephson Junctions being driven by electrical pulses to produce quantum-accurate output signals with high spectral purity and low noise [1]. It has been subject of research for many years and is well established at output frequencies in the kHz and low MHz range. However, the extension to GHz frequencies, which could prove to be very important for quantum applications and metrology, has just recently started [2, 3]. This effort requires completely new circuit designs. Moreover, at high frequencies part of the input signal is fed through to the output signal and it is essential to accurately determine and minimize this so-called feedthrough error. We will present the status of the GHz-JAWS development at PTB, including new approaches to circuit design and feedthrough reduction.

[1] O. Kieler, Encyclopedia of Condensed Matter Physics, 2e 1 Oxford: Elsevier (2024). DOI: 10.1016/B978-0-323-90800-9.00001-9
[2] C. Donnelly et al., IEEE Trans. Appl. Supercond. 30 (2020). DOI: 10.1109/TASC.2019.2932342
[3] A. Babenko et al., IEEE Trans. Appl. Supercond. 32 (2022). DOI: 10.1109/TASC.2022.3201188

TT 38.6 Wed 18:00 H32

Characterization of stacked Josephson junction arrays for the Josephson Arbitrary Waveform Synthesizer with integrated on-chip power dividers — •Omar M. Aladdin[1], Oliver Kieler[1], Abdulrahman Widaa[1], Hannes Preissler[1], Erasmus Wolf[2], Marco Schubert[2], Johannes Kohlmann[1], and Mark Bieler[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Supracon AG, An der Lehmgrube 11, 07751 Jena, Germany

The Josephson Arbitrary Waveform Synthesizer (JAWS) is based on pulse-driven Josephson junction (JJ) arrays and provides precisely controlled, spectrally pure quantum-based AC voltages with low noise and no drift. Being widely used at National Metrology Institutes, increasing the output voltage of JAWS might significantly expand its application range. In this contribution, we describe our current efforts towards reaching JAWS output voltage of 1 V RMS. We are improving the existing on-chip RF power dividers enabling up to 8 parallel JJ arrays to operate simultaneously per chip with sufficient operation margins. Additionally, we are increasing the number of active junctions by means of fabricating of up to 5-stacked SNS-type JJ with Nb_xSi_{1-x} as barrier material. The target is to integrate about 50 000 to 60 000 JJ per chip. The circuit layout with integrated on-chip power dividers, the fabrication technology and first measurement results will be presented at the conference.

TT 38.7 Wed 18:15 H32

High-temperature superconducting Josephson junctions for optical neuromorphic computing — •Elena Vinnemeier[1], Sebastian Schaper[1], Malik Ayachi[2], Vincent Humbert[2], Javier Villegas[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, Palaiseau, France

Josephson Junctions (JJ) offer a promising platform for neuromorphic computing, owing to their inherent ability to emulate key neuronal behaviours such as spiking and bursting. When coupled with high-temperature superconductors and reconfigurable interconnects, these junctions present a viable alternative to traditional CMOS-based approaches, providing a low-power solution that is both faster and more efficient. The integration of high-temperature superconductors into the JJs enhances energy efficiency while exploiting their sensitivity to external stimuli. The currently missing integrated memory element is addressed by replacing passive interconnections with active links, which can be tuned by external stimuli. Our goal is to achieve optical modulation of the critical current I_C through light irradiation. To explore this capability, we characterize semiconducting materials from the transition metal dichalcogenide (TMDCs) family in combination with superconducting JJs using Raman spectroscopy and photoluminescence (PL), contrasting their properties as a function of environmental conditions.

This project was supported by the EIC pathfinder grant No. 101130224 'JOSEPHINE'.

TT 39: Twisted Materials / Systems (joint session TT/HL)

Time: Wednesday 17:00–18:30 Location: H31

TT 39.1 Wed 17:00 H31

Formation, persistence and ordering of local moments in magic angle twisted bilayer graphene — •Lorenzo Crippa[1,2], Gautam Rai[1], Dumitru Călugăru[3,13], Haoyu Hu[4], Luca de' Medici[5], Antoine Georges[6,7,8,9], Bogdan Andrei Bernevig[3,4,10], Roser Valentí[11], Giorgio Sangiovanni[2], and Tim Wehling[1,12] — [1]University of Hamburg — [2]University of Würzburg — [3]Princeton University — [4]DIPC, Donostia-San Sebastian — [5]ESPCI, Paris — [6]Collège de France, Paris — [7]Flatiron Institute, New York — [8]École Polytechnique, Palaiseau Cedex — [9]Université de Genève — [10]IKERBASQUE, Bilbao — [11]Goethe University Frankfurt — [12]Hamburg CUI — [13]University of Oxford

The physics of magic angle twisted bilayer graphene (MATBLG) is remarkably diverse across a wide range of dopings and temperatures.

By means of a Dynamical Mean-Field Theory (DMFT) approach, we study the effect of electronic correlations in MATBLG, with particular focus on the physics of local spin and valley isospin moments. We analyze their magnitude and screening across a broad temperature range, discuss the limits of very low and infinite temperature, and obtain two different scales for their formation (around 100 K) and ordering (around 10 K).

We discuss their implications in terms of transport properties of the system (e.g. resistivity) and of spectral features (resonance peaks) and contextualize our findings with recent experimental results.

TT 39.2 Wed 17:15 H31

Nematic versus Kekulé phases in twisted bilayer graphene under hydrostatic pressure — Miguel Sánchez Sánchez[1], Israel Díaz[1], José González[2], and •Tobias Stauber[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC — [2]Instituto de Ciencia de Materiales, CSIC

We address the precise determination of the phase diagram of magic angle twisted bilayer graphene under hydrostatic pressure within a self-consistent Hartree-Fock method in real space, including all the remote bands of the system. We further present a novel algorithm that maps the full real-space density matrix to a 4x4 density matrix based on a SU(4) symmetry of sublattice and valley degrees of freedom. We find a quantum critical point between a nematic and a Kekulé phase, and show also that our microscopic approach displays a strong particle-hole asymmetry in the weak coupling regime. We arrive then at the prediction that the superconductivity should be Ising-like in the hole-doped nematic regime, with spin-valley locking, and spin-triplet in the electron-doped regime [1].

[1] M. Sánchez Sánchez, I. Díaz, J. González, T. Stauber, Phys. Rev. Lett. (in press), arXiv:2403.03140.

TT 39.3 Wed 17:30 H31

Quantum diffusion in sheared bilayer graphene — •Taher Rhouma[1], Florie Mesple[2], Vincent Renard[3], and Guy Trambly de Laissardière[1] — [1]LPTM, CY Cergy Paris Univ., CNRS, Cergy-Pontoise, France. — [2]Dept. Physics, Univ. of Washington, USA — [3]CEA, Univ. Grenoble Alpes, IRIG, PHELIQS, Grenoble, France

The identification of correlated insulators and superconductivity in magic-angle twisted bilayer graphene (MATBG) has sparked significant interest in its electronic properties [1]. When examining the MATBG moiré patterns along the line with alternating regions of AA, AB, and BA, we observe striking similarities to those found in a 1D moiré of a sheared bilayer graphene, where one layer is laterally displaced. That may lead to a localization of the electronic states [2]. In this study, we investigate numerically the electronic and quantum transport properties in sheared bilayer graphene, focusing on how the degree of shear influences these characteristics.

[1] Y. Cao, et al., Nature **556**, 43 (2018); Nature **556**, 80 (2018).

[2] J. Gonzalez, Phys. Rev. B **94**, 165401 (2016).

TT 39.4 Wed 17:45 H31

Ab-initio fRG study on $tWSe_2$ — •Hannes Braun — Max Planck Institut für Festkörperforschung — Technische Universität München

The recent experimental reports on superconductivity in twisted WSe_2 have served to justify the already considerable interest in twisted TMD systems. From a theoretical standpoint, there have been numerous attempts to describe these systems. To study the phase diagram and analyse the governing physics, we employ the functional renormalisation group method. This approach allows us to gain an unbiased understanding of the interplay between fluctuations leading to symmetry-broken phases. To develop a model capable of describing the material, we integrate *ab-initio* results as initial conditions. In this talk, we present method developments for a more efficient momentum integration and results on the interplay between magnet and pairing instabilities.

TT 39.5 Wed 18:00 H31

Mott transitions and doping asymmetry in twisted bilayer WSe_2 — •Siheon Ryee[1], Lennart Klebl[2,1], Valentin Crépel[3], Ammon Fischer[4], Lede Xian[5,6], Angel Rubio[6,3], Dante Kennes[4,6], Andrew Millis[3,7], Antoine Georges[8,3], Roser Valentí[9], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany — [3]Flatiron Institute, New York, USA — [4]RWTH Aachen University, Aachen, Germany — [5]Tsientang Institute for Advanced Study, Zhejiang, China — [6]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [7]Columbia University, New York, USA — [8]Collège de France, Paris, France — [9]Goethe Universität Frankfurt, Frankfurt am Main, Germany

The recent discovery of superconductivity in twisted bilayer WSe_2 ($tWSe_2$) at two distinct twist angles (3.65 deg and 5 deg) along with previous reports of metal-insulator transitions, spin density wave states, and fractional Chern insulators raises deep questions in correlated electron physics. We present results of a dynamical mean-field theory-based investigation of a model that faithfully captures the band structure and topology of twisted transition metal dichalcogenides as functions of twist angle and displacement field. We find good agreement with several key aspects of the experimental data. Focusing further on the twist angle of 3.65 deg, we discuss the nature of the electric-field-induced metal-insulator transition, the experimentally observed coherence temperature, and the origin of the observed doping asymmetry in resistivity.

TT 39.6 Wed 18:15 H31

Twisted bilayer MoS_2 under electric fields: A system with tunable symmetry — •Aitor Garcia-Ruiz[1,2] and Ming-Hao Liu[1] — [1]National Cheng Kung University, Tainan, Taiwan — [2]National Graphene Institute, University of Manchester, Manchester, United Kingdom

Gate voltages take full advantage of two-dimensional systems, making it possible to explore novel states of matter by controlling their electron concentration or applying perpendicular electric fields. Here, we study the electronic properties of small-angle twisted bilayer MoS_2 under a strong electric field. We show that the transport across one of its constituent layers can be effectively regarded as a two-dimensional electron gas under a nanoscale potential. We find that the band structure of such system reconstructs following two fundamentally different symmetries depending on the orientation of the external electric field, namely, hexagonal or honeycomb. By studying this system under magnetic fields, we demonstrate that this duality not only translates into two different transport responses, but also results in having two different Hofstadter's spectra. Our work opens up a new route for the creation of controllable artificial superlattices in van der Waals heterostructures.

TT 40: Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)

Time: Wednesday 17:30–19:00 Location: H19

TT 40.1 Wed 17:30 H19

Orbital torques and orbital pumping in two-dimensional rare-earth dichalcogenides — •Mahmoud Zeer[1,2,3], Dongwook Go[3], Mathias Kläui[3,4], Wulf Wulfhekel[5], Stefan Blügel[1], and Yuriy Yuriy Mokrousov[1,3] — [1]Peter Gr *unberg Institute, Forschungszentrum J *ulich, 52425 J *ulich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, German — [3]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [4]Centre for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway — [5]5Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The design of spin-orbit torque (SOT) properties in two-dimensional (2D) materials represents a key challenge in modern spintronics. We now explore ferromagnetic Janus H-phase monolayers of 4f-Eu rare-earth dichalcogenides

EuSP, EuSSe, and EuSCl using first-principles calculations. Our findings reveal that these compounds exhibit substantial SOT, primarily driven by the colossal current-induced orbital response of Eu f-electrons. Additionally, the resulting orbital torques can generate strong in-plane currents of orbital angular momentum with non-trivial orbital polarization directions. These results establish f-based 2D materials as a highly promising platform for in-plane orbital pumping and SOT applications, positioning f-based 2D materials as a promising platform for next-generation orbitronic and spintronic technologies with 2D materials.

TT 40.2 Wed 17:45 H19

Orbital Topology of Chiral Crystals for Orbitronics — •Ying-Jiun Chen[1], Kenta Hagiwara[1,2], Dongwook Go[3], Xin Liang Tan[1,2], Sergii Grytsiuk[1], Kui-Hon Ou Yang[4], Guo-Jiun Shu[5], Jing Chien[4], Yi-Hsin Shen[4], Xiang-Lin Huang[5], Iulia Cojocariu[1], Vitaliy Feyer[1,2], Minn-Tsong Lin[4,6], Stefan Blügel[1], Claus Michael Schneider[1,2], Yuriy Mokrousov[1,3], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich — [2]University of Duisburg-Essen — [3]Johannes Gutenberg University Mainz — [4]National Taiwan University, Taiwan — [5]National Taipei University of Technology, Taiwan — [6]Academia Sinica, Taiwan

Chirality is ubiquitous in nature and manifests in a wide range of phenomena including chemical reactions, biological processes, and quantum transport of electrons. In quantum materials, the chirality of fermions, given by the relative directions between the electron spin and momentum, is connected to the band topology of electronic states. Here, we show that in structurally chiral materials like CoSi, the orbital angular momentum (OAM) serves as the main driver of a nontrivial band topology in this new class of unconventional topological semimetals, even when spin-orbit coupling is negligible. A nontrivial orbital-momentum locking of multifold chiral fermions in the bulk leads to a pronounced OAM texture of the helicoid Fermi arcs at the surface. Our findings highlight the pivotal role of the orbital degree of freedom for the chirality and topology of electron states, in general, and pave the way towards the application of topological chiral semimetals in orbitronic devices.

TT 40.3 Wed 18:00 H19

Vectorial flow of the Berry curvature and its relation to the transport and band structure — •Jaroslav Hamrle[1,2], Ondřej Stejskal[1], Milan Vrána[2,1], and Martin Veis[2] — [1]Czech Technical University, Prague, Czechia — [2]Charles University, Prague, Czechia

Berry curvature expresses the curvature of the reciprocal space, in a similar manner as magnetic field express curvature of the real space, resulting in a curved transport of electrons in solids. Therefore, Berry curvature is a base of various lossless transport phenomena such as anomalous Hall effect, anomalous Nerst effect, orbital magnetization or electric polarization. Here, in model materials bcc Fe and Fe_3Ga, we demonstrate details of the vectorial flow of the Berry curvature (monopole source, 1-dimensional flow, 2-dimensional flow), and its relations to the band structure, orbital magnetization as well as anomalous Hall and Nerst effects.

[1] O. Stejskal, M. Veis, J. Hamrle, Sci Rep **12**, 97 (2022) [doi: 10.1038/s41598-021-04076-z]

[2] O. Stejskal, M. Veis, J. Hamrle, Phys. Rev. Materials **7**, 084403 (2023) [doi:10.1103/PhysRevMaterials.7.084403]

TT 40.4 Wed 18:15 H19

Finite-temperature transport properties of magnetic/non-magnetic alloys: trends in the longitudinal and in the transverse charge and spin currents — •Alberto Marmodoro[1], Yang Wang[2], Yuqing Lin[3], and Ilja Turek[4] — [1]Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czech Republic — [2]Pittsburgh Supercomputer Center (PSC), Carnegie Mellon University, Pittsburgh, USA — [3]Mellon College of Science, Carnegie Mellon University, Pittsburgh, USA — [4]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic

Alloys composed of magnetic and non-magnetic metals exhibit non-trivial transport trends as a function of composition and temperature. The stoichiometry controls not only the Curie point, but also the slope of resistivity vs. temperature. Beside affecting longitudinal currents, this has further implications also for transverse charge and spin currents, i.e. on anomalous Hall effects [1]. We report first-principles results based on density functional theory (DFT), relativistic linear response and Green function methods based on the multiple scattering Korringa-Kohn-Rostoker (KKR) or linear muffin tin orbitals (LMTO) frameworks.

[1] "Large anomalous Hall angle in the Fe(60),Al(40) alloy induced by substitutional atomic disorder" by J.Kudrnovsky et al. PRB 101, 054437 (2020); "Exploiting Spin Fluctuations for Enhanced Pure Spin Current" by P.Wu et al. PRL 128, 227203 (2022); "Critical enhancement of the spin Hall effect by spin fluctuations" by S.Okamoto et al. Quantum Materials 29, 9 (2024).

TT 40.5 Wed 18:30 H19

Impact of the substrate on angular momentum transport between separated ferromagnets — •Fiona Sosa Barth[1,2], Matthias Grammer[1,2], Richard Schlitz[3], Tobias Wimmer[1,2], Janine Gückelhorn[1,2], Luis Flacke[1,2], Sebastian T.B. Goennenwein[3], Rudolf Gross[1,2,4], Hans Huebl[1,2,4], Akashdeep Kamra[5], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]Department of Physics, University of Konstanz, Konstanz, Germany — [4]Munich Center for Quantum Science and Technology, München, Germany — [5]RPTU Kaiserslautern-Landau, Kaiserslautern, Germany

Spintronics relies on the transfer of angular momentum between electrons and solid state excitations such as magnons and phonons. In our recent work, we demonstrate angular momentum transfer between two ferromagnetic strips on diamagnetic substrates [1] by converting a DC current at one of the electrodes to a non-equilibrium magnon accumulation. Due to dipolar and potentially phononic coupling, angular momentum is transferred to the magnonic system of the second FM electrode and measured by the inverse processes. In this work, we investigate the substrate influence on the angular momentum transport by comparing our results for SiOx and SiN layers on Si substrates. As a next step, we investigate substrate-supported strips versus freestanding strings to separate phononic contributions from dipolar coupling. [1] R. Schlitz et al., Phys. Rev. Lett. 132, 256701 (2024)

TT 40.6 Wed 18:45 H19

Orbital Edelstein contribution to the spin-charge conversion in Germanium Telluride — •Sergio Leiva-Montecinos[1], Libor Vojáek[2], Jing Li[2], Mairbeck Chshiev[2], Ingrid Mertig[1], and Annika Johansson[3] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Université. Grenoble Alpes, CEA, CNRS, SPINTEC, Grenoble, France — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Edelstein effect (EE) is a promising mechanism for generating spin and orbital polarization from charge currents in systems without inversion symmetry. In ferroelectric materials, such as Germanium Telluride (GeTe), the combination of bulk Rashba splitting and voltage-controlled ferroelectric polarization provides a pathway for reversible spin-charge interconversion [1, 2].

In this work, we investigate current-induced spin and orbital magnetization in bulk GeTe using Wannier-based tight-binding models derived from DFT calculations and semiclassical Boltzmann theory. Employing the modern theory of orbital magnetization (MTOM), we demonstrate that the orbital Edelstein effect (OEE) entirely dominates its spin counterpart (SEE). This difference is visualized through the spin and orbital textures at the Fermi surfaces, where the orbital moment surpasses the spin moment by one order of magnitude. Moreover, the OEE remains largely unaffected when we suppress the spin-orbit coupling, highlighting its distinct physical origin compared to the SEE.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2012).

[2] C. Rinaldi *et al.*, Nano Lett. **18**, 2751 (2018).

TT 41: Quantum-Critical Phenomena (joint session TT/DY)

Time: Thursday 9:30–12:45 Location: H31

TT 41.1 Thu 9:30 H31

Missing Spectral Weight in a Paramagnetic Heavy-Fermion System — •Debankit Priyadarshi[1], Jingwen Li[1], Chia-Jung Yang[1], Ulli Pohl[2], Oliver Stockert[3], Hilbert von Löhneysen[4], Shovon Pal[5], Manfred Fiebig[1], and Johann Kroha[2,6] — [1]ETH Zurich, Switzerland. — [2]University of Bonn, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Karlsruhe Institute of Technology, Germany — [5]NISER, HBNI, Jatni, India. — [6]University of St. Andrews, UK

Time-resolved terahertz spectroscopy (THz-TDS) has proven to be a powerful method to study the correlation dynamics in many-body systems, particularly heavy-fermions [1]. The competition between the Kondo screening effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in these materials drives a quantum phase transition (QPT) between a magnetically ordered and a liquid-like ground state of heavy Kondo quasiparticles. These quasiparticles disintegrate near a quantum critical point (QCP). Using THz-TDS, we report a suppression in the quasiparticle spectral weight in $CeCu_{6-x}Au_x$ on the antiferromagnetic side of the QPT at temperatures much higher than the Neel temperature, which has a different origin from the suppression at QCP [2]. We study the paramagnetic phase of $CeCu_{6-x}Au_x$ with x = 0.2, 0.3, and 0.5 samples, and show that the suppression results from a quantum frustration effect induced by the temperature-independent RKKY interaction, which may influence material properties at QCP.

[1] C. Wetli *et al.*, Nat. Phys. 14, 1103 (2018);
[2] J.Li *et al.*, arXiv:2408.07345 (2024).

TT 41.2 Thu 9:45 H31

Terahertz Crystal Electric Field Transitions in a Kondo-Lattice Antiferromagnet — •Payel Shee[1], Chia-Jung Yang[2], Shishir Kumar Pandey[3], Ashis Kumar Nandy[1], Ruta Kulkarni[4], Arumugam Thamizhavel[4], Manfred Fiebig[2], and Shovon Pal[1] — [1]NISER, HBNI, Jatni, India. — [2]ETH Zurich, Switzerland. — [3]Artificial Intelligence for Science Institute, Beijing, China. — [4]Tata Institute of Fundamental Research, Mumbai, India.

The interplay between the Kondo effect and Ruderman-Kittel-Kasuya-Yosida (RKKY) leads to the emergence of many intriguing phenomena in strongly correlated systems. Metallic materials doped with magnetic impurities are ideal for such studies. These impurities interact with the crystal electric field (CEF) produced by neighboring ions, lifting the degeneracy of their energy levels and creating CEF states. Given that CEF excitations occur in the millielectronvolt (meV) range, the terahertz (THz) frequency range is particularly suited for these investigations. Using time-domain THz reflection spectroscopy, we show the first direct evidence of two low-energy CEF transitions at 0.6 THz (2.5 meV) and 2.1 THz (8.7 meV) in $CeAg_2Ge_2$, a prototype Kondo-lattice antiferromagnet. In addition, we also observe that the lower CEF transition peak undergoes a blue-shift once the sample enters into the antiferromagnetic phase. The temporal spectral weights obtained directly from the THz time traces corroborate the corresponding CEF energy scales of the compound [2].

[1] S. Pal *et al.*, Phys. Rev. Lett. 122, 096401 (2019);
[2] P. Shee *et al.*, Phys. Rev. B 109, 075133 (2024).

TT 41.3 Thu 10:00 H31

Tuning a ferromagnetic quantum phase transition by interface engineering in artificial heterostructures — Robin Heumann[1], Robert Gruhl[1], Ludwig Scheuchenpflug[1], Leonard Schüler[2], Vasily Moshnyaga[2], and •Philipp Gegenwart[1] — [1]Lehrstuhl für Experimentalphysik VI, Universität Augsburg — [2]Erstes Physikalisches Institut, Georg-August-Universität-Göttingen

The substitution series $Sr_{1-x}Ca_xRuO_3$ between the itinerant ferromagnet $SrRuO_3$ (SRO) and the non-Fermi liquid paramagnetic metal $CaRuO_3$ (CRO) constitutes a broadly smeared quantum phase transition (QPT) between $x = 0.7$ and 1. To avoid the impact of structural disorder we explore the possibility of tuning ferromagnetism by confining SRO to thin layers placed in between those of CRO. Ordered epitaxial $[SRO_n/CRO_m]_K$ superlattices, with n ranging from 8 down to the monolayer limit, keeping $m/n = 2$ and 3 with $K = 32/n$, were grown on $SrTiO_3$ (100) substrates, characterized and investigated by electrical transport and Hall effect measurements. We observe stable ferromagnetism from SRO layers for $n \geq 3$ and fragile low-temperature ferromagnetism due to the SRO/CRO interfaces. The latter survives down to the monolayer limit $n = 1$, explaining the difficulty to cross a ferromagnetic QPT in $Sr_{1-x}Ca_xRuO_3$. We also find that the effective interface density $K/(n+m)$ is a new suitable control parameter and construct the T_C vs $K/(n+m)$ phase diagram.

TT 41.4 Thu 10:15 H31

Interplay of nematic fluctuations and transverse phonons near a nematic quantum critical point — •Morten H. Christensen[1], Michael Schütt[2], Avraham Klein[3], and Rafael M. Fernandes[4] — [1]Niels Bohr Institute, University of Copenhagen — [2]University of Minnesota — [3]Ariel University — [4]University of Illinois Urbana-Champaign

In an electronic fluid absent an atomic lattice, an electronic nematic transition can be described as a consequence of a Pomeranchuk instability of the Fermi surface with an associated critical nematic mode. As a coupling to an atomic lattice is introduced, the nematic transition is accompanied by a structural distortion of the lattice. Here, we study the fluctuation spectra near such a coupled nematic-structural transition driven primarily by the electronic nematic fluctuations. This requires coupling the nematic fluctuations to transverse phonons which implies that the transition is no longer accompanied by a critical nematic mode, but rather by the vanishing of the transverse phonon velocity along a certain direction. To understand how, e.g., superconductivity is affected by this, knowledge of the dynamic behaviour of the hybrid nematic/phonon soft excitation is crucial. The purpose of this presentation is to elucidate the properties of this mode. We find that the low-energy fluctuations are generally overdamped except near the soft lattice directions where they become underdamped. How the transition from overdamped to underdamped takes place depends on the proximity to the nematic quantum critical point.

TT 41.5 Thu 10:30 H31

Chiral Heisenberg Gross-Neveu-Yukawa criticality: Honeycomb vs. SLAC fermions — •Thomas C. Lang[1] and Andreas M. Läuchli[2,3] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Laboratory for Theoretical and Computational Physics, Paul Scherrer Institute, Switzerland — [3]Institute of Physics, École Polytechnique Féedérale de Lausanne, Switzerland

We perform large scale quantum Monte Carlo simulations of the Hubbard model at half filling with a single Dirac cone close to the critical point, which separates a Dirac semi-metal from an antiferromagnetically ordered phase where SU(2) spin rotational symmetry is spontaneously broken. We discuss the implementation of a single Dirac cone in the SLAC formulation for eight Dirac components and the influence of dynamically induced long-range super-exchange interactions. The finite size behavior of dimensionless ratios and the finite size scaling properties of the Hubbard model with a single Dirac cone are shown to be superior compared to the honeycomb lattice. We extract the critical exponents believed to belong to the chiral Heisenberg Gross-Neveu-Yukawa universality class which coincide for the two lattice types once honeycomb lattices of sufficient linear dimension are considered.

TT 41.6 Thu 10:45 H31

Fractionalized multicriticality in Kitaev spin-orbital liquids — •Max Fornoville[1,2] and Lukas Janssen[3] — [1]Max Planck Insti- tute for Solid State Research, 70569 Stuttgart, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Two-dimensional spin-orbital magnets with Kitaev-like exchange frustration realize spin-orbital liquid ground states that are characterized by the appearance of gapless Majorana fermions and a static $\mathbb{Z}_2$ gauge field. It has been shown that the introduction of an antiferromagnetic Heisenberg interaction between nearest-neighbor spin degrees of freedom facilitates a transition towards a partially ordered spin-orbital liquid state with a spontaneously broken spin-rotation symmetry. The associated quantum critical point belongs to the fractionalized fermionic Gross-Neveu-SO(3)* universality class and only partially gaps out the fermionic spectrum. Here, we consider an enlarged theory space, introducing an anisotropic XXZ interaction in the spin sector. The explicit breakdown of spin-rotation symmetry allows for two types of antiferromagnetic order, depending on the nature of the anisotropy. By means of Majorana mean-field theory and ε-expansion to leading order, we uncover the phase diagram of the model and characterize its multicritical behavior. Additionally, we present evidence for the appearance of a symmetry-enhanced first-order transition between the two ordered phases.

15 min. break

TT 41.7 Thu 11:15 H31

One-loop perturbative structure of a (2+1)D bosonized non-Fermi liquid — •Parasar R. Thulasiram[1,2], Chris Hooley[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Centre for Fluid and Complex Systems, Coventry University, Coventry, United Kingdom

Non-Fermi liquids are a class of metals with no quasiparticle excitations often arising from the interaction of slow collective modes, such as an emergent critical boson, with a Fermi surface. Minimal models of this type are called Hertz-Millis-Moriya models and historically suffer from uncontrolled approximations in perturbation theory and patchy treatments of the Fermi surface, preventing the study of global-Fermi surface physics. Delacrétaz et al. (2022) recast Fermi liquid theory in any dimension via a bosonic field that parametrizes macroscopic particle-hole excitations about the whole Fermi surface. This bosonized field theory is suggested to reduce the order in perturbation theory necessary to calculate important quantities and is considerate of whole Fermi surface fluctuations, potentially providing the first robust results of a Hertz-Millis-Moriya theory when coupled to a critical boson. We present initial results of the one-loop critical boson self-energy in 2+1D for calculating the dynamical critical exponent and discuss the benefits and challenges of this theory.

TT 41.8 Thu 11:30 H31

Exotic quantum criticality in Luttinger semimetals — •David Moser and Lukas Janssen — TU Dresden, Deutschland

Luttinger semimetals are three-dimensional strongly-spin-orbit-coupled systems, in which valence and conduction bands touch quadratically at the Fermi level. They provide a rich playground for highly unconventional physics and serve as a parent state to a number of exotic states of matter, such as Weyl semimetals, topological insulators, or spin ice. Here, we discuss various quantum critical phenomena beyond standard quantum criticality, including quasiuniversality, fixed-point annihilation scenarios, and large-N aspects. Our results are relevant for the low-temperature behavior of rare-earth pyrochlore iridates, such as $Pr_2Ir_2O_7$ or $Nd_2Ir_2O_7$.

TT 41.9 Thu 11:45 H31

Examination of the antiferromagnetic superradiant intermediate phase and the effects of geometrical frustration in the Dicke-Ising model — •Jonas Leibig, Anja Langheld, Andreas Schellenberger, and Kai Phillip Schmidt — Chair for Theoretical Physics V, FAU Erlangen-Nürnberg, Germany

We map the Dicke-Ising model to a self-consistent matter Hamiltonian in the thermodynamic limit [1, 2] and solve it using a variety of methods, including ex-

act diagonalization, perturbative and numerical linked-cluster expansions, and density matrix renormalization group. In one dimension, we explore the intermediate phase in the antiferromagnetic model and the multi-critical point in the ferromagnetic model, comparing our results with complementary quantum Monte Carlo simulations [2]. Additionally, we investigate the antiferromagnetic model on the frustrated geometry of the sawtooth chain. We employ high-order series expansions in the strong coupling limit, where the mapping to the self-consistent matter Hamiltonian is definitively valid. Independently, we analyze in greater detail whether the mapping also holds in the specific regime emerging from the frustrated Ising limit induced by an infinitesimal light-matter perturbation.

[1] K. Lenk, J. Li, P. Werner, M. Eckstein, arXiv:2205.05559;
[2] A. Langheld, M. Hörmann, K. P. Schmidt, arXiv:2409.15082.

TT 41.10 Thu 12:00 H31

Critical behavior of the 1d superconductor in the FLEX approximation — •Šimon Kos[1], Sunil D'Souza[1], Jan Gebel[1], Ján Minár[1], and Václav Janiš[2] — [1]University of West Bohemia, Univerzitní 8, CZ-301 00 Plzeň, Czech Republic — [2]Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, CZ-18200 Praha 8, Czech Republic

The dynamical quantum fluctuations below the lower critical dimension push the superconducting critical point to zero temperature. We study the quantum critical behavior of the 1d superconductor with one-particle self-consistency provided by the FLEX approximation within the canonical Baym-Kadanoff scheme. We use the non-interacting singlet electron-electron bubble in the two-particle vertex of the Schwinger-Dyson equation, allowing for a qualitatively correct and tractable treatment of the low-energy critical behavior compatible with the Mermin-Wagner theorem. We use a polar approximation to transform the convolutive Schwinger-Dyson equation into an algebraic one that can be solved semi-analytically. We confirm the position of the critical point and assess the low-temperature behavior of the Hubbard model with attractive interaction.

TT 41.11 Thu 12:15 H31

Tunable criticality and pseudo-criticality in a quantum dissipative spin system — •Manuel Weber — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

The study of competing orders in two-dimensional quantum magnets was strongly motivated by the prediction of non-Landau quantum phase transitions, but often we found symmetry-enhanced first-order transitions or pseudocriticality with a logarithmic drift of critical exponents. Here we present results for a (0+1) dimensional spin-boson model where all of these phenomena occur due to a fixed-point annihilation within the critical manifold. Our recently-developed wormhole quantum Monte Carlo method for retarded interactions allows us to study the critical properties of this model with unprecedented precision. We find a tunable transition between two ordered phases that can be continuous or first-order, and even becomes weakly first-order in an extended regime close to the fixed-point collision. We provide direct numerical evidence for pseudo-critical scaling on both sides of the collision manifesting in an extremely slow drift of critical exponents. We also find scaling behavior at the symmetry-enhanced first-order transition as described by a discontinuity fixed point. Our study motivates future work in higher-dimensional quantum dissipative spin systems.

TT 41.12 Thu 12:30 H31

Universality of the quantum Heisenberg model with sub-volume long-range couplings — •Daniel Resch and Thomas C. Lang — Institute for Theoretical Physics, University of Innsbruck, Austria

We investigate the critical properties of effective spin models which emerge from low energy band structures, or momentum space patches of strongly interacting fermions. As representative worst case scenario we present quantum Monte Carlo simulations of phase transitions in the major-axis coupled, long-range quantum Heisenberg model in two spatial dimensions at finite and zero temperature. We quantify the effects of sub-volume anisotropic long range spin-coupling with power-law form $1/r^{\alpha}$ on the critical exponents of the transitions where SU(2) spin symmetry is spontaneously broken for at low, finite temperatures in accordance with the Mermin Wagner Hohenberg theorem. Performing finite-size scaling analyses for different α we determine the extent of the regimes where the (quantum) phase transitions are represented by Gaussian fixed point, short-range Wilson-Fisher, or continuously varying long-range non-Gaussian critical exponents.

TT 42: Superconductivity: Tunneling and Josephson Junctions

Time: Thursday 9:30–13:15 Location: H32

TT 42.1 Thu 9:30 H32

Extraction of the Density of States and the Gap Function on a Temperature Smearing Scale from the Tunneling Conductance Data — •Lucia Geleneky-ová and František Herman — Comenius University in Bratislava

The aim of our work is to extract the density of states (DOS) and the gap function from the tunneling conductance data at higher temperatures. It is known that if the temperature approaches zero, the DOS function is proportional to the tunneling conductance, and therefore, it can be easily extracted. However, with increasing temperature, the temperature smearing causes that this approximation can no longer be used. Thus, we have developed an algorithm that was designed to extract the details of the DOS function and the gap function on a typical temperature scale, which can be used approximately up to 1/2 of T_c. Moreover, knowledge of the DOS in its normal state plays an important role. Hence, we present the results of the testing data sets and also the outcome from experimentally measured tunneling conductance data of the NbN superconductor.

This work has been supported by the Slovak Research and Development Agency under the Contract no. APVV-23-0515, by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 945478.

TT 42.2 Thu 9:45 H32

Superconductivity of α-Gallium Probed on the Atomic Scale by Normal and Josephson Tunneling — Corinna Fohn[1], David Wander[1], Danilo Nikolic[2,3], Stéphanie Garaudée[1], Hervé Courtois[1], Wolfgang Belzig[3], Claude Chapelier[4], Vincent Renard[4], and •Clemens B. Winkelmann[1,4] — [1]Université Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, F-38000 Grenoble, France — [2]Institut für Physik, Universität Greifswald, Felix-Hausdorff-Strasse 6, D-17489 Greifswald, Germany — [3]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [4]Université Grenoble Alpes, CEA, Grenoble INP, IRIG/DEPHY/PHELIQS, F-38000 Grenoble, France

We investigate superconducting gallium in its α phase using scanning tunneling microscopy and spectroscopy at temperatures down to about 100 mK. High-resolution tunneling spectroscopies using both superconducting and normal tips show that superconducting α-Ga is accurately described by Bardeen-Cooper-Schrieffer theory, with a gap $\Delta_{\mathrm{Ga}} = 163\ \mu$eV on the α–Ga(112) facet, with highly homogeneous spectra over the surface, including atomic defects and step edges. Using a superconducting Pb tip, we furthermore study the low-bias conductance features of the Josephson junction formed between tip and sample. The features are accurately described by dynamical Coulomb blockade theory, highlighting α–Ga as a possible platform for surface science studies of mesoscopic superconductivity.

TT 42.3 Thu 10:00 H32

Current Phase Relation of HgTe Nanowire Josephson Junctions in an Axial Magnetic Field — •Niklas Hüttner[1], Wolfgang Himmler[1], Ralf Fischer[1], Dmitriy Kozlov[1], Michael Barth[2], Jacob Fuchs[2], Andreas Costa[2], Klaus Richter[2], Leandro Tosi[1], Nicola Paradiso[1], Dieter Weiss[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg — [2]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

Proximitized semiconductor nanowires are expected to show Anomalous Josephson effect by spin-orbit interaction and Zeeman effect in a magnetic field parallel to the wire direction [1]. The φ_0 shift is accompanied by a direction dependent critical current (Superconducting diode effect).[1] We directly probe the current phase relation (CPR) of HgTe nanowires proximitized by niobium leads via an asymmetric SQUID measurement. The topological surface states additionally pick up an Aharanov Bohm phase for $B_{\parallel}$ in wire direction [2]. We observe an highly tunable φ_0 shift, a 0-π transition, and a superconducting diode effect from the corresponding CPRs. Additionally a strong modulation of both the critical current and the content of higher harmonics is observed for magnetic flux between 0 and $1.5\Phi_0$.

[1] T. Yokoyama et al., Phys. Rev. B 89, 195407 (2014).
[2] W. Himmler et al., Phys. Rev. Res. 5, 043021 (2023).

TT 42.4 Thu 10:15 H32

Theory of Josephson Scanning Tunneling Microscopy with s-Wave Tip on a Cuprate Surface — •Peayush Kumar Choubey[1] and Peter Hirschfeld[2] — [1]Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India — [2]University of Florida, Gainesville, Florida 32611, USA

The Josephson scanning tunneling microscopy (JSTM) is a direct local probe of superconducting gap order parameter (SCOP). JSTM studies have been largely limited to the cases where superconducting sample and superconducting tip,

both, have the same gap symmetry- either s-wave or d-wave. It has been generally assumed that in an s-to-d SJTS study of cuprates the critical current would vanish everywhere owing to the orthogonality of tip and sample SCOPs. We show here that this is not the case. Using first-principles Wannier functions for $Bi_2Sr_2CaCu_2O_8$, we develop a scheme to compute Josephson critical current (I_c) measured by a JSTM setup employing an s-wave tip with sub-angstrom resolution. We show that I_c remains finite everywhere in the unit cell except along Cu-Cu directions, changes sign under four-fold rotation, and attains largest magnitude above O sites, which can be regarded as a hallmark of the d-wave gap symmetry. Further, we find that I_c is suppressed near a strong scatterer like Zn and modulations in I_c around an impurity occur at wavevectors distinct from quasi-particle interference (QPI). Our work provides a theoretical foundation for probing unconventional superconductivity using JSTM set-up with s-wave tip.

TT 42.5 Thu 10:30 H32

Optimal Parametric Control of Transport Across a Josephson Junction — •Hannah Victoria Kleine-Pollmann, Guido Homann, and Ludwig Mathey — Zentrum für Optische Quantentechnologien and Institut für Quantenphysik, *Universität Hamburg, 22761 Hamburg, Germany

We present optimal control strategies for the DC transport across a Josephson junction. Specifically, we consider a junction in which the Josephson coupling is driven parametrically, with either a bichromatic or a trichromatic driving protocol, and optimize the prefactor of the $1/\omega$ divergence of the imaginary part of the conductivity. We demonstrate that for an optimal bichromatic protocol an enhancement of 70 can be reached, and for an optimal trichromatic protocol an enhancement of 135. This is motivated by pump-probe experiments that have demonstrated light-enhanced superconductivity along the c-axis of underdoped YBCO, where the junction serves as a minimal model for the c-axis coupling of superconducting layers. Therefore, the significant enhancement of superconductivity that we show for multi-frequency protocols demonstrates that the advancement of pump-probe technology towards these strategies is highly desirable.

TT 42.6 Thu 10:45 H32

Gate-Controlled Superconductivity: Mechanisms, Parameters and Technological Potential — Leon Ruf, Jennifer Koch, Elke Scheer, and •Angelo Di Bernardo — University of Konstanz, Universitätsstraße 10, 78464 Konstanz

Over the past few years, several research groups have demonstrated the reversible control of the superconducting current flowing through a nanoscale-size constriction under the application of a gate voltage (V_G) - currently known as gate-controlled supercurrent (GCS) [1].

The numerous differences between fabrication protocols, device parameters and measurement setups adopted by these groups, however, have made it difficult to find universal features of the GCS effect.

In this talk, I will discuss the results of systematic studies carried by our group [2-4] that have allowed us to identify parameters that are key for the GCS observation and to achieve high reproducibility in the functioning of GCS devices [4]. In addition, I will review the progress that we have made towards the optimization of performance parameters that are important for the future development of technological applications based on the GCS.

[1] L. Ruf et al., Appl. Phys. Rev. **11**, 041314 (2024).
[2] L. Ruf et al., APL Mater. **11**, 091113 (2023).
[3] J. Koch et al., Nano Res. **17**, 6575 (2024).
[4] L. Ruf et al., ACS Nano **18**, 20600 (2024).

TT 42.7 Thu 11:00 H32

Gate-Controlled Supercurrents in Three-Terminal Devices Made on Industrial Grade SiO_2 and Al_2O_3 — •Leon Ruf, Jennifer Koch, Elke Scheer, and Angelo Di Bernardo — University of Konstanz, Universitätsstraße 10, 78457 Konstanz

Gate-controlled supercurrent (GCS) is a growing, highly debated field of research. It was found that in gated three-terminal devices made of Ti and Al the supercurrent could be modulated by the application of a gate voltage [1]. The authors attribute their observation to a direct electric field effect, which would pave the way for future CMOS compatible transistors. Contrary, other works reported about a leakage related effect: high-energy quasiparticle emission through vacuum [2], phonon-induced heating of the electronic system [3], out-of-equilibrium state induced by phonons and/or high energy electrons without sizeable heating [4]. Here we are studying the GCS in Nb and NbRe Dayem bridges on industrial grade SiO_2 and Al_2O_3. Our results reveal a strong correlation between the substrate material and the GCS parameters, such as suppression voltage and stability. Herby, SiO_2 and Al_2O_3 show major differences. Further, our results suggest that for both SiO_2 and Al_2O_3 the leakage current is mediated via defects giving rise to trap-assisted tunneling. We discuss our results in the light of the above-mentioned mechanism [1-4].

[1] De Simoni et al., Nat. Nanotechnol. **13**, 802 (2018);
[2] Alegria et al., Nat. Nanotechnol. **16**, 404 (2021);
[3] Ritter et al., Nat. Electron. **5**, 71 (2022);
[4] Basset et al., Phys. Rev. Rese. **3**, 043169 (2021).

15 min. break

TT 42.8 Thu 11:30 H32

Transport Measurements on Arrays of Four-Terminal Nb-Pt-Nb Josephson Junctions — •Justus Teller[1,2], Christian Schäfer[1,2], Benjamin Bennemann[1], Matvey Lyatti[1,2], Kristof Moors[1,2], Detlev Grützmacher[1,2], Roman-Pascal Riwar[1], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9, PGI-10, PGI-2), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

Arrays of interconnected two-terminal Josephson junctions have been investigated since the 1980's. Usually, the array is realized as a square lattice with four two-terminal Josephson junctions connected in a square unit cell. Recently, Graziano et al. [1] showed that a multi-terminal Josephson junction can be described as a network of interconnected two-terminal Josephson junctions. Based on that concept, we present an array made of 30×30 four-terminal Nb-Pt-Nb Josephson junctions. The in-situ fabrication of large networks of Josephson junctions, using molecular beam epitaxy, is described. For this process, a periodically patterned shadow mask of Si_3N_4 has been developed. The physical concept of a multi-terminal Josephson junction array is introduced. Its theoretical explanation is based on a lattice of interconnected two-terminal Josephson junctions, each described as a resistively-capacitively-shunted junction. Critical current and resistance of the array show oscillations connected to its unit cell.

[1] G. V. Graziano et al., Phys. Rev. B 101, 054510 (2020).

TT 42.9 Thu 11:45 H32

Superconducting Atomic Contacts under Microwave Irradiation, Photon-Assisted Tunneling and Fractional Shapiro Steps — •Oliver Irtenkauf[1], Patrick Raif[1,2], Carlos Cuevas[1,3], and Elke Scheer[1] — [1]University of Konstanz, Germany — [2]University of Basel, Switzerland — [3]Universidad Autónoma de Madrid, Spain

We form an atomic contact from a mechanically controlled aluminum break junction and irradiate it with microwaves in its superconducting state [1]. In the dI/dV spectra, we observe the well-known structures caused by photon-assisted tunneling, which, in the case of tunnel contacts, are fully explained by the Tien-Gordon (TG) model [2]. However, for higher-order transport processes, the model requires extensions, as shown in simulations based on the TG model [3,4]. Shapiro steps, i.e., replicas of the supercurrent, reveal deviations from the theoretical predictions described in references [5,6]. Fractional Shapiro steps, which we observe in atomic contacts with high-transmission channels at high frequencies, differ from traditional Shapiro steps and represent a new phenomenon.

[1] P. Raif, Master Thesis, *Uni. Konstanz* (2024);
[2] P. K. Tien & J. P. Gordon, *PR* **129**, 647 (1963);
[3] P. E. Gregers-Hansen et al., *PRL* **31**, 524 (1973);
[4] J.C. Cuevas et al., *PRL* **88**, 157001 (2002);
[5] G. Falci, V. Bubanja & G. Schön, *Z. Phys.* **85**, 451 (1991);
[6] P. Kot et al., *PRB* **101**, 134507 (2020).

TT 42.10 Thu 12:00 H32

High-Frequency Irradiation of Single-Atom Josephson Junctions — •Martina Trahms[1,2], Bharti Mahendru[2], Clemens B. Winkelmann[1], and Katharina J. Franke[2] — [1]University Grenoble Alpes, LATEQS, 38042 Grenoble, France — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Understanding superconducting junctions on the atomic scale yields significant insights for the prospect of using superconducting circuits in future technological applications. Here, we investigate the influence of single magnetic adatoms (Mn) on the phase dynamics of current-biased Pb-Pb Josephson junctions in a scanning tunneling microscope (STM) in the presence of high-frequency (HF) irradiation that is applied via an antenna close to the junction. We observe Shapiro steps that indicate coherent absorption of the irradiation while at the same time phase diffusion is enhanced due to incoherent absorption. In the presence of a magnetic adatom, phase diffusion is more prominently enhanced compared to the pristine junction which indicates that the quantum spin of the magnetic impurity influences the coherence of the tunneling processes in the junction.

TT 42.11 Thu 12:15 H32

Amplification Schemes for Single Microwave Photons — •Lukas Danner[1,2], Hanna Zeller[2], Ciprian Padurariu[2], Joachim Ankerhold[2], and Björn Kubala[1,2] — [1]Institute for Quantum Technologies, German Aerospace Center (DLR), Ulm (Germany) — [2]Institute for Complex Quantum Systems and IQST, University of Ulm, Ulm (Germany)

The detection of single microwave photons plays a crucial role in a wide range of envisioned technological applications of quantum microwaves. However, this is challenging because of the large thermal background and the low energy of a single photon. Here, we investigate schemes to amplify single itinerant mircowave photons using Josephson photonics devices [1, 2]. These devices consist of a

dc-voltage biased Josephson junction, connected in series with two microwave cavities. By tuning the dc voltage, various resonances can easily be accessed, such that e.g. a Cooper pair tunneling through the junction enables a coherent transfer between one excitation in the first cavity and n excitations in the second cavity. We show that a single photon pulse absorbed by the device effectively triggers the emission of multiple photons from the second cavity that can subsequently be detected. To study such processes theoretically, we use a recently developed formalism [3] to describe arbitrary traveling photon pulses interacting with a quantum system in a cascaded manner.

[1] Leppäkangas et al., Phys. Rev. A 97, 013855 (2018)
[2] Albert et al., Phys. Rev. X, 14, 011011 (2024)
[3] Kiilerich and Mølmer, Phys. Rev. Lett. 123, 123604 (2019)

TT 42.12 Thu 12:30 H32

Tunneling in Altermagnet/Superconductor/Altermagnet Junctions — •Marcel Polák[1], František Herman[1], Andreas Costa[2], and Jaroslav Fabian[2] — [1]Comenius University Bratislava, Slovakia — [2]University of Regensburg, Germany

Their unprecedented spectral characteristics—particularly their large local magnetic exchange splittings in momentum space without rising an overall net spin polarization—make altermagnets promising candidates for engineering strongly spin-polarized currents in superconducting heterostructures.

In this talk, we will focus on lateral altermagnet/superconductor/ altermagnet junctions in the ballistic limit to theoretically explore the ramifications of their d-wave-like spin-split Fermi surfaces on superconducting transport. We will demonstrate that the subgap interplay of Andreev and quasiparticle tunnelings, and thereby the experimentally accessible tunneling conductance, is tunable through the absolute and relative orientations of the altermagnets' Fermi surfaces, recovering the two important limiting cases in which the altermagnets behave either rather like normal metals or ferromagnets. Finally, we will also investigate geometrical conductance oscillations at supergap voltages in the presence of resonant scattering and compare our results against the ferromagnetic junction counterpart.

This work has been supported by Contract no. APVV-23-0515, by the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 945478 and by DFG Grants 314695032 (SFB 1277) and 454646522.

TT 42.13 Thu 12:45 H32

Chiral Interference Pattern in Tunneling Junctions and SQUIDs Made of Time-Reversal Invariant Weyl Superconductors — •Anastasiia Chyzhykova[1,2], Vira Shyta[1], Jeroen van den Brink[1], and Flavio Nogueira[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Technische Universität Dresden

In recent years a number of experiments have reported superconductivity in various Weyl semimetals. The low-energy electromagnetic response of Weyl semimetals is governed by the axion term in the action arising due to the chiral anomaly. A recent publication [1] demonstrated that the time-reversal invariant Weyl superconductors (SCs) exhibit a chiral Meissner state. In our work we explore the influence of the chiral Meissner state on the tunnel junctions and squids made of time-reversal invariant Weyl SCs. We derive a modified Fraunhofer interference pattern in such a junction and demonstrate how the presence of the axion term affects Josephson energy in asymmetric squids and Berry phase in charge qubits. The effect of the chiral Meissner state manifests as a temperature-dependent deficit flux, which provides a new tuning parameter compared to ordinary squids.

[1] V.Shyta, J.van den Brink, F.S.Nogueira, Phys.Rev.Res. 6, 013240 (2024).

TT 42.14 Thu 13:00 H32

Superconductor-Altermagnet Proximity Effect with Nonmagnetic Impurities — •Christian Wiedemann[1], Danilo Nikolić[2], Matthias Eschrig[2], and Wolfgang Belzig[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Universität Greifswald, Greifswald, Germany

Altermagnetism is a novel magnetic phase with zero net magnetization and momentum-dependent (e.g. d-wave) spin-split Fermi surface which has been recently discovered [1]. Similarly to ferromagnets [2,3], when brought to the proximity of a superconductor (S) an altermagnet (AM) modifies the spectral properties of the former [4,5]. However, most works in the field of superconducting spintronics involving altermagnets have assumed the absence of impurities that are, however, typically unavoidable in experiments. In this talk, we address this question explicitly presenting a systematic analysis of the inverse proximity effect in an S/AM bilayer in the presence of nonmagnetic impurities. Utilizing the quasiclassical Green's function theory, we investigate the effect of impurities on observables, e.g., the self-consistently calculated order parameter and the density of states. We observe interesting phenomena such as the gapless superconductivity and an impurity-enhanced critical temperature.

[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 040501 (2022).
[2] A. I. Buzdin, Rev. Mod. Phys. **77**, 935 (2005).
[3] M. Eschrig, Rep. Prog. Phys. **78**, 104501 (2015).
[4] S. Chourasia *et al.*, arXiv:2403.10456.
[5] M. Wei *et al.*, Phys. Rev. B **109**, L201404 (2024).

TT 43: Correlated Electrons: Other Theoretical Topics

Time: Thursday 9:30–13:00 Location: H33

TT 43.1 Thu 9:30 H33

Fragility of local moments for singular hybridizations — •Max Fischer[1,2], Arianna Poli[3], Lorenzo Crippa[1,2], Sergio Ciuchi[3,4], Matthias Vojta[2,5], Alessandro Toschi[6], and Giorgio Sangiovanni[1,2] — [1]Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Università dell'Aquila, Italy — [4]CNR, Italy — [5]TU Dresden, Germany — [6]TU Wien, Austria

Some transition-metal phtalocyanines on an Ag(001) surface show hybridizations for xz/yz-orbitals with sharp peaks superimposed on a rather constant z^2 contribution. These sharp peaks in the hybridization correspond to an Anderson impurity model with one impurity site hybridized with one bath site. Investigating only a constant hybridization this typically shows rich physics arising from the Kondo effect yielding local moments and screening of them at low temperatures. Expanding the constant hybridization by a peak at the Fermi level, the formation of the local moment is shifted to lower temperatures with increasing weight of the peak. With such a toy model we analyze the vanishing of the local moment at large weights of the peak. Here, we find the evolution from screening of the local moment to the formation of a singlet ground state for the two site AIM.

TT 43.2 Thu 9:45 H33

Inducing strong electronic correlation by charged impurities in weakly interacting two-dimensional electron system — Junho Bang[1], Byeongin Lee[1], João Augusto Sobral[2], Sayan Banerjee[2], Mathias Scheurer[2], •Jianfeng Ge[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Korea — [2]Institute for Theoretical Physics III, University of Stuttgart, 70550 Stuttgart, Germany — [3]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

When translational invariance is broken, e.g. in the presence of impurities, an ordered state can emerge where the electronic charge density modulates spatially. While conventional charge modulations are explained by weak-impurity scattering of Landau quasiparticles, strong correlations may drive the electrons to depart from the Fermi liquid behavior. Using scanning tunneling microscopy and spectroscopy, we switch the ionization state of individual surface impurities and discover a local phase transition induced by the impurity potential. A nanoscale charge-ordered phase, which breaks the symmetry of the underneath hosting lattice, spontaneously emerges from the otherwise uniform two-dimensional electron system. Further, the charge modulations appear with an anisotropy distinct from that of the Fermi surface, excluding any Fermi-surface-related interpretations for the ordered phase. While the exact origin of the solid-like electronic phase remains a mystery, our work demonstrates a microscopic approach for creating and manipulating strongly correlated electrons in two-dimensional systems even with weak intrinsic interactions.

TT 43.3 Thu 10:00 H33

Anomalous quantum oscillations from boson-mediated interband scattering — •Léo Mangeolle[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Quantum oscillations (QO) in metals refer to the periodic variation of thermodynamic and transport properties as a function of inverse applied magnetic field. QO frequencies are normally associated with semi-classical trajectories of Fermi surface orbits but recent experiments challenge the canonical description. We

develop a theory of composite frequency quantum oscillations (CFQO) in two-dimensional Fermi liquids with several Fermi surfaces and interband scattering mediated by a dynamical boson, e.g. phonons or spin fluctuations. Specifically, we show that CFQO arise from oscillations in the fermionic self-energy with anomalous frequency splitting and distinct strongly non-Lifshitz-Kosevich temperature dependencies. Our theory goes beyond the framework of semi-classical Fermi surface trajectories highlighting the role of many-body effects. We provide experimental predictions and discuss the effect of non-equilibrium boson occupation in driven systems.

TT 43.4 Thu 10:15 H33

Disentangling real space fluctuations: The diagnostics of metal-insulator transitions beyond single-particle spectral functions — •Michael Meixner[1], Marcel Krämer[1,2], Nils Wentzell[3], Pietro Bonetti[1,4], Sabine Andergassen[2], Alessandro Toschi[2], and Thomas Schäfer[1] — [1]Max-Planck-Insitut für Festkörperforschung, Stuttgart, Germany — [2]TU Wien, Vienna, Austria — [3]CCQ at Flatiron Institut, New York NY, USA — [4]Harvard University, Cabridge MA, USA

The destruction of metallicity due to the mutual Coulomb interaction of quasiparticles gives rise to fascinating phenomena of solid state physics such as the Mott metal-insulator transition and the pseudogap. A key observable characterizing their occurrences is the single-particle spectral function, determined by the fermionic self-energy. In this paper we investigate in detail how real space fluctuations constitute a self-energy that drives the Mott-Hubbard metal-insulator transition. To this aim we first introduce a real space fluctuation diagnostics approach to the Hedin equation, which connects the fermion-boson coupling vertex λ to the self-energy Σ. Second, by using cellular dynamical mean-field theory calculations for λ we identify the leading physical processes responsible for the destruction of metallicity across the transition. Eventually, to pave the way for relating our findings to the pseudogap phenomenology, we discuss the influence of real space fluctuations on the momentum-dependence of correlations.

TT 43.5 Thu 10:30 H33

Numerical indications for two-channel physics in the lightly doped t-J model — •Pit Bermes[1,2], Lukas Homeier[1,2], Sebastian Paeckel[1,2], Annabelle Bohrdt[2,3], and Fabian Grusdt[1,2] — [1]Department of Physics, Arnold Sommerfeld Center of Theoretical Physics, University of Munich, Theresienstrasse 37, 80333 Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, 80799 München, Germany — [3]University of Regensburg, Universitätsstr. 31, Regensburg D-93053, Germany

The infamous cuprate superconductors at low doping are effectively described by hole doped antiferromagnets. Due to strong correlations however, standard techniques fail to describe these materials and full understanding of the microscopic mechanism remains elusive. Here we analyze numerical simulations of the lightly doped t-J model in two dimensions and present indications for two effective scattering channels in the simulated pair spectrum. We employ a previously proposed effective model whose degrees of freedom are given by magnetic polarons and bipolarons and show that it qualitatively reproduces the two branches in the pair spectrum. In addition, we propose a scheme to experimentally measure these signatures. The understanding of the effective quasiparticles presents an important step to unravel the elusive phases of high Tc superconductors.

TT 43.6 Thu 10:45 H33

Interplay of local and non-local electronic correlations in the Hubbard model — •Maria Chatzieleftheriou[1], Silke Biermann[2], and Evgeny Stepanov[2] — [1]Goethe University Frankfurt, Germany — [2]Ecole Polytechnique, IP Paris, France

Strongly correlated electronic systems exhibit intriguing properties and highly complex phase diagrams, including metal-to-insulator transitions, magnetic/charge orderings and the field's holy grail: high temperature superconductivity. Their theoretical description is very challenging and various many-body methods have been developed to this direction. I will present results using state-of-the-art numerical techniques that allow for an accurate description of both strong local electronic correlations and spatial fluctuations. I will discuss the application of this approach on the study of the Hubbard model, relevant for a series of materials, where we have analyzed the interplay of Mott physics and magnetic fluctuations at half-filling. We have identified the Slater and Heisenberg regimes in the phase diagram, which are separated by a crossover region of competing spatial and local electronic correlations. This bridging of the two limits (the spin-fluctuation dominated Slater regime at weak coupling and the Mott insulator at strong-coupling) had been a key missing ingredient to our understanding of metal-insulator transitions in real materials. Lastly, I will present recently obtained results on the evolution of the system's magnetic and charge susceptibility as a function of doping.

TT 43.7 Thu 11:00 H33

Fracton and topological order in the XY checkerboard toric code — Max Vieweg and •Kai Phillip Schmidt — Frichdrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

Topological and fraction phases are of great importance in current research due to their fascinating physical properties like entangled ground states, exotic excitations with non-trivial particle statistics or restricted mobility as well as potential applications in quantum technologies. The 2D toric code is the most paradigmatic, simplest, and exactly solvable model displaying topological order, which has been proposed as quantum memory and is relevant for quantum error correction. Consequently, the toric code plays an important role in several domains of research covering condensed matter physics, quantum optics, and quantum information.

However, the toric code has so far not been linked to the field of fracton physics. Here we introduce the XY checkerboard toric code (XYTC) connecting for the first time topological and fracton order in two dimensions within the same model. The XYTC represents a generalization of the conventional toric code with two types of star operators and two anisotropic star sublattices forming a checkerboard lattice. The quantum phase diagram is deduced exactly by a duality transformation displaying topological and type-I fracton phases.

15 min. break

TT 43.8 Thu 11:30 H33

Deconfinement Phase Transitions in a nematic two dimensional XY model with Long-range couplings — •Luis Walther[1], Josef Willsher[1,2], and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, 80799 Munchen, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The Modified XY model is an illustrative example of the interplay between ferromagnetic and nematic couplings, hosting both vortex and half-vortex excitations. The model gives rise to an exotic second order phase transition driven by the deconfinement of vortices into half-vortices. This transition is in the universality class of the Ising model, displaying features of the 'Deconfined Criticality' scenario. We analyse the effect of long-range algebraically decaying couplings $\sim r^{-2-\sigma}$ on the model. Long-range couplings enrichen the phase diagram and influence the deconfinement phase transition. We find that the transition persists for long-range couplings decaying fast enough so that $\sigma > 2 - \eta$ holds, where η is the the correlation function exponent of the short-range XY model. Our results are based on Landau Peierls type arguments as well as Renormalisation Group flow techniques. Long-range couplings appear in many experimental setups including 2D Rydberg simulators. Therefore we hope our work contributes to enable the experimental observation of the deconfinement phase transition present in the model.

TT 43.9 Thu 11:45 H33

Mapping out Localization Phases in Bond-Disordered XXZ Models — Adrian Braemer[1], •Javad Vahedi[2], and Martin Gärttner[2] — [1]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Historically, the phenomenon of many-body localization (MBL) has been studied in spin systems subject to random, local magnetic fields. At strong disorder, the system is found to be localized, with the local integrals of motion (LIOMs) consisting of single spins. However, this is not the only type of MBL: in bond-disordered Heisenberg models, the LIOMs have been shown to involve pairs of spins.

In this talk, we show that the bond-disordered XXZ model also exhibits a single-spin localized phase at strong anisotropy and map out the transitions between these three phases. To this end, we generalize the notion of occupation distance introduced by Hopjan et al. [1] to different observables, enabling us to characterize all three phases.

[1] Phys. Rev. B 104, 235112 (2021).

TT 43.10 Thu 12:00 H33

Melting of Devil's Staircases in the Long-Range Dicke-Ising Model — •Jan Alexander Koziol and Kai Phillip Schmidt — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstraße 7, 91058 Erlangen, Germany

We present ground-state phase diagrams of the antiferromagnetic long-range Ising model under a linear coupling to a single bosonic mode on the square and triangular lattice. In the limit of zero coupling the ground state magnetization forms a Devil's staircase structure of magnetization plateaux as a function of an applied longitudinal field in Ising direction. The linear coupling to a single bosonic mode melts this structure to a so-called superradiant phase with a finite photon density in the ground state. The long-range interactions lead to a plethora of intermediate phases that break the translational symmetry of the lattice, as well as having a finite photon density. To study the ground-state phase diagram we apply an adaption of the unit-cell-based mean-field calculations [1,2], which capture all possible magnetic unit cells up to a chosen extent. Further, we exploit a mapping of the non-superradiant phases to the Dicke model in order to calcu-

late upper bounds for phase transitions towards superradiant phases [3]. In the case of second-order phase transitions, these bounds agree with the boundaries determined by the mean-field calculations.
[1] J. A. Koziol et al., SciPost Phys. 14, 136 (2023);
[2] J. A. Koziol et al., SciPost Phys. 17, 111 (2024);
[3] A. Schellenberger et al., SciPost Phys. Core 7, 038 (2024).

TT 43.11 Thu 12:15 H33

Anyonic phase transitions in the 1D extended Hubbard model with fractional statistics — •Sebastian Eggert[1], Martin Bonkhoff[2], Kevin Jägering[1], Shi-Jie Hu[3], Axel Pelster[1], and Imke Schneider[1] — [1]University of Kaiserslautern-Landau — [2]Theoretische Physik, Univ. Hamburg — [3]Beijing Computational Science Research Center

Recent advances in quantum technology allow the realization of "lattice anyons", which have enjoyed large interest as particles which interpolate between bosonic and fermionic behavior. We now study the interplay of such fractional statistics with strong correlations in the one-dimensional extended Anyon Hubbard model at unit filling by developing a tailored bosonization theory and employing large-scale numerical simulations. The resulting quantum phase diagram shows several distinct phases, which show an interesting transition through a multicritical point. As the anyonic exchange phase is tuned from bosons to fermions, an intermediate coupling phase changes from Haldane insulator to a dimerized phase. Detailed results on the universality classes of the phase transitions are presented.

TT 43.12 Thu 12:30 H33

Nonlinear effects on the transport of fractional charges in quantum wires — •Imke Schneider[1], Flavia Braga Ramos[1], Rodrigo Gonçalves Pereira[2], and Sebastian Eggert[1] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern-Landau, Kaiserslautern, Germany — [2]International Institute of Physics and Departamento de Física Teórica e Ex- perimental, Universidade Federal do Rio Grande do Norte, Natal, Brazil

We investigate the transport properties of one-dimensional systems be- yond linear response, focusing on the fractionalization of propagating charges. Starting from a right-moving unit charge, we predict its evo- lution into at least three distinct stable parts: a fractionally charged particle with freeparticle dynamics, a left-moving signal, and a right- moving low-energy excitation, which can carry positive or negative charge depending on the interaction strength and energy regime. Our findings provide deep insights into the universal correlated nature of these emergent particles and pave the way for out-of-equilibrium transport measurements, offering a direct method to extract the interaction parameters governing correlations in the system.

TT 43.13 Thu 12:45 H33

To Infinity and Back - $1/N$ Graph Expansion of Light-Matter Systems — •Andreas Schellenberger and Kai Phillip Schmidt — FAU Erlangen-Nürnberg, Erlangen, Deutschland

We present a method for performing a full graph expansion for light-matter systems, utilizing the linked-cluster theorem. This enables us to explore $1/N$ corrections to the thermodynamic limit $N \to \infty$, giving us access to the mesoscopic regime. This region is yet largely unexplored, as it is challenging to tackle with established solid-state methods. However, it hosts intriguing features, such as entanglement between light and matter that vanishes in the thermodynamic limit [1-3]. We calculate physical quantities of interest for paradigmatic light-matter systems like generalized Dicke models by accompanying the graph expansion by both exact diagonalization (NLCE [4]) and perturbation theory (pcst++ [5]), benchmarking our approach against other techniques.
[1] J.Vidal, S.Dusuel, EPL 74, 817 (2006).
[2] K.Lenk, J.Li, P.Werner, M.Eckstein, arXiv:2205.05559 (2022).
[3] A.Kudos,D.Novokreschenov,I.Iorsh,I.Tokatly,arXiv:2304.00805(2023).
[4] M.Rigol, T.Bryant, R.R.P.Singh, PRL 97, 187202 (2006).
[5] L.Lenke, A.Schellenberger, K.P.Schmidt, PRA, 108 (2023).

TT 44: Focus Session: Ising Superconductivity in Monolayer Transition Metal Dichalcogenides (joint session TT/HL/MA)

Superconducting monolayer transition metal dichalcogenides (TMDs) like $NbSe_2$, TaS_2, and gated WSe_2 or MoS_2, have attracted lot of interest in recent years. On the one hand Ising spin-orbit coupling pins the electron's spin out of plane, and hence is responsible for critical in-plane magnetic fields by far exceeding the Pauli limit. On the other hand, while the underlying pairing mechanism is still under debate, recent experiments provide strong evidence for its unconventional, multiband, nature. The Focus Session will feature experimental and theoretical advances on the superconductivity in monolayer TMDs, with focus on universal features, a possible Luttinger-Kohn mechanism, a nodal or even chiral nature of the gap functions, and their phase diagram.

Organizers: Milena Grifoni (Universität Regensburg), Julian Siegl (Universität Regensburg)

Time: Thursday 9:30–12:45 Location: H36

Topical Talk TT 44.1 Thu 9:30 H36

Evidence of Unconventional Superconductivity in Monolayer and Bulk van der Waals Material TaS_2 — •Somesh Chandra Ganguli[1], Viliam Vano[1,2], Yuxiao Ding[1], Maryam Khosravian[1], Jose Lado[1], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University FI-00076 Aalto, Finland — [2]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, NJ, USA

Unconventional superconductors are at the forefront of modern quantum materials' research. Even though unconventional superconductivity has been discovered in a large number of bulk systems, intrinsic unconventional superconductivity in the monolayer limit has remained elusive.

In our work, we demonstrate the evidence of nodal f-wave superconductivity in monolayer 1H-TaS_2. We also observe the emergence of many-body excitations potentially associated to its unconventional pairing mechanism. Furthermore, the nodal f-wave superconducting state in the pristine monolayer 1H-TaS_2 is driven to a conventional gapped s-wave state by the inclusion of non-magnetic disorder. I will also briefly describe our recent results on bulk layered superconductor 6R-TaS_2 where alternating metallic and Mott insulating layers gives rise to unconventional superconductivity.

Our results demonstrate the emergence of unconventional superconductivity in van der Waals (vdW) materials and therefore opens possibilities to create designer unconventional superconductivity in vdW heterostructures.

Topical Talk TT 44.2 Thu 10:00 H36

Signatures of Unconventional Superconductivity in Transition Metal Dichalcogenides — •Miguel Ugeda — Donostia International Physics Center, San Sebastián, Spain

Lowering the dimensionality of a material is an effective strategy to boost electronic correlations that fail to be captured by conventional pictures. In this arena, two-dimensional (2D) materials provide an ideal platform for the exploration of quantum collective phenomena arising from such strong interactions due to their simple synthesis and modelling. In this talk, I will review the rich physics that emerges in the family of transition metal dichalcogenide (TMD) metals in the superconducting state in the 2D limit. While many of these TMD metals exhibit superconductivity in both the bulk form down to the monolayer, the latter limit stores exciting surprises beyond the BCS frameworks that have been revealed in the last years. I will focus on our $NbSe_2$, the most representative TMD superconductor, where I will describe our recent STM/STS experiments. Lastly, I will briefly describe our current efforts to induce unconventional superconductivity in more complex TMD heterostructures.

Topical Talk TT 44.3 Thu 10:30 H36

Friedel Oscillations and Chiral Superconductivity in Monolayer $NbSe_2$ — •Magdalena Marganska[1,2], Julian Siegl[1], Anton Bleibaum[1], Marcin Kurpas[3], Wen Wan[4], John Schliemann[1], Miguel M. Ugeda[4,5], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93 053 Regensburg — [2]Institute for Theoretical Physics, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland — [4]Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao 48013, Spain

In 1965 Kohn and Luttinger proposed a mechanism for superconductivity, based on the electronic Coulomb interaction alone. The screening effects, which cause

Friedel oscillations of charge density around impurities, modulate also the interaction between moving electrons. If it has attractive regions, superconductivity can arise by exploiting them. This mechanism, negligible in 3D metals, can become much stronger in 2D electronic systems. In a monolayer of $NbSe_2$ the screening is further suppressed, due to the multi-orbital nature of the electronic band at the Fermi level. We show how this, and the presence of K/K' Fermi surfaces, leads to superconducting pairing. The dominant gap solution at $T = 0$ has the chiral p+ip symmetry. It evolves with increasing temperature, turning from fully chiral at T=0 to a nematic solution with p-like symmetry close to the critical temperature. Our results are also consistent with our tunneling spectroscopy measurements in $NbSe_2$.

15 min. break

Topical Talk TT 44.4 Thu 11:15 H36

Unconventional Pairing in Ising Superconductors — •Andreas Kreisel[1], Subhojit Roy[2,3,4], Brian M. Andersen[1], and Shantanu Mukherjee[2,3,4] — [1]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [2]Department of Physics, Indian Institute of Technology Madras, Chennai, 600036, India — [3]Center for Atomistic Modelling and Materials Design, IIT Madras, Chennai 600036, India — [4]Quantum Centers in Diamond and Emergent Materials (QCenDiem)-Group, IIT Madras, Chennai, 600036 India

Ising spin orbit coupling arises in materials with non-centrosymmetric crystal structure in conjunction of an in-plane mirror symmetry and is realized in some two dimension transition metal dichalcogenides. Example materials are monolayer $NbSe_2$, MoS_2, TaS_2, and $PbTe_2$, where signatures of unconventional superconductivity are found in contrast to their three dimensional bulk counterparts. In this talk, I present a microscopic formalism to calculate the superconducting instability from a momentum-dependent spin- and charge-fluctuation-mediated pairing interaction in presence of spin orbit coupling that induces a spin splitting. This pairing is then applied to the electronic structure of transition metal dichalcogenides. We provide a quantitative measure of the mixing between the even- and odd-parity superconducting states which varies with Coulomb interaction. The pairing scenario from spin fluctuations together with the mixing of the odd-parity superconducting state gives rise to an enhancement of the critical magnetic field.

Topical Talk TT 44.5 Thu 11:45 H36

High-Field Study of Ising Superconductivity in TMDs — •Oleksandr Zheliuk[1,2], Xiaoli Peng[3], Andrew Ammerlaan[1,2], Puhua Wan[3], Yulia Kreminska[3], Steffen Wiedmann[1,2], Uli Zeitler[1,2], and Jianting Ye[3] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, Nijmegen 6525 ED, The Netherlands — [2]Radboud University, Institute for Molecules and Materials, Nijmegen 6525 AJ, The Netherlands — [3]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands

Semiconducting transition metal dichalcogenides are known for their strong spin-orbit coupling, the possibility of hosting a variety of quantum phases such as two-dimensional superconductivity with upper critical fields that by far bypasses the Pauli limit, Josephson coupled states, and high mobility electron gasses accessed in electric double-layer transistor (EDLT) configuration. Despite its well-established electronic structure, the dome-shaped superconducting phase diagram where the critical temperature T_c can be modulated by carrier concentration is yet to be understood. This talk will sharpen the understanding of the electronic structure of the electron-doped MoS_2, covering recent insights into superconductivity in MoS_2 probed via the multivalley transport phenomena accessed in high magnetic field.

TT 44.6 Thu 12:15 H36

Unconventional Pairing in Ising Superconductors: Application to Monolayer $NbSe_2$ — •Subhojit Roy[1], Andreas Kreisel[2], Brian Andersen[3], and Shantanu Mukherjee[4] — [1]Indian Instititute of Technology Madras, Chennai, 600036, India — [2]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [3]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark — [4]Indian Instititute of Technology Madras, Chennai, 600036, India

The presence of a non-centrosymmetric crystal structure and in-plane mirror symmetry allows an Ising spin-orbit coupling to form in some two-dimensional materials, where a nontrivial nature of the superconducting state is currently being explored. In this study(1), we develop a microscopic formalism for Ising superconductors that captures the superconducting instability arising from a momentum-dependent spin- and charge-fluctuation-mediated pairing interaction. We apply our pairing model to the electronic structure of monolayer $NbSe_2$, where first-principles calculations reveal the presence of strong paramagnetic fluctuations. Our calculations provide a quantitative measure of the mixing between the even- and odd-parity superconducting states and its variation with Coulomb interaction. Further, numerical analysis in the presence of an external Zeeman field reveals the role of Ising spin-orbit coupling and mixing of odd-parity superconducting state in influencing the low-temperature enhancement of the critical magnetic field.

[1] S. Roy et al., 2D Mater. 12 015004 (2025).

TT 44.7 Thu 12:30 H36

Emergence of Unconventional Superconductivity and Doped Mott Physics in 6R-TaS_2 — •Yuxiao Ding[1], Amritroop Achari[2], Jonas Bekaert[3], Jose Lado[1], Rahul R. Nair[2], Peter Liljeroth[1], and Somesh C. Ganguli[1] — [1]Aalto University, Finland — [2]University of Manchester, UK — [3]University of Antwerp, Belgium

Discovery of Unconventional superconductivity in van der Waals (vdW) materials have brought about a paradigm shift in modern condensed matter research for their tunability and potential application in quantum computing. Among these, most prevalent are 4Hb-TaS_2 and 6R-TaS_2. They comprise of alternating Mott insulating and metallic layers and give rise to exotic quantum states such as topological superconductivity, anomalous Hall effect potentially associated with hidden magnetism etc. We have studied, using low temperature STM/STS, the newly discovered vdW superconductor 6R-TaS_2. For the 1T phase, a doped Mott phase was observed with potential charge order occurring due to hybridisation between 1T and underlying 1H layer. We also observe Kondo sites in the half-filled regime, which unlike 4Hb-TaS_2, were more robust under the application of tip-induced electric field. This indicates significantly different interlayer interactions in these two systems. We also observe evidence of unconventional superconductivity in the 1H phase, indicated by the presence of V-shaped superconducting gap and many-body excitations. Our results pave a new direction in understanding the role of interplay between magnetism and superconductivity in layered unconventional superconductors.

TT 45: 2D Materials: Electronic Structure and Exitations III (joint session O/HL/TT)

Time: Thursday 10:30–12:30 Location: H11

TT 45.1 Thu 10:30 H11

Charge ordered phases in the hole-doped triangular Mott insulator 4*Hb*-TaS_2 — •Byeongin Lee[1], Junho Bang[1], Hyungryul Yang[1], Sunghun Kim[2], Dirk Wulferding[3], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, Ajou University, Suwon 16499, Republic of Korea — [3]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Republic of Korea

4*Hb*-TaS_2 has a unique layered structure, featuring a heterojunction between a 2D triangular Mott insulator and a charge density wave metal. Since a frustrated spin state in the correlated insulating layer is susceptible to charge ordering with carrier doping, it is required to investigate the charge distribution driven by interlayer charge transfer to understand its various phases. In this study, we utilize scanning tunneling microscopy and spectroscopy (STM/S) to examine the charge-ordered phases of 1*T*-TaS_2 layers within 4*Hb*-TaS_2, explicitly focusing on the non-half-filled regime. Our STS findings reveal an energy gap that exhibits an out-of-phase relation of the charge density. We attribute the emergence of the charge-ordered insulating phase in a doped triangular Mott insulator to the interplay between on-site and nonlocal Coulomb repulsion.

TT 45.2 Thu 10:45 H11

Superlattice engineering in graphene and 1T-$NbSe_2$ heterostructures — •Keda Jin[1,2], Lennart Klebl[3], Junting Zhao[1,2], Tobias Wichmann[1,5], F. Stefan Tautz[1,5], Felix Lüpke[1], Dante Kennes[4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [3]I. Institute for Theoretical Physics, Universität Hamburg, 22607 Hamburg, Germany — [4]Institut für Theorie der statistischen Physik, RWTH Aachen, 52074 Aachen — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

Superlattice engineering has become a major branch of condensed matter research, not at least due to the variety of exotic states observed twisted in van der Waals heterostructures. We here present a new method to periodically modulate graphene by stacking it on 1T/2H-$NbSe_2$. By tuning the twist angle, we realized two near-commensurate superlattices: $\sqrt{3}\times\sqrt{3}$ and 2×2 aligned with the charge density wave (CDW) of 1T-$NbSe_2$. Using scanning tunnelling microscopy, we visualized local stacking configurations for these two superlattices. We applied a newly developed symmetry analysis method to track rotational symmetry breaking as a function of bias. In the 2×2 superlattice, C_3 rotational symmetry was

preserved. However, in the $\sqrt{3} \times \sqrt{3}$, a strong strip phase occurs. This symmetry breaking is explained by our tight-binding model. Our findings highlight a mechanism for superlattice-induced symmetry breaking that hints towards exotic states of matter.

TT 45.3 Thu 11:00 H11

Influence of Edge Termination on the Electronic Structure of Single Layer MoS_2 on Graphene/Ir(111) — •Alice Bremerich[1], Marco Thaler[2], Thais Chagas[1], Borna Pielic[1], Laerte Patera[2], and Carsten Busse[1] — [1]Universität Siegen, Deutschland — [2]Universität Innsbruck, Österreich

MoS_2 is the prototypical semiconducting single-layer transition-metal dichalcogenide (TMDC). It exhibits a metallic edge state that induces partial charge accumulation at its edges, resulting in band bending effects. This 1D state acts as a barrier to electron transport across the edge and contributes significantly to quantum confinement effects in TMDC islands. In this study, we tune the edge state and the associated band bending by altering the edge termination of MoS_2/gr/Ir(111) and investigate the resulting changes in the electronic structure by Scanning Tunneling Microscopy and Spectroscopy (STM and STS) at 8 K.

Quasi-freestanding MoS_2 is grown on gr/Ir(111) by Molecular Beam Epitaxy (MBE). We prepare hexagonal islands that exhibit two geometrically different edge types (Mo- and S-type). We vary the chemical potential of sulfur and thereby modify the chemical environment of the boundaries. The partial charge at the perimeter depends on edge type as well as edge chemistry. In consequence, also the upward bending of both valence and conduction band shows distinct variations.

TT 45.4 Thu 11:15 H11

magnetic-field-induced dimensionality transition of charge density waves in strained 2H-NbSe2 — •Ryo Ichikawa[1], Yukiko Takahashi[2], Eiichi Inami[3], and Toyo Kazu Yamada[1,4] — [1]Department of Material Science, Chiba University — [2]National Institute for Material Science, Tsukuba — [3]School of system Engineering, Kochi University of Technology — [4]Molecular Chirality Research center, Chiba University

Layered transition metal dichalcogenides (TMDs) exhibit various correlated phases, including charge density waves (CDW), superconductivity, and magnetic orders. Bulk 2H-NbSe2 (2H niobium diselenide) is one of the most extensively studied TMDs, showing a triangular (3Q) incommensurate CDW with a 3a period in real space (3 * 3, TCDW ~ 33 K). Electric and magnetic fields have been used to manipulate spatial or time inversion symmetry, while the CDW in 2H-NbSe2 remains robust even under large magnetic fields on the order of tens of Tesla. However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe2, where a weak magnetic field of approximately 30 mT can switch the electronic phase within the thin film, resulting in a supercurrent diode effect. This study investigates the strained 2H-NbSe2 exhibiting the 2*2 CDW phase. We utilize low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) in ultrahigh vacuum (UHV). STS maps reveal the coherence of the 2*2 CDW patterns. However, applying an out-of-plane magnetic field induces a dramatic transformation akin to that observed in 1T-NbSe2, shifting the metallic 2D CDW pattern to a 1D CDW pattern.

TT 45.5 Thu 11:30 H11

Ultrafast phonons dynamics of monolayer transition metal dichalcogenides — •yiming pan and fabio caruso — Kiel University, Germany

Valley degrees of freedom in transition-metal dichalcogenides influence thoroughly electron-phonon coupling and its nonequilibrium dynamics. Here we present a time-resolved ab-initio study of the ultrafast dynamics of chiral phonons following carrier excitation with circularly-polarized light. By investigating the valley depolarization dynamics of monolayer MoS_2 and WS_2, we find that a population imbalance of carriers distributed at K and K' can lead to valley polarized phonons persisting beyond 10 ps, and characterized by a distinctive chirality [1]. Additionally, we find that strain can be exploited as a tool to control the phonon emission and the relaxation channels of hot carriers [2]. Finally, we briefly discuss available opportunities for experimental detection of these phenomena

[1] Y. Pan and F. Caruso, Nano Lett. 23, 7463 (2023)
[2] Y. Pan and F. Caruso, npj 2D Mater. Appl. 8, 42 (2024)

TT 45.6 Thu 11:45 H11

Probing Excitonic Properties and Structural Effects in WS_2-Graphene Heterostructures Using EELS and DFT-BSE Modeling — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Robin Günkel, Badrosadat Ojaghi Dogahe, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the excitonic properties of WS_2 epitaxially grown on graphene by metal-organic chemical vapor deposition. We focus on understanding the effects of structural changes, such as variations in the number of WS_2 layers. Using monochromatic electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), we observe in the monolayer region of WS_2 an excitonic spectrum with excitonic peaks at 2.0 eV and 2.4 eV, as well as additional spectral features at higher energies. Measurements in the bilayer region show a small redshift of these features due to the additional layer. Complementary density functional theory and Bethe-Salpeter calculations show that this redshift in the K-valley excitons is due to both a change in quantum confinement and a change in the WS_2 lattice constant, with the latter being the dominant effect. Using STEM, this lattice distortion can be attributed to the heteroepitaxial alignment of the lower WS_2 layer to the graphene substrate, while the upper layer is relaxed. This study provides valuable insights into the relationship between atomic structure and optical properties in complex material systems, providing essential knowledge for the design and optimization of 2D heterostructures for advanced device applications.

TT 45.7 Thu 12:00 H11

Optical excitations in 2H-MoS_2 bilayers under pressure — •Jan-Hauke Graalmann[1], Paul Steeger[2], Rudolf Bratschitsch[2], and Michael Rohlfing[1] — [1]University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]University of Münster, Institute of Physics and Center for Nanotechnology, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Theoretical and experimental investigations have shown several changes in the optical spectrum of the 2H-MoS_2 bilayer under pressure [1].

By using density functional theory (DFT) and many-body perturbation theory in combination with linear elasticity, our computational investigations show an effective shift of the A exciton under pressure. It is strongly connected to the behavior of the direct band gap at the K point, which shifts in energy under pressure. The direction of this shift depends on the stress condition. While a hydrostatic pressure leads to a blueshift, a suppression of the in-plane contraction, as it appears in diamond anvil cell-experiments due to the interaction between the sample and the substrate, shows a redshift.

Moreover, we observe a similar behavior for the interlayer exciton, whereas the shift rate is smaller than that of the A exciton, which results in a decreasing A-IL splitting for an increasing pressure.

[1] P. Steeger, J. Graalmann et al., Nano Lett., 23, (2023)

TT 45.8 Thu 12:15 H11

Visualizing and controlling charge states of metal nanoislands on a two dimensional semiconductor — •Junho Bang[1], Byeongin Lee[1], Jian-Feng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul, Korea — [2]Department of Topological Quantum Chemistry, Max Planck Institute for Chemical Physics of Solids, München ,Germany

Nanoscale objects show unique electronic behaviors when weakly coupled to electrodes. Coulomb blockade (CB) can occur in such systems, where the repulsive Coulomb interaction between electrons prevents additional electrons from entering the quantum dots, hindering their flow. Single electron tunneling occurs by these correlated electron transports, leading to the discrete charge states of objects in double barrier tunneling junctions. Despite enormous progress, challenges remain in precisely controlling the interplay between objects' charge states and tunneling dynamics under varying conditions. Here, we visualize the charge states and their spatial variation on the random array of the indium islands on two-dimensional semiconductor black phosphorus using scanning tunneling microscopy and spectroscopy. Our spatially resolved tunneling spectra reveal that the junction capacitance varies across the islands. Furthermore, we find that the CB features are visible outside the islands, which is attributed to the remote gating of the islands. Our work advances the manipulation of electron transport at the nanoscale, which will be helpful in the application of nanoscale object-based single-electron devices.

TT 46: Transport Properties (joint session HL/TT)

Time: Thursday 15:00–17:15 Location: H13

TT 46.1 Thu 15:00 H13

Quasi-Ballistic Transport in Phase-Pure GaAs/InAs Core/Shell Nanowires — •Farah Basarić[1,2], Vladan Brajović[1,2], Gerrit Behner[1,2], Kristof Moors[1], William Schaarman[1], Raghavendra Juluri[3], Ana M. Sanchez[3], Hans Lüth[1,2], Detlev Grützmacher[1,2], Alexander Pawlis[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Core/shell GaAs/InAs nanowires represent tubular conductors due to their insulating core and confined conducting states in the InAs shell. We investigate nanowires with a crystalline phase purity of the InAs shell, where reduced scattering in electronic transport is expected. Low-temperature gate-dependent transport measurements give us insight into different contributions to the oscillatory behavior in the magnetoconductance, as well as the possibility to probe non-local transport phenomena due to large phase coherence length. With temperature-dependent measurements, we resolved the quasi-ballistic transport regime, and estimate the phase coherence length. Both measurements indicate superior transport properties of phase-pure GaAs/InAs nanowires in contrast to previous reports on non-phase pure nanowires. Our findings are an important optimization step for further development of nanowire-based hybrid devices.

TT 46.2 Thu 15:15 H13

Influence of defects and shape of thin InAs nanowires on their thermal conductivity, assessed via machine-learning potentials — •Sandro Wieser[1], Yujie Cen[1], Georg K. H. Madsen[1], and Jesús Carrete[2] — [1]Institute of Materials Chemistry, TU Wien, Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Nanowires (NWs) grown from the zincblende (ZB) phase of InAs in the (111) direction commonly contain twin boundary defects consisting of narrow wurtzite (WZ) (001) phase regions between ZB sections. To investigate the impact of these and other defects on heat transport, we employ Green-Kubo equilibrium molecular dynamics simulations utilizing cepstral analysis to efficiently process the noise, and an accurate MACE model trained via active learning strategies to achieve transferability for a wide range of surface conditions.

We show that these twin boundaries reduce the thermal conductivity with respect to that of defect-free WZ-phase (001) NWs by a factor of more than two and that surface conditions lead to lower thermal conductivity values for defect-free ultrathin InAs ZB NWs. Analysis of the shape of twinning NWs reveals that structures mimicking experimentally measured surface configurations can enhance heat transport compared to strictly hexagonal NWs. Additional insights are gained from an analysis of line-group symmetries and vibrational properties for various NW shapes. Furthermore, experimentally motivated symmetric and symmetry-breaking surface defects are studied to reveal more and less influential defect sites.

TT 46.3 Thu 15:30 H13

Ab-initio heat transport in defect-laden quasi-1D systems from a symmetry-adapted perspective — •Yujie Cen[1], Sandro Wieser[1], Georg Kent Hellerup Madsen[1], and Jesús Carrete Montaña[2] — [1]Institute of Materials Chemistry, TU Wien, A-1060 Wien, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

Due to their aspect ratio and wide range of thermal conductivities, nanotubes hold significant promise as heat-management nanocomponents. However, one major limitation preventing their widespread use is the typically high thermal resistance that arises from defects or contact with other materials. An intriguing question is the role that structural symmetry plays in thermal transport through those defect-laden sections. However, the ab-initio study of lattice thermal transport is hindered by factors such as the large number of atoms involved and the artifacts introduced by formalism designed for 3D systems.

We employ an Allegro-based machine learning potential to calculate the force constants and phonons of single and multi-layer MoS_2-WS_2 nanotube with near-DFT accuracy and efficient scaling. Subsequently, we combine representation theory with the mode-resolved Green's function method to calculate detailed phonon transmission profiles across defects, and connect the transmission probability of each mode to structural symmetry. while more drastic symmetry breakdowns might be expected to increase scattering and thermal resistance, our results show they actually reduce it by the suppression of selection rules and opening more phonon transmission channels.

TT 46.4 Thu 15:45 H13

Analysis of the electrical transport properties of MBE grown cubic Galliumnitride (c-GaN) sample structures — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor system for 'more-than-Moore' applications such as high-power electronics or optoelectronic devices. The analysis of its electrical transport properties is challenging since the molecular beam epitaxy (MBE) growth of high-quality c-GaN thin films requires a complex substrate architecture in order to accommodate the lattice mismatch between c-GaN and the 3C-SiC template. However, a reliable characterization of the electrical transport properties of c-GaN is crucial for the design of advanced functional devices. Here we analyze the electrical transport properties of the whole sample structure (MBE grown c-GaN/c-AlN thin films onto a 3C-SiC/Si template) with different c-GaN thicknessses using electrochemical impedance spectroscopy (EIS) as well as angle- and temperature-dependent magnetoresistance (MR) measurements. MR measurements reveal the existence of a highly conductive channel while EIS measurements allow the determination of the position of the channel between the c-AlN thin film and the 3C-SiC layer.

15 min. break

TT 46.5 Thu 16:15 H13

Fabrication and Characterisation of Short-channel Junctionless Nanowire Transistors — •Alessandro Puddu — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The downscaling limitations of conventional planar transistors require the investigation of alternative device configurations. Because of their excellent electrostatic control and intrinsic scalability, junctionless nanowire transistors (JNTs) present a feasible solution and are highly desirable for next-generation electronics. The key factor that characterizes the JNTs is the absence of pn-junctions. This provides several benefits, such as an easier fabrication process since the devices do not require abrupt doping profiles within the nanowire channel, which is now uniformly doped.

This work focuses on the fabrication and characterisation of short-channel Si JNTs. A top-down approach based on e-beam lithography (EBL) and inductively coupled plasma reactive ion etching (ICP-RIE) was used to fabricate the Si nanowires. The device characterisation showed improved performances due to the channel length shrinking.

TT 46.6 Thu 16:30 H13

***Ab initio* investigation of drag effect in germanium** — •Dwaipayan Paul and Nakib Protik — Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany

In a system of interacting electrons and phonons, the transport of one induces transport in the other. This phenomenon is known as the electron-phonon drag effect [1]. Now, an important milestone in the history of drag physics is the first recorded measurement of this phenomenon in germanium [2]. Here we present the results of our *ab initio* computations of the thermoelectric transport coefficients of germanium for various temperatures and charge carrier concentrations using the `elphbolt` code [3]. We investigate how the various scattering channels in the system enable this material to exhibit strong drag phenomena.

[1] Gurevich, Yu G., and O. L. Mashkevich. "The electron-phonon drag and transport phenomena in semiconductors." Physics Reports 181.6 (1989): 327-394.

[2] Frederikse, H. P. R. "Thermoelectric power of germanium below room temperature." Physical Review 92.2 (1953): 248.

[3] Protik, Nakib H., et al. "The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations." npj Computational Materials 8.1 (2022): 28.

TT 46.7 Thu 16:45 H13

Anomalous Knudsen effect signaling long-lived modes in 2D electron gases — •Grigorii Starkov and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

Careful analysis of electron collisions in two spatial dimensions leads to the conclusion, that the odd harmonics of the electron distribution function decay much slower in comparison to the even ones at finite temperatures. Focusing on a channel geometry with boundary scattering, we show, that such behaviour of

the odd decay rates leads to a characteristic behaviour of the resistance that we dub anomalous Knudsen effect: increasing temperature leads to decreasing resistance, that quickly slows down and turns into growth. The further increase of temperature exhibits the usual Gurzhi peak in the resistance related to the crossover from ballistic to hydrodynamic transport. The simultaneous observation of the Gurzhi peak preceded by an anomalous Knudsen dip can serve as a concrete signature of the long-lived modes in the 2D electron transport at low temperatures.

TT 46.8 Thu 17:00 H13

Quantum confinement and stoichiometry fluctuations in nm-thin SiGe layers — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

We simulate biaxially strained SiGe layers of varying thickness in the range of a few nanometers, as found in the base layer of heterojunction bipolar transistors (HBTs). At this length scale, local fluctuations in atomic concentrations can strongly influence the electronic properties of the device, especially the distribution of dopants like e.g. boron. Even at high doping concentrations, only a single atom is present at a 1 nm^2 cross section of the layer on average.

Employing a new parameterization of silicon and germanium in the framework of extended Hückel theory (EHT), we calculate the local band gap for different permutations of the atomic structure. Various distributions of boron atoms are simulated. We study the impact of locally increased and decreased concentrations on the band gap. By varying layer thickness, we evaluate the effects of quantum confinement and how it impacts transport properties of the thin layer in contrast to bulk material.

TT 47: Fluctuations, Noise and Other Transport Topics (joint session TT/DY)

Time: Thursday 15:00–18:30 Location: H31

TT 47.1 Thu 15:00 H31

Noise and reliability characterization of ferroelectric field-effect transistors under cryogenic conditions — •Yannick Raffel[1], Shouzhuo Yang[1], Oliver Ostien[1], Maik Simon[1], Thomas Kämpfe[1], Konrad Seidel[1], Maximilian Lederer[1], and Johannes Heitmann[2] — [1]Fraunhofer Institute IPMS-CNT, Dresden, Germany — [2]TU Bergakademie Freiberg, Freiberg, Germany

This study explores the impact of defects in the ferroelectric (FE) hafnium oxide (HfO_2) layer on the low-frequency noise (LFN) characteristics of HfO_2-based ferroelectric field-effect transistors (FeFETs), which show great potential as memory devices for quantum computing applications under cryogenic conditions. The investigation focuses on device degradation and material-dependent changes under various temperature conditions, including cryogenic temperatures as low as 2 K. A clear link between device reliability and flicker noise was identified. Initially, the endurance of the devices was evaluated across a range of temperatures, including cryogenic conditions. Subsequently, their data retention behavior was characterized, revealing a notably prolonged electron detrapping time at 2 K. In addition, flicker noise trends were analyzed and discussed, shedding light on key factors influencing device optimization and reliability.

TT 47.2 Thu 15:15 H31

Charge dissipation in Josephson systems and its impact on phase diffusion — •Johannes Hauff, Joachim Ankerhold, and Dominik Maile — Institut für komplexe Quantensysteme, Universität Ulm

We theoretically investigate the dynamics of the Josephson phase for different quantum circuits in the presence of dissipative couplings. Thereby, we study the environmental assisted quantum tunneling of the superconducting phase in a current-biased Josephson junction and consider Ohmic resistors inducing dissipation both in the phase and in the charge of the quantum circuit. We find that the charge dissipation leads to an enhancement of the quantum escape rate, which is strongly dependent on the shape of the potential. This effect appears already in the low Ohmic regime and also occurs in the presence of phase dissipation that favors localization [1]. Inserting realistic circuit parameters, we address the question of its experimental observability, the impact of temperature and discuss suitable parameter spaces for the observation of the enhanced rate. Furthermore, we show how the interplay of thermal and quantum fluctuations in such nonlinear systems can lead to an interesting stochastic cooling process. In this context, we also discuss the relevance of dissipative couplings for quantum annealing procedures.

[1] D. Maile et al., Phys. Rev. B 106, 045408 (2022)

TT 47.3 Thu 15:30 H31

Thermodynamic and energetic constraints on out-of-equilibrium tunneling rates — Ludovico Tesser[1], •Matteo Acciai[2,1], Christian Spånslätt[3,1], Inès Safi[4], and Janine Splettstoesser[1] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy — [3]Department of Engineering and Physics, Karlstad University, Karlstad, Sweden — [4]Laboratoire de Physique des Solides, CNRS-Université Paris-Sud and Paris-Saclay, Orsay, France

We consider a bipartite quantum system, where the two parts are kept at different temperatures and are connected by a tunnel coupling. In this setup, we show that the out-of-equilibrium tunneling rates between the two subsystems (depending on the applied temperature bias) are bounded by two constraints. The derived bounds are related to the dissipated heat and the absorbed energy neede to establish and deplete the temperature bias, thus providing a thermodynamic and energetic constraint on the tunneling rates.

Except for the restriction to the tunneling regime, our results are valid for arbitrary Hamiltonians of the two subsystems, that can include generic many-body interactions. The derived bounds thus apply to a large class of systems, such as molecular junctions and coupled cavities, and can be tested by measuring the out-of-equilibrium tunneling current and its fluctuations.

Based on: arXiv:2409.00981

TT 47.4 Thu 15:45 H31

Colored noise Langevin equation for photon counting — •Steven Kim and Fabian Hassler — Institute for Quantum Information, RWTH Aachen, Germany

For open quantum systems, obtaining the photon counting statistics of the emitted radiation is central to obtain insights into phenomena such as entanglement and correlations, in particular super- and anti-bunching. Typically, these systems are described by a Lindblad master equation, which allows the counting statistics to be derived from normal-ordered number operators. However, the Lindblad equation relies on the rotating wave approximation (RWA), which assumes that the dissipation rate is much smaller than the characteristic photon frequency. While this requirement is always fulfilled at optical frequencies, microwave cavities can have broader linewidths, making the RWA inaccurate. Alternatively, such systems can be effectively described by an equivalent Langevin equation with correlated (colored) noise, which bypasses the need for the RWA. In this work, we derive the photon counting statistics directly from the Langevin equation, providing a broader framework for understanding photon emission in open quantum systems.

TT 47.5 Thu 16:00 H31

Quantum stochastic resonance in a periodically-driven quantum dot — •Johann Zöllner[1], Hendrik Mannel[1], Eric Kleinherbers[2], Marcel Zöllner[1], Nico Schwarz[1], Fabio Rimek[1], Andreas Wieck[3], Arne Ludwig[3], Axel Lorke[1], Martin Geller[1], and Jürgen König[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Physics and Astronomy, University of California, Los Angeles — [3]Faculty of Physics and Astronomy, Ruhr University Bochum

The combination of periodic driving and fluctuations in a system with an inherent noise source leads to stochastic resonance, where the synchronization of the system dynamics with the external drive leads to an enhanced signal-to-noise ratio. This phenomenon has been found in many different noisy systems in palaeoclimatology, biology, medicine and physics. The classical stochastic resonance with thermal noise has recently been experimentally extended to the quantum regime, where the fundamental randomness of individual quantum events is the noise source [1]. Here we demonstrate quantum stochastic resonance in the single-electron tunneling dynamics of a periodically driven single self-assembled quantum dot, tunnel-coupled to an electron reservoir [2]. We extend the statistical evaluation to factorial cumulants to gain a deeper understanding of the transition between stochastic and deterministic transport through the quantum dot.

[1] T. Wagner et al., Nat. Phys. 15, 330 (2019).
[2] A. Kurzmann et. al., Phys. Rev. Lett. 122, 247403 (2019).

TT 47.6 Thu 16:15 H31

Curvature-assisted high harmonic generation in strongly-driven superconductors — •Björn Niedzielski and Jamal Berakdar — Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle/Saale 06099, Germany

Superconductors (SCs) under strong driving fields show inherently nonlinear dynamics, offering potential for nonlinear optics and high harmonic generation. However, the weak coupling of SCs to homogeneous transverse fields limits their efficiency. Here, we show that introducing curvature to mesoscopic type-II SC structures enables enhanced coupling to strong THz fields. Applied transport currents further allow for controlled emission of even and odd-order harmonic light modes.

The enhanced coupling of SCs and light arises from geometric and finite-size effects steering supercurrents while preserving the coherence of the SC state. Using the time-dependent Ginzburg-Landau framework, we simulate the dynamics of the superconducting order parameter in nanostructures with large coherence lengths under near-gap driving frequencies. Our simulations reveal the time-dependent supercurrents and their contributions to dipole radiation and high harmonic generation.

Our results highlight the role of the SC geometry and finite-size effects for amplifying nonlinear optical responses, offering a new method to use SCs for nonlinear THz optics.

15 min. break

TT 47.7 Thu 16:45 H31

Quantum oscillations in magneto-thermoelectrical conductivities of 2DEG: The Keldysh field-theoretical approach — •Kitinan Pongsangangan — Mahidol University, Bangkok, Thailand

The purpose of this work is to formulate a kinetic theory describing transport properties of interacting electrons in a uniform magnetic field of arbitrary magnitude. Exposing an electronic system to a constant magnetic field quenches its energy bands into a series of discrete energy levels, known as Landau levels. Following Keldysh formalism, we derive the quantum kinetic equation with the Landau-level basis. The Landau-level states, exact solutions of the Schroedinger equation in a constant background magnetic field, are natural and suitable basis to use, especially, for the investigation of strong-magnetic-field phenomena. In the weak-field limit, the lowest order approximation of the quantum kinetic equation reduces to a Boltzmann equation into which the magnetic field enters as the Lorentz force. As an application of our quantum transport equation, we calculate magneto-thermoelectric coefficients of a disordered two-dimensional electron gas (2DEG) in the quantum hall regime interacting with acoustic phonons.

TT 47.8 Thu 17:00 H31

Typical medium theory for disordered electronic systems on simple lattices with Cauchy distribution of on-site potentials — Andreas Ostlin[1], Hanna Terletska[2], Dylan Jones[1], and •Liviu Chioncel[1,3] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Middle Tennessee State University, Murfreesboro, Tennessee, USA — [3]ACIT, University of Augsburg, Augsburg, Germany

Effective medium approaches using single-site averaging procedures of various kinds contributed substantially in understanding the density of states of electronically disordered systems in models and materials. The nature and the conditions for appearance of single-particle (Anderson) localization seems to be qualitatively understood, yet discussions concerning special applied methods and quantitative results for the critical conditions are still ongoing. Here we present results using the typical medium theory for the one-particle and two-particle Green's function (conductivities) for the special case of Cauchy-distribution.

TT 47.9 Thu 17:15 H31

Dynamical current as tool to distinghuish degenerate spin states in open-shell graphene nanoribbons — •Nico Leumer, Thomas Frederiksen, and Geza Giedke — Donostia International Physics Center

The recent advances of surface synthesis unlocked the potential of open-shell physics in graphene nanoribbons (GNRs) which ever since have gained significant attention. Normally chemically unstable, these structures feature unpaired, localized p_z-electrons pinned at zero energy, giving rise to the unique phenomenon of π-magnetism. Intrinsically low spin-orbit/hyperfine interactions suppress spin relaxation, making GNRs ideal for tunable spin physics and spintronics applications. Although scanning probe techniques provide the necessary access to electron's spins and their interactions, state preparation, manipulation and detection remains an open challenge. Our ambition addresses the latter.

At half-filling certain GNRs host quasi degenerate spin singlets/triplets states with a vanishing energy gap for long ribbons. Without significantly increasing the gap, e.g., via magnetic fields, conventional current-based measurements hardly distinguish these spin textures. However, and even for absent gap, we demonstrate that in our setup $I(t)$ discriminates between the responsible states by exploiting the states's distinct spatial profiles. To probe the spatial information, we apply a constant bias between two STM tips. The scheme is suitable for single shot measurements and a quantum master equation (Hubbard model) accounts for the time evolution (GNR).

TT 47.10 Thu 17:30 H31

Josephson force in a vibrating carbon nanotube Josephson junction — •Andreas K. Hüttel[1,2], Jukka-Pekka Kaikkonen[2], Keijo Korhonen[2], and Pertti Hakonen[2] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Low Temperature Laboratory, Dept. of Applied Physics, Aalto University, Espoo, Finland

A single carbon nanotube suspended between superconducting electrodes acts simultaneously as nanomechanical resonator and as Josephson junction. Its energy-dependent density of states and thus displacement-dependent Josephson energy couple electronics and mechanics. Measurements on such a system display complex behaviour of the vibrational resonance with respect to junction biasing; strikingly, the resonance frequency decreases in a distinct parameter region where the bias is similar in size to the junction switching current.

We numerically solve the coupled differential equation system of the driven (via an ac gate voltage and an ac bias) system for realistic device parameters, using highly parallelized Julia code, and characterize the evolving steady state. Specific attention is given to the effect of the Josephson junction behaviour on the mechanical resonance frequency and the vibration amplitude. In the numerical results, we observe a clear impact of superconductivity on the mechanical response, with a rather counterintuitive dependence on externally tunable parameters.

TT 47.11 Thu 17:45 H31

Tunable nonlinear Duffing response of a driven carbon nanotube nanomechanical resonator — •Akong Loh, Furkan Özyigit, Fabian Stadler, Katrin Burkert, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Extremely lightweight and with very high quality factors, Carbon nanotube nanomechanical resonators have been used as ultrasensitive force, mass, and charge sensors [1-5]. When suspended on source and drain leads and gated, a CNT nanomechanical resonator can also be operated as a quantum dot. The motion of the nanotube is strongly coupled to single electron tunneling, dominating the nonlinear response [1-5]. Control of the strong nonlinear dynamics of a CNT will be useful for engineering mechanical qubits with information stored in the vibrations and mechanical Schrödinger's cat states [3]. Here, we analyze the nonlinear vibrational response of a driven CNT quantum dot, at ~10mK in a dilution refrigerator and with opaque tunnel barriers to minimize dissipation. We demonstrate how the nonlinearity parameters of the coupled system can be controlled via Coulomb blockade and the associated gate voltage, leading to a rich interplay of frequency, damping, and Duffing behavior.

[1] A. K. Hüttel *et al.*, Nano Lett. 9, 2547 (2009).
[2] G. A. Steele *et al.*, Science 325, 1103 (2009).
[3] C. Samanta *et al*, Nat. Phys. 19, 1340 (2023).
[4] S. Blien *et al.*, Nat. Commun. 11, 1636 (2020).
[5] N. Hüttner *et al.*, Phys. Rev. Appl. 20, 064019 (2023).

TT 47.12 Thu 18:00 H31

Vibrational instabilities in molecular nanojunctions: A mixed quantum-classical analysis — •Martin Mäck, Samuel Rudge, Riley Preston, and Michael Thoss — Institute of Physics, University of Freiburg

Understanding the current-induced vibrational dynamics in molecular nanojunctions is critical for gaining insight into the stability of such systems. While it is well known that Joule at higher bias voltages plays an important role for the stability of the nanojunction, a different mechanism caused by current-induced nonconservative forces has been reported to cause vibrational instabilities already at much lower voltages [1].

In this contribution, we apply a mixed quantum-classical approach based on electronic friction and Langevin dynamics [2,3] to a model system for which vibrational instabilities have previously been reported. Such a mixed quantum-classical description has the benefit of giving valuable insight into the electronic forces acting on the molecular vibrations. We analyze the possible occurrence of vibrational instabilities and compare our results to previous approaches, which were limited to small amplitude motion of the vibrational degrees of freedom [1].

[1] J.-T.Lü, M.Brandbyge, P.Hedegård, Nano Lett. **10**, 1657 (2010).
[2] S.L.Rudge, C.Kaspar, R.L.Grether, S.Wolf, G.Stock, M.Thoss, J.Chem. Phys.**160**, 184106 (2024).
[3] R.J.Preston, D.S.Kosov, J.Chem.Phys.**158**, 224106 (2023).

TT 47.13 Thu 18:15 H31

Vortex shedding in superfluid He-4 and in a Bose-Einstein condensate — •Wilfried Schoepe — Fakultät für Physik, Universität Regensburg, D-93040 Regensburg, Germany

Our experiments on vortex shedding from a microsphere oscillating in superfluid He-4 at mK temperatures is compared with experiments on vortex shedding from a laser beam moving in a Bose-Einstein condensate as observed by other authors. In either case a linear dependence of the shedding frequency fv=a(v-vc) is observed a above some critical velocity vc for the onset of turbulence and the

coefficient a is proportional to the oscillation frequency f above some characteristic value and assumes a finite value for steady state motion f=0. An analytical relation between the superfluid Reynolds number and the superfluid Strouhal number is presented.

TT 48: Topology: Majorana Physics

Time: Thursday 15:00–16:30 Location: H32

Invited Talk TT 48.1 Thu 15:00 H32

Optical Conductivity as a Probe for Chiral Majorana Edge Modes — •Lina Johnsen Kamra[1,2,3], Bo Lu[4], Jacob Linder[1], Yukio Tanaka[5], and Naoto Nagaosa[6] — [1]Norwegian University of Science and Technology, Trondheim, Norway — [2]Universidad Autónoma de Madrid, Madrid, Spain — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Tianjin University, Tianjin, China — [5]Nagoya University, Nagoya, Japan — [6]RIKEN, Saitama, Japan

Recent years have seen considerable progress towards realizing nonabelian particles for topological quantum devices. A prominent example is the chiral Majorana mode at the edge of topological superconductors. It introduces the possibility of using wave packets propagating at high speed as an alternative to the braiding of zero-dimensional Majorana bound states. However, a weak spot in detecting them lies in reliably capturing quantitative measures such as a quantized conductivity. Recent advances in microwave microscopy [1] have opened a promising new avenue for observing distinct qualitative signatures in their optical conductivity [2,3]. These emerge due to the unique dispersion of the Majorana edge mode that allows photons to break up Cooper pairs into propagating Majorana fermions [2]. As a guide to future experiments, we have shown how the local optical conductivity presents distinct and tunable qualitative features that depend on the symmetry of the superconductivity [3].

[1] K. Lee et al., Sci. Adv. 6, eabd1919 (2020);
[2] J. J. He et al., Phys. Rev. Lett. 126, 237002 (2021);
[3] L. J. Kamra et al., Proc. Natl. Acad. Sci. 121, e2404009121 (2024).

TT 48.2 Thu 15:30 H32

Interedge backscattering in time-reversal symmetric quantum spin Hall Josephson junctions — •Cajetan Heinz[1], Patrik Recher[1,2], and Fernando Dominguez[1,3] — [1]Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, D-38106 Braunschweig, Germany — [3]University of Würzburg, D-97074 Würzburg, Germany

Using standard tight-binding methods, we investigate a novel backscattering mechanism taking place on quantum spin Hall N'SNSN' Josephson junctions in the presence of time-reversal symmetry. This extended geometry allows for the interplay between two types of Andreev bound states (ABS): the usual phase-dependent ABS localized at the edges of the central SNS junction *and* phase-independent ABS localized at the edges of the N'S regions. Crucially, the latter arise at discrete energies E_n and mediate a backscattering process between opposite edges on the SNS junction, yielding gap openings when both types of ABS are at resonance. In this scenario, a 4π-periodic ABS decouples from the rest of the spectrum, and thus, it can be probed preventing the emission to the quasicontinuum. Interestingly, this backscattering mechanism introduces a new length scale, determining the ratio between 4π- and 2π-periodic supercurrent contributions and distorts the superconducting quantum interference (SQI) pattern. Finally, to prove the participation of these ABS, we propose to use a magnetic flux to tune E_n to zero, resulting in the selective lifting of the fractional Josephson effect.

TT 48.3 Thu 15:45 H32

Geometric measure of entanglement in systems with poor man's Majorana modes — •Vimalesh Vimal and Jorge Cayao — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

The physical realization of minimal Kitaev chains has recently opened an alternative avenue for engineering Majorana physics with interesting applications in quantum computing. Central to these applications is the utilization of the Majorana-like quasiparticles in these systems, known as poor man's Majorana modes, for realizing qubits and highly entangled states. In this work we consider a minimal Kitaev chain hosting poor man's Majorana modes and investigate the generation of maximally entangled quantum states by using an entirely geometric approach [1]. In particular, for pure states, the geometric measure of entanglement is quantified by its distance from the nearest separable state and provides an advantageous approach for quantifying entanglement in multipartite mixed states, in contrast to conventional bipartite measures. We characterize regimes with maximally entangled states, which surprisingly emerge with and without poor man's Majorana modes. We also discuss the generation and control of maximally entangled states by the Josephson effect in a Josephson junction based on minimal Kitaev chains. Our work thus demonstrates the potential of minimal Kitaev chains for applications in quantum information.

[1] V. K. Vimal and J. Cayao, Manuscript in preparation.

TT 48.4 Thu 16:00 H32

Emerging Majorana bound states in superconducting Haldane nanoribbons — •Simone Traverso[1], Niccolò Traverso Ziani[1], Maura Sassetti[1], and Fernando Dominguez[2] — [1]Physics Department, University of Genoa and CNR-SPIN, 16146 Genoa, Italy — [2]Faculty of Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, 97074 Würzburg, Germany

In the rapidly evolving field of quantum technologies, topological superconductors are promising platforms for topologically protected quantum computation. In this context, manipulating Majorana bound states (MBSs) would be a significant breakthrough.

We introduce a novel approach to designing MBSs, based on the geometric confinement of 2D nodal topological superconductors. We illustrate this mechanism in a superconducting extension of the Haldane model. In 2D, the model displays a nodal topological superconducting phase with chiral Majorana modes. However, by confining one of the dimensions the bulk bands gap out faster than the edge states, allowing for their hybridization and potentially resulting in Majorana zero modes. We assess their emergence by computing the topogical invariant for the quasi-1D setup and inspecting the energy spectrum of open flakes. Their topological nature is confirmed by the zero bias conductance in a normal-superconducting junction, precisely quantized to $2\frac{e^2}{h}$ in presence of an MBS. Our findings indicate quantum confinement as a crucial ingredient for developing quasi-1D topological superconducting phases starting from 2D nodal topological superconductors.

TT 48.5 Thu 16:15 H32

Absence of gapless Majorana edge modes in few-leg bosonic flux ladders — •Felix A. Palm[1,2], Cécile Repellin[3], Nathan Goldman[2,4], and Fabian Grusdt[1] — [1]LMU Munich & MCQST, Munich, Germany — [2]Université Libre de Bruxelles, Brussels, Belgium — [3]Université Grenoble-Alpes, Grenoble, France — [4]Laboratoire Kastler Brossel, Collège de France, Paris, France

Non-Abelian phases of matter, such as certain fractional quantum Hall states, are a promising framework to realize exotic Majorana fermions. Quantum simulators provide unprecedented controllability and versatility to investigate such states, and developing experimentally feasible schemes to realize and identify them is of immediate relevance. Motivated by recent experiments, we consider bosons on coupled chains, subjected to a magnetic flux and experiencing Hubbard repulsion. At magnetic filling factor $\nu = 1$, similar systems on cylinders have been found to host the non-Abelian Moore-Read Pfaffian state in the bulk.

Here, we address the question whether more realistic few-leg ladders can host this exotic state and its chiral Majorana edge states. We perform extensive DMRG simulations and determine the central charge of the ground state. While we do not find any evidence of gapless Majorana edge modes in systems of up to six legs, exact diagonalization of small systems reveals evidence for the Pfaffian state in the entanglement structure. By systematically varying the number of legs and monitoring the appearance and disappearance of this signal, our work highlights the importance of finite-size effects for the realization of exotic states in experimentally realistic systems.

TT 49: Graphene and 2D Materials (joint session TT/HL)

Time: Thursday 15:00–18:30 Location: H33

TT 49.1 Thu 15:00 H33

Magnetotransport of the Radial Rashba Spin-Orbit Coupling in Proximitized Graphene — •Wun-Hao Kang[1,2], Ming-Hao Liu[1,2], and Denis Kochan[2,3] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

Graphene-based van der Waals heterostructures take advantage of tailoring spin-orbit coupling (SOC) in the graphene layer by the proximity effect. The proximity effect can be effectively modeled by the tight-binding Hamiltonian involving novel SOC terms[1] and allows for an admixture of the tangential and radial spin-textures[2]. Taking such effective models we perform realistic large-scale magnetotransport calculations–transverse magnetic focusing–and show that there are unique qualitative and quantitative features allowing for an unbiased experimental disentanglement of the conventional Rashba SOC from its novel radial counterpart, called here the radial Rashba SOC. Along with that, we propose a scheme for a direct estimation of the Rashba angle by exploring the magneto response symmetries when swapping an in-plane magnetic field[3].

[1] M. Gmitra et al., Phys. Rev. B 93, 155104 (2016).
[2] K. Zollner et al., Phys. Rev. B 108, 235166 (2023).
[3] W.-H. Kang et al., Phys. Rev. Lett. 133, 216201 (2024).

TT 49.2 Thu 15:15 H33

Nonequilibrium Spin Transport in Graphene Proximitized by WSe_2 — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Spin-orbit coupling (SOC) in graphene is known to be negligibly weak, on the order of 0.1 meV, due to its composed atom, carbon, a light element of atomic number only 6. A decade ago, it was found that the SOC in graphene can be significantly enhanced simply by attaching it to a transition metal dichalcogenide of strong SOC, known as the spin-orbit proximity effect. Our recent theoretical work in collaboration with a transport experiment on graphene proximitized by WSe_2 reported a supporting number for the SOC as strong as 12.6 meV [1]. Inspired by this finding, here I present numerical results on nonequilibrium spin Hall accumulation in graphene/WSe_2 heterostructures based on the Landauer-Keldysh formalism [2]. Combined with the recently discussed radial Rashba SOC [3], nonequilibrium spin precession will be shown, paving an alternative way to realize the Datta-Das spin transistor.

[1] Q.Rao *et al.*, Nat. Commun. **14**, 6124 (2023);
[2] B.K.Nikolic *et al.*, Phys. Rev. Lett. **95**, 046601 (2005);
[3] W.-H.Kang,M.Barth,A.Costa,A.Garcia-Ruiz,A.Mrenca-Kolasinska, M.-H.Liu, D.Kochan, Phys. Rev. Lett. **133**, 216201 (2024).

TT 49.3 Thu 15:30 H33

Resistively Detected Electron Spin Resonance and g Factor in Few-Layer Exfoliated MoS_2 Devices — •Chithra H. Sharma[1,2], Appanna Parvangada[2], Lars Tiemann[2], Kai Rossnagel[1,3], Jens Martin[4], and Robert H. Blick[2,5] — [1]Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany — [5]University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA

MoS_2 has recently emerged as a promising material for enabling quantum devices and spintronic applications. In this context, the demonstration of resistively detected electron spin resonance (RD-ESR) and the determination and improved physical understanding of the g factor are of great importance. However, its application and RD-ESR studies have been limited so far by Schotttky or high-resistance contacts to MoS_2. Here, we exploit naturally n-doped few-layer MoS_2 devices with ohmic tin (Sn) contacts that allow the electrical study of spin phenomena. Resonant excitation of electron spins and resistive detection is a possible path to exploit the spin effects in MoS_2 devices. Using RD-ESR, we determine the g factor of few-layer MoS_2 to be ≈1.92 and observe that the g factor value is independent of the charge carrier density within the limits of our measurements.

TT 49.4 Thu 15:45 H33

Unifying Recent Experiments on Spin-Valley Locking in TMDC Quantum Dots — Aakash Shandilya[1], Sundeep Kapila[2], Radha Krishnan[3], Bent Weber[3], and •Bhaskaran Muralidharan[2] — [1]Department of Physics, IIT Bombay, Powai, Mumbai-400076, India — [2]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [3]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

The spin-valley qubit promises significantly enhanced spin-valley lifetimes due to strong coupling of the electrons* spin to their momentum (valley) degrees of freedom. Very recently, few experiments on TMDC quantum dots have, for the first time, shared evidence for spin-valley locking at the few-electron limit. Employing quantum transport theory, we numerically simulate the ground- and excited-state transport spectroscopy signatures of these experiments under diverse conditions through a unified theoretical framework, and reveal the operating conditions, based on intrinsic properties, for spin- valley locking. We thus provide a method to experimentally deduce the degree of spin-valley locking based on the SOC strength, inter-valley mixing, and the spin and valley g-factors. Our theoretical analysis provides an important milestone towards the next challenge of experimentally confirming valley-relaxation times using single-shot projective measurements.

[1] A.Shandilya, S.Kapila, R.Krishna, B.Weber B.Muralidharan, ArXiv:2410.21814 (2024).

TT 49.5 Thu 16:00 H33

Estimation of Relaxation Parameters of Spin-Valley Qubits Via Readout Simulations — •Sundeep Kapila, Aparajita Modak, and Bhaskaran Muralidharan — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

Two dimensional (2D)-material quantum dot systems, can host multiple qubit possibilities, namely, spin, valley and the spin-valley qubits. The spin-valley qubit, often referred to as the Kramers qubit, is of special interest due to the possibility of long relaxation and coherence times. Experimentally, such long relaxation times (T_1) have been demonstrated in the bilayer graphene (BLG) platform via Elzerman single-shot readout techniques [1-3]. However, there is a lack of comprehensive synergy in explaining the experimental trends in the relaxation times of different types of qubit possibilities, especially at low magnetic fields [1-3]. Here, we present a detailed master equation-based simulation approach to mimic the Elzerman readout schemes to understand the experimental data presented and to characterize the relaxation processes. Our approach allows us to directly extract from the experimental data, the relaxation rates for individual decay processes. We then extend our analysis to unify various experimental data observed across varying conditions in the BLG platform [1-3]. Our analysis backed up by dedicated machine learning algorithms also enables the extension of the model to qubit systems in the transition metal dichalcogenide platform.

[1] Ennslin et al., Arxiv, Mar 2024
[2] Stampfer et al., Arxiv, Feb 2024
[3] Stampfer et al., Nat. Commun. (2022)

TT 49.6 Thu 16:15 H33

Quantum transport in graphene-based Chern mosaics — •Patrick Wittig[1], Fernando Dominguez[1,2], and Patrik Recher[1,3] — [1]Institute of Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Faculty of Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, 97074 Würzburg, Germany — [3]Laboratory of Emerging Nanometrology, 38106 Braunschweig, Germany

Chern mosaics [1] are systems composed of domains with different Chern numbers within the bulk of the material. Here, the difference in the Chern number between neighboring domains leads to the emergence of chiral boundary modes that propagate along their interface. In our research, we construct a phenomenological scattering network theory based on the symmetries of the system to model the propagation of these chiral modes in triangular and kagome lattice structures, which can arise in graphene-based systems with characteristic valley-chiral edge modes. In particular, we investigate effects such as energy-dependent scattering [2] and spin-orbit coupling [3] within these networks to analyze the spectrum and transport properties.

[1] S. Grover et al., Nat. Phys. **18**, 885 (2022).
[2] P. Wittig et al., Phys. Rev. B **108**, 085431 (2023).
[3] P. Wittig et al., Phys. Rev. B **109**, 245429 (2024).

TT 49.7 Thu 16:30 H33

Effects of relaxation in deformed graphene structures — Jan Verlage[1], Thomas Stegmann[2], and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, Mexico

It is known that locally deformed graphene creates strong pseudomagnetic fields (of over 100 T) giving rise to Landau levels and being crucial elements of various valleytronic devices. However, taking into account the atomic relaxation of such structures may lead to reduction and regularization of the strain. Here, we revise these effects in various previously studied setups, including membranes and bumps. Our numerical simulations indicate that the atomic relaxation induces a reduction of the pseudomagnetic field by a factor of $5 \div 10$. It may have several consequences for applications.

15 min. break

TT 49.8 Thu 17:00 H33

Landau level mixing in moderately disordered graphene junctions — •Yu-Ting Hsiao and Ming-Hao Liu — Department of Physics,National Cheng Kung University,Tainan 70101,Taiwan

Landau levels are quantized eigenenergy levels in two-dimensional (2D) systems in the presence of an applied perpendicular magnetic field. They are the basic origin of the (integer) quantum Hall effect (QHE). To observe the QHE, i.e., electrical conductance quantized into a sequence of an integer multiple of the universal conductance quantum $\nu * \frac{e^2}{h}$, the sample quality and the strength of the magnetic field typically play the most decisive roles. The cleaner the sample, the weaker the magnetic field required to form the Landau levels. Collaborating with the experiment group led by Prof. Wei Yang from the Institute of Physics(CAS), China, who observed phase shifts of quantized conductance plateaus in ultra-clean two-terminal, single-gated graphene devices. From our quantum transport simulations with a systematic tuning of different parameters that could influence the conductance behavior of the graphene device, we found that the experimentally observed phase shift shall arise from the mixing of Landau levels across two neighboring regions with slightly different doping concentrations. Interestingly, we found that the Landau level mixing occurs only when the graphene sample is moderately disordered. In the purely ballistic regime or under strong disorder, the Landau levels mixing fails to form. Our finding reveals a counter-intuitive role played by disorder, possibly also required in other fundamental transport phenomena, such as the Shubnikov-de Haas oscillation.

TT 49.9 Thu 17:15 H33

Dirac meets flat bands: Topological Mottness swap over through hybridization control — Siheon Ryee[1], •Niklas Witt[2,1,3], Lennart Klebl[2,1], Jennifer Cano[4,5], Giorgio Sangiovanni[2], and Tim Wehling[1,3] — [1]Universität Hamburg — [2]JMU Würzburg — [3]Hamburg Centre for Ultrafast Imaging — [4]Stony Brook University — [5]CCQ

Graphene-based multilayer systems provide a versatile platform to explore the interplay between correlation physics and topology. These systems' unique electronic properties arise from their low-energy bands, characterized by significant Berry curvature originating from graphene's Dirac bands, which is believed to play a crucial role in stabilizing emergent correlated states such as superconducting order and various pseudomagnetic states. In this work, we investigate single-site functionalized graphene, where the Dirac bands hybridize with a correlated flat band of localized orbitals. Our findings based on dynamical mean-field theory (DMFT) calculations reveal a hybridization-driven transition between two symmetry-distinct Mott insulators with a protected metallic state emerging in between. Density functional theory (DFT) calculations suggest that the topological transition observed in our model system is achievable in real materials, specifically through the proximity coupling of epitaxial graphene on SiC with group IV intercalants. Unlike phenomena in other correlated graphene-based platforms, such as twisted bilayer graphene and rhombohedral graphene multilayers, the topology-enforced Mottness swap over occurs at a much higher energy scale of electron-volts.

TT 49.10 Thu 17:30 H33

Magnetism in monolayer graphene near 1/4 doping — •Maxime Lucas, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France

Recent studies of twisted bilayer graphene (or other 2D materials) have been stimulated by the discovery of correlations between electronic flat-band states due to a moiré pattern [1]. It is shown experimentally and theoretically that the filling of the flat bands affects their magnetic properties significantly. On the other hand, the effect of doping on a simple graphene layer is still unclear. Indeed, its half-filled case is well known [2], but unlike other lattices [3] its magnetic properties beyond half filling are mostly unexplored, except at 1/4 doping [4]. Here, we present our analysis of graphene magnetism using a combination of the Hubbard model and Hartree-Fock mean-field theory. We work at density values around 1/4 doping (average number of electron per site N_e=0.75) as it puts the system right into one of the Van Hove singularities found in graphene's density of states, giving rise to interesting magnetic properties. We present an interaction-density phase diagram and its associated magnetic orders, described by their band structure and spin structure factor.

[1] Y. Cao et al., Nature 556, 43 (2018); Nature 556, 80 (2018).
[2] M. Raczkowski et al., Phys. Rev. B 101, 125103 (2020), and Refs. therein.
[3] R. Scholle et al., Phys. Rev. B 108, 035139 (2023).
[4] S. Jiang, A. Mesaros, Y. Ran, Phys. Rev. X 4, 031040 (2014).

TT 49.11 Thu 17:45 H33

Electronic transport and anti-super-Klein tunneling in few-layer black phosphorus — •Jorge Alfonso Lizarraga Brito[1], Yonatan Bentancur Ocampo[2], and Thomas Stegmann[1] — [1]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México — [2]Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México, México

The electronic transport of few-layer black phosphorus is analyzed theoretically. This work was performed using recent experimental results obtained by μ-ARPES, where tight-binding parameters up to the 4th nearest neighbors within and between the layers were estimated. It is confirmed that the anisotropic band structure of few-layer black phosphorus leads to highly anisotropic transport properties. Most prominently, it is found that the electrons can pass through a potential barrier aligned in a certain crystallographic direction, while for potential barriers rotated by 90 degrees, the transport is completely blocked (anti-super-Klein tunneling). Finally, the study was extended to the case where the top layer of the system is oxidized, showing that the electronic transport is significantly reduced in the oxidized layers, whereas it can be largely unaffected in the central layers.

TT 49.12 Thu 18:00 H33

Pressure-induced structural phase transitions in the van der Waals multiferroic $CuCrP_2S_6$ — •Swarnamayee Mishra[1] and Jochen Geck[1,2] — [1]Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062 Dresden, Germany

Two-dimensional (2D) crystals with strong in-plane covalent bonds and weak van der Waals (vdW) interlayer interactions have garnered significant attention following the discovery of graphene and its remarkable properties. $CuCrP_2S_6$ (CCPS) is a promising 2D material exhibiting antiferromagnetic behavior due to the collective ordering of Cr^{3+} spins and antiferroelectric properties driven by Cu+ ion ordering. As a type-I multiferroic, CCPS is particularly notable for its coexistence of antiferroelectricity and antiferromagnetism, coupled with strong polarization-magnetization interactions. These ferroic properties arise from spin-orbit coupling associated with crystal symmetry breaking. Despite its potential, a detailed pressure-dependent crystallographic study of CCPS remains unexplored. In this work, we address this gap using high-pressure single-crystal X-ray diffraction (XRD) to investigate the interplay between structural changes and the material's ferroic behaviors. Our study reveals a phase transition from the low-pressure monoclinic Pc phase to the high-pressure monoclinic C2/c phase at low temperatures, providing new insights into the structure-property relationships of this promising 2D vdW material.

TT 49.13 Thu 18:15 H33

^{31}P NMR studies of quasi-two-dimensional (2D) magnetic correlations in $ACrP_2S_6$ (A = Cu, Ag) — •Saramgi Sivan[1,2], Kizhake Malayil Ranjith[1], Lukas Prager[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2], and Hans-Joachim Grafe[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062

The $AA'P_2S_6$ (A, A' = transition metal ions) family of quasi-2D van der Waals materials has proven to be a model system for low-dimensional magnetism. Here we present detailed ^{31}P NMR measurements on the single crystals of $ACrP_2S_6$. The high-temperature single narrow NMR line shows a splitting at about 160 K for $CuCrP_2S_6$, which is attributed to the antiferroelectric (AFE) transition, while a pake-doublet NMR spectrum is observed for $AgCrP_2S_6$ at room temperature, but no AFE transition at lower temperatures. In $CuCrP_2S_6$, we observed further line splitting below 30 K, reflecting the antiferromagnetic (AFM) order. At T_N = 30 K, the NMR spin-lattice relaxation rate $T_1^{-1}(T)$ in $CuCrP_2S_6$ measured at 2.5 T shows a sharp peak due to the critical fluctuations. The T_N is suppressed towards lower temperatures when measured at higher magnetic fields. The $(T_1T)^{-1}(T)$ measured at 7 T shows a broad maximum at about 60 K and a critical enhancement at T_N. On the other hand, $AgCrP_2S_6$ exhibits in-plane AFM order at 20 K, as evidenced by the clear splitting of the NMR spectra, the divergence of $T_1^{-1}(T)$ at T_N, and a broad maximum in the NMR Knight shift. In contrast to $CuCrP_2S_6$, the $(T_1T)^{-1}(T)$ shows only a critical enhancement around T_N without a broad anomaly.

TT 50: Superconducting Electronics: SQUIDs, Qubits, Circuit QED II

Time: Thursday 15:00–18:30 Location: H36

TT 50.1 Thu 15:00 H36

Development of ultrasensitive dc SQUIDs with sub-micrometric circuit elements — •Mauro Esattore[1], Michael Paulsen[2], Jörn Beyer[2], Oliver Kieler[1], Mark Bieler[1], Patryk Krzysteczko[2], and Rainer Körber[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-10, 10587 Berlin, Germany

The dc SQUID is one of the most established applications of superconductor technology. Their sensitivity to magnetic flux allows for numerous applications, such as low-temperature thermometry or current sensing for electrical metrology. In this contribution, we present superconducting "fine-pitch" input coils with sub-micrometric parameters to be integrated into existing Nb/Al-AlO_x/Nb-based SQUID sensor designs. The aim is to reduce inductive losses of the signal-to-SQUID coupling, without compromising the overall device layout. In a SQUID current sensor, to maximize the inductive coupling constant k between the signal input coil and the SQUID loop means to achieve a low coupled energy sensitivity $\epsilon_c = (1/k^2)\times\epsilon$ - where ϵ is the SQUID-intrinsic energy sensitivity. Fine-pitch input coils will increase k, as well as extend the range of input coil inductances for our existing devices. The energy sensitivity $\epsilon \propto \sqrt{C}$: reduced Josephson junction (JJ) sizes will lower the capacitance C and improve ϵ_c. Thus, we are refining our JJ definition process to obtain JJs with sub-micrometric lateral size. The contribution will provide details on the fabrication process and design aspect of the sensors, as well as characterization results.

TT 50.2 Thu 15:15 H36

Superconducting Pb stripline resonators: Role of coupling and applications in spectroscopy — Elies Ben Achour, Cenk Beydeda, Gabriele Untereiner, Martin Dressel, and •Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Planar superconducting microwave resonators play an important role for various research directions in solid state physics and quantum technologies. Here we investigate superconducting lead (Pb) stripline resonators, which we probe at various harmonics between 0.7 GHz and 6 GHz and at temperatures between 1.5 K and 7 K.

We discuss on general grounds how the loaded quality factor Q_L of a planar microwave resonator made of a conventional superconductor should depend on temperature and frequency. We consider contributions due to dissipation by thermal quasiparticles Q_{QP}, due to residual dissipation Q_{Res}, and due to coupling Q_C. We focus on the role of coupling, and we compare resonators with different coupling capacitance. For the Pb resonators, we find a strongly frequency- and temperature-dependent Q_L, which we can describe by a lumped element model. For certain resonators at the lowest studied temperatures we observe a maximum in the frequency-dependent Q_L when Q_{Res} and Q_C match, and here the measured Q_L can exceed 2×10^5.

We also present the application of such Pb stripline resonators for microwave spectroscopy at temperatures down to the mK range.

TT 50.3 Thu 15:30 H36

Hybrid Microwave Resonators Integrated with van der Waals Superconductors — •Yejin Lee[1], Haolin Jin[1,2], Giuseppe Serpico[1,3], Tommaso Confalone[2,4], Berit Goodge[1], Edouard Lesne[1], Kornelius Nielsch[2,4], Nicola Poccia[3,4], and Uri Vool[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]University of Naples Federico II, Italy — [4]Leibniz Institute for Solid State and Materials Science Dresden, Germany

Superconducting microwave resonators are highly coherent devices that are extensively used in quantum circuits. Their robustness and sensitivity also make them excellent probes for exploring novel materials, which are coupled to them in a hybrid system. Particularly good candidates are van der Waals materials, whose microscopic size makes them incompatible with conventional bulk measurement methods. However, such hybrid platforms require the development of a new process to maintain the high quality of the circuit. We present a technique to integrate a microwave resonator with a superconducting thin van der Waals flake with a crystalline-preserved interface. We investigate their microwave response as a function of temperature under various microwave powers and magnetic field. The hybrid resonator exhibits a significant modification in its resonant mode with the presence of the flake while maintaining a high-quality factor. Hybrid superconducting circuits integrated with vdW crystals offer an extensive potential in probing materials' unique properties and for developing high-quality devices for quantum technology.

TT 50.4 Thu 15:45 H36

Two-level system involved nonlinear response in van der Waals hybrid microwave resonators — •Haolin Jin[1,3], Giuseppe Serpico[1,2], Yejin Lee[1], Berit Goodge[1], Edouard Lesne[1], Nicola Poccia[2,3], and Uri Vool[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of Naples Federico II, Italy — [3]Leibniz Institute for Solid State and Materials Science Dresden, Germany

Two-level system (TLS) bath is considered as the main loss channel in coplanar superconducting microwave resonators and is often associated with an upshift in resonance frequency as the temperature increases. The individual TLS can be saturated at the high input power, improving the quality factor of the resonator. However, the resonance frequency upshift remains unaffected by driving power because all TLS at different energy can contribute to the frequency shift, whereas only those close to the resonance frequency can be saturated. Here, we observed a positive nonlinearity in a van der Waals superconductor integrated hybrid resonator device. The hybrid device exhibited a significant upshift in resonance frequency with increasing temperature, indicating strong coupling to a TLS bath. It maintained a high-quality factor despite this coupling. These findings suggest that the resonance mode in the hybrid device is coupled to an off-resonant TLS bath and the hybrid system provides a new source of lossless nonlinearity unrelated to the Josephson effect. This work opens a path towards high quality hybrid superconducting circuits with vdW materials and highlights the development of new devices for quantum technology.

TT 50.5 Thu 16:00 H36

Dielectric waveguide setup tested with a superconducting millimeter-wave Fabry-Pérot interferometer at milli-Kelvin temperatures — •Jakob Lenschen[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie — [2]Institut für Quantenmaterialien und Technologie (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Superconducting quantum circuits operating at mm-wave frequencies of around 100 GHz may offer many interesting new possibilities. The order of magnitude higher photon energy compared to current implementations and the wider bandwidth would not only improve the resilience to thermal fluctuations, but could also speed up qubit manipulation. Millimeter-wave measurements at ultra-low temperatures are largely unexplored due to several technical difficulties, such as a difficult signal path isolation and thermalization. We have developed a cryogenic setup consisting of dielectric waveguides and a superconducting Fabry-Pérot cavity located at the dilution cryostat base temperature. We show that the quality of the mm-wave signal guided to and from a temperature of 10 mK is sufficient to measure resonator cavity quality factors of over one million at 110 GHz in the few photon limit.

TT 50.6 Thu 16:15 H36

Resonant escape in Josephson tunnel junctions under millimeter-wave irradiation — •Jonas N. Kämmerer[1], Sergei Masis[1], Karo Hambardzumyan[1], Philipp Lenhard[1], Urs Strobel[1], Jürgen Lisenfeld[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für QuantenMaterialien und Technologien (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Operating superconducting quantum circuits at mm-wave frequencies around 100 GHz promises several advantages. For example, it may allow for much higher operating temperatures above 1 K and faster qubit manipulation. We study the microwave-driven dynamics of a superconducting phase qubit made of Nb/AlO_x/Nb junction. In particular, we have measured the switching current distributions at radiation frequencies above 100 GHz and observed clear double-peak structures. The data indicate a resonant escape of the phase as well as an irradiation-induced suppression of the potential barrier. This behavior is well described by the strong-driving model of the resonant escape[1]. While being measured in the quasi-classical regime of thermally activated escape, our results point towards a feasibility of operating phase qubits at mm-wave frequencies.

[1] M.V.Fistul,A.Wallraff,A.V.Ustinov, Phys.Rev.B**68**, 060504 (2003).

15 min. break

TT 50.7 Thu 16:45 H36

Heat transport in the quantum Rabi model: Universality and ultrastrong coupling effects — Luca Magazzu[1], Elisabetta Paladino[2,3], and •Milena Grifoni[1] — [1]University of Regensburg — [2]Università di Catania, Italy — [3]INFN, Sez. Catania, Italy

Heat transport in a qubit-oscillator junction weakly coupled to heat baths displays a rich variety of effects depending on the junction parameters. Signatures of

the transition to the regime of ultrastrong qubit-oscillator coupling appear in the thermal conductance, current, and rectification. For example, upon increasing the coupling, the conductance as a function of a bias applied to the qubit undergoes a transition from a resonant to a broadened, zero-bias peak behavior. At low temperatures, coherent heat transfer via virtual processes yields a universal power-law behavior in the linear conductance as a function of the temperature. In addition, the low-temperature conductance is modulated by a prefactor which unravels the multilevel nature of the junction: A coherent suppression arises in the presence of quasi-degeneracies in the spectrum. At higher temperatures, sequential processes dominate heat transfer and a scaling regime is found when quantities are scaled with a coupling-dependent Kondo-like temperature.

[1] L.Magazzù, E.Paladino, M.Grifoni, Phys.Rev.B110, 085419 (2024);
[2] L.Magazzù, E.Paladino, M.Grifoni, arXiv:2403.06909 (2024).

TT 50.8 Thu 17:00 H36

Gauging away the ground-state photon content of the quantum Rabi model — •Arka Dutta, Daniel Braak, and Marcus Kollar — Theoretische Physik III, University of Augsburg

The quantum Rabi model (QRM) features the simplest type of coupling between a single cavity light mode and an atomic electron. It is integrable if the electronic degree of freedom is truncated to just two states [1]. The derivation of the effective Hamiltonian leads to different forms depending on the chosen gauge [2]. In the dipole gauge, the ground state of the QRM exhibits non-zero photon number in contrast to its weak coupling approximation, the Jaynes-Cummings model. We compute the exact photon content for all eigenstates in an arbitrary gauge and obtain a gauge for which the ground state contains no photons. Thus only this gauge fits the intuitive understanding that the cavity should be empty in the lowest energy state even for strong light-matter interaction.

[1] D. Braak, Phys. Rev. Lett. **107**, 100401 (2011).
[2] O. Di Stefano et al., Nat. Phys. **15**, 803 (2019).

TT 50.9 Thu 17:15 H36

Dispersive and dissipative interactions in niobium-based photon-pressure circuits — •Zisu Emily Guo, Mohamad el Kazouini, Janis Peter, Kevin Uhl, Dieter Koelle, Reinhold Kleiner, and Daniel Bothner — Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen

Photon-pressure (PP) circuits consist of one superconducting microwave resonator in the GHz range and one low-frequency (LF) circuit in the MHz range and are the cQED analog of cavity optomechanics. The LC circuits in a PP device are coupled to each other via a superconducting quantum interference device (SQUID), emulating an optomechanical interaction and offering access to sensing and control of MHz photons with potential applications in axion dark matter detection and quantum information technologies. Here, we report the realization of niobium- and nanoconstriction-based photon-pressure circuits operated in the thermal regime. In contrast to previous implementations, we observe in our experiments both dispersive and dissipative PP coupling - meaning that not only frequency but also linewidth modulations contribute significantly to the overall interaction. We investigate dynamical backaction effects with these dissipative contributions as well as sideband-cooling of the LF mode, measured through photon-pressure-induced transparency and output noise thermometry, respectively. Additionally, our circuit design with on-chip flux-bias line allows the parametric modulation of the LF mode resonance frequency, which may be used for LF squeezing and (phase-sensitive) amplification of the PP coupling rate.

TT 50.10 Thu 17:30 H36

Exact and Dispersive Models for Superconducting Networks — •Adrian Parra-Rodriguez — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain — Institut Quantique and Département de Physique, Université de Sherbrooke, Sherbrooke, Quebec J1K 2R1, Canada

In this presentation, I will address the construction of exact quantum mechanical models for quasi-lumped electrical networks [1,2], comprising (nonlinear) capacitors, inductors, nonreciprocal elements (circulators), and transmission lines (TLs). Traditional quantization methods, such as node-flux or loop-charge approaches, often lead to singularities and unphysical predictions, stemming from incorrect identification of the TLs' infinite-dimensional Hilbert space. Using a geometrical description [1] and the Faddeev-Jackiw method, we resolve these issues via a mixed charge-flux first-order quantization. I will also introduce a systematic method to construct effective dispersive Lindblad master equations for weakly anharmonic superconducting circuits coupled by generic linear nonreciprocal systems, deriving coupling parameters and decay rates from the coupler's immittance parameters [3]. Extending the work of Solgun et al. (2019) on reciprocal couplers, this approach includes nonreciprocal elements, stray coupling, and collective dissipative effects from external environments, while avoiding potential singularities.

[1] A. Parra-Rodriguez et al., Quantum 8, 1466 (2024);
[2] A. Parra-Rodriguezet al., arxiv:2401.09120;
[3] Labarca et al., Phys. Rev. App. 22, 034038 (2024).

TT 50.11 Thu 17:45 H36

Nonlinear High-Kinetic-Inductance Microstrips for Integrated Non-Reciprocal Devices — •Niklas Gaiser[1], Ciprian Padurariu[1], Björn Kubala[1,2], Nadav Katz[3], and Joachim Ankerhold[1] — [1]ICQ and IQST, University of Ulm, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany — [3]The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Superconducting microwave circuits offer a rich platform for many quantum information devices and quantum-technological applications. Recently, nonlinear properties of circuit elements have become of increasing interest as they allow new functionalities, such as frequency mixing or self-interaction of waves. Microstrip waveguides with high-kinetic-inductance, as experimentally realized in [1], possess strong nonlinear features. Moreover, they yield a greatly reduced phase velocity which addresses the challenge of long wavelengths in the microwave regime and enable highly compact and integrated on-chip solutions.

Here, we present a theoretical proposal for a devices that utilizes a nonlinear high-kinetic-inductance to achieve a non-reciprocal effect. Diode-like behaviour is proven with markedly dissimilar transmission spectra for signals propagating through the device in different directions. We discuss the nonlinearities' power dependence as well as the special boundary conditions posed by the nonlinear propagation problem.

[1] S. Goldstein, G. Pardo, N. Kirsh, N. Gaiser, C. Padurariu, B. Kubala, J. Ankerhold, N. Katz, New J. Phys. 24, 023022 (2022).

TT 50.12 Thu 18:00 H36

Observation and Modelling of Self-Sustained Oscillations in Non-Linear Cavity-Optomechanics — •Korbinian Rubenbauer[1,2], Shivangi Dhiman[4], Thomas Luschmann[1,2], Achim Marx[1,2], Rudolf Gross[1,2,3], Anja Metelmann[4,5], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]Institute for Theory of Condensed Matter and Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [5]Institut de Science et d'Ingénierie Supramoléculaires, University of Strasbourg and CNRS

Quantum sensing uses quantum elements or quantum principles to detect an external stimulus. In this context, cavity-electromechanics focuses on mechanical sensor elements dispersively coupled to a microwave resonator. This setting typically uses linear mechanical elements and linear microwave cavities. Here, we discuss the case of a non-linear or Kerr microwave resonator as a readout circuit. Our device integrates a mechanically compliant nanostring into a superconducting quantum interference device (SQUID), which is part of a flux-tunable superconducting resonator. This enables large tunable single-photon optomechanical coupling. We present an experimental and theoretical study investigating the impact of the Kerr nonlinearity on the device performance, particularly in the context of mechanical instabilities. We find excellent quantitative agreement.

TT 50.13 Thu 18:15 H36

Engineering Cooper Pair Bunching Using an Anharmonic Environment — •Surangana Sengupta[1], Björn Kubala[1,2], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]ICQ and IQST,Ulm University,Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

The electromagnetic environment of superconducting circuits provides exciting opportunities to engineer the tunneling of Cooper pairs. The simplest example is a dc biased Josephson junction in series with a microwave cavity. There has been extensive work showing that when the dc bias is chosen to be resonant with a well-defined cavity mode, the transport of Cooper pairs has the same statistics in the long time limit as that of the photon emission from the cavity mode [1].

In my talk, I extend this study to the case when the cavity mode is anharmonic. I investigate the case when the voltage bias is detuned from the transition between Fock states 0 and 1. Due to the anharmonicity however, this voltage can be resonant with half the transition between Fock states 0 and 2. Therefore, the process of coherent two-Cooper pair tunneling accompanied by two-photon creation is favored compared to single Cooper pair tunneling and single photon creation. This results in bunched Cooper pair tunneling, with Fano factor approaching $F = 2$, and in a squeezed cavity state. I will compare this effect to a similar and competing inelastic co-tunneling process arising from second-order rotating wave approximation.

[1] M. Hofheinz *et al.*, Phys. Rev. Lett. **106**, 217005 (2011).

TT 51: Topological Superconductors

Time: Thursday 16:45–18:15 Location: H32

TT 51.1 Thu 16:45 H32

Disentangling the Individual Junctions in Multi-Terminal Devices — •Josua Thieme[1,2], Nisha Shahi[1], Abdur Rehman Jalil[1], Benedikt Frohn[1], Detlev Grützmacher[1,2], and Peter Schüffelgen[1] — [1]Forschungszentrum Jülich, Germany — [2]RWTH Aachen, Germany

One avenue towards building a topological qubit, is by creating and manipulating Majorana zero modes in a hybrid device made from s-wave superconductors and 3D topological insulators (TIs). Such hybrid multi-terminal devices possess an increased number of interfaces and the coupling between all electrodes needs to be assured. We present low-temperature measurements of a TI-based three-terminal Josephson device fabricated by a combination of selective-are growth of $(BiSb)_2Te_3$ and shadow evaporation of Nb. This approach allows for the in-situ fabrication of Josephson devices with an exceptional interface quality, which is important for obtaining a strong proximity effect. In our measurements, we find quartet resonances, formed by two entangled Cooper pairs. Additionally, we present a method on how to disentangle the contributions of individual junctions in a multi-terminal device.

TT 51.2 Thu 17:00 H32

Non-Hermitian Topology in Multi-Terminal Superconducting Junctions — •Valentin Wilhelm, David Christian Ohnmacht, Hannes Weisbrich, and Wolfgang Belzig — Universität Konstanz, Konstanz, Germany

Recent experimental advancements in dissipation control have yielded significant insights into nonhermitian Hamiltonians for open quantum systems. Of particular interest are the topological characteristics exhibited by these non-hermitian systems, that arise from exceptional points–distinct degeneracies unique to such systems. In this study, we focus on Andreev bound states in multiterminal Josephson junctions with non-hermiticity induced by normal metal or ferromagnetic leads [1]. By investigating several systems of different synthetic dimensions and symmetries, we predict fragile and stable non-hermitian topological phases in these engineered superconducting systems.

[1] D.C. Ohnmacht, V. Wilhelm, H. Weisbrich, W. Belzig, arXiv:2408.01289 (2024).

TT 51.3 Thu 17:15 H32

Localized Edge States in Antiferromagnet-Superconductor Hybrid Structures — •Ignacio Sardinero[1,2], Yuriko Baba[1,2], Rubén Seoane-Souto[3], and Pablo Burset[1,2,4] — [1]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Sor Juana Inés de la Cruz, 3, 28049 Madrid, Spain — [4]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Topological superconductors (TSCs) are promising building blocks for robust and reliable quantum information processing [1]. Most approaches to implement TSCs focus on materials with intrinsic spin-orbit coupling (SOC). However, a recent alternative strategy relies on synthetically engineering spin orbit using spatially varying magnetic fields [2]. Such proximitized structures need to be carefully designed so that the magnetic and superconducting orders coexist, avoiding stray fields detrimental for superconductivity. Here, we circumvent this challenge by investigating the role of antiferromagnetic (AF) textures in proximity to 2-dimensional superconducting surfaces. Our results reveal that the interplay between AF order and the SC coherence length impacts the density of states at the Fermi level. We show that lattice symmetry plays a crucial role for emerging topological phases, with higher-order phases arising when interlayer SOC is considered.

[1] S. Das Sarma et al., npj Quantum Inf. 1, 15001 (2015);
[2] I. Sardinero, R. Seoane-Souto, P. Burset, PRB 110, L060505 (2024).

TT 51.4 Thu 17:30 H32

Proximity-Induced Superconductivity into Thin Films of Magnetic Topological Insulators — •Daniele Di Miceli[1,2], Eduárd Zsurka[1,3], and Thomas Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Department of Physics, University of the Balearic Islands, E-07122 Palma, Spain — [3]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany

Inducing superconducting (SC) correlations into magnetic topological insulators (MTIs) is becoming a promising route toward topological superconductivity and the realization of topologically protected Majorana bound states. However, a detailed understanding of the proximity effect in such MTI-SC heterostructures is still missing.

To address this question, we have developed a theory for the SC pairing induced by a conventional BCS superconductor on top of a 3D MTI thin film. By performing a perturbation series expansion in the electron tunneling between the SC and the MTI, we computed the corrections to the normal and anomalous Green's functions in the MTI in terms of the unperturbed propagators in the two isolated materials. Since the latter can be obtained exactly as a solution to the Gor'kov equations, this makes it possible to evaluate the Green's functions in the full MTI-SC heterostructures.

Our results provide a detailed description of the induced pairing, in particular showing the existence of p-wave correlations in the MTI.

TT 51.5 Thu 17:45 H32

Topological Classification of Chiral Symmetric One Dimensional Interfaces — •Harry MullineauxSanders and Bernd Braunecker — University of St. Andrews, St. Andrews, United Kingdom

Low dimensional topological phases can be engineered by placing a scattering interface into a higher dimensional bulk where the in-gap bands of quasi low dimensional interface modes can be tuned to a topologically non-trivial phase. However the classification of such modes cannot be done through low-dimensional conventional methods due to the dimensional mismatch and local nature of the topological bands. We demonstrate that there exists a simple and efficient classification method through the local Green's function at the interface, that sidesteps numerically heavy real space computations. We show that the Green's function maintains the protecting symmetries of the Hamiltonian and produces the correct phase diagram, together with a formula disentangling the contributions to the topological invariant from the substrate and the interface. For illustration we apply our method to a model of a spiral magnetic interface in an s-wave superconductor. Furthermore we compare with an alternative classification scheme derived from the spatially reduced ground state projector and show that it can produce an erroneous topological classification due to gap closures driven by the strong entanglement between the internal and spatial degrees of freedom which are naturally contained in the local Green's function. [arXiv:2407.01223]

TT 51.6 Thu 18:00 H32

Role of Spin-Orbit Coupling on Topological Superconductivity from First Principles — •András Lászlóffy[1], Bendegúz Nyári[2], Levente Rózsa[1], László Szunyogh[2], and Balázs Újfalussy[1] — [1]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary

Recent developments on magnetic structures on superconductors paved the way to explore topological phases in real materials [1,2]. This was achieved by solving the Kohn-Sham-Dirac Bogoliubov-de Gennes equations within the Korringa-Kohn-Rostoker multiple scattering theory. By investigating 1D magnetic chains on superconductors we demonstrate that the spin-orbit coupling plays a key role in the formation of a topological phase, however, it is challenging to scale it up, because SOC is implicitly included in the Dirac equation. To circumvent this, we calculate the superconducting order parameter and the Shiba band structure of magnetic chains on a Ta overlayer on Nb. Ta has a very similar crystal structure and lattice constant to Nb. It is also a superconductor with a much smaller gap size and a considerably larger SOC. With varying the Ta layer thickness SOC can be tuned in a way which is in principle reproducible in experiments. We show that a few layers of Ta has tiny effects on the energy of the Yu-Shiba-Rusinov states of single adatoms, however, varying the SOC can tune the chains into a topologically non-trivial domain.

[1] Nyári et. al., PRB 108, 134512 (2023);
[2] Lászlóffy et. al., PRB 108, 134513 (2023).

TT 52: Nickelates and Other Complex Oxides

Time: Friday 9:30–11:15 Location: H31

TT 52.1 Fri 9:30 H31

High-temperature superconductivity and polymorph structures in $La_3Ni_2O_7$ — •Matthias Hepting[1], Pascal Puphal[1], Pascal Reiss[1], Niklas Enderlein[2], Yu-Mi Wu[1], Vignesh Sundaramurthy[1], Peter A. van Aken[1], Hidenori Takagi[1], Bernhard Keimer[1], Y. Eren Suyolcu[1], Björn Wehinger[3], and Philipp Hansmann[2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]University of Erlangen-Nürnberg, Erlangen, Germany — [3]ESRF, Grenoble, France

The recent discovery of high-temperature superconductivity in $La_3Ni_2O_7$ under high pressure has drawn considerable interest [1]. Using high-resolution synchrotron x-ray diffraction and scanning transmission electron microscopy, we observed that $La_3Ni_2O_7$ single crystals which show signs of filamentary superconductivity exhibit a crystal structure composed of alternating monolayer (ML) and trilayer (TL) units [2]. This lattice architecture diverges significantly from the previously assumed bilayer configuration [1]. In addition, we employed density functional theory to examine the distinct contributions of the ML and TL structural units to the electronic structure of the $La_3Ni_2O_7$ polymorph. In combination with recent angle resolved photoemission spectroscopy experiments [3], our findings set the stage for future investigations into unique properties of the ML-TL polymorph and the possibility of bulk high-temperature superconductivity.

[1] H. Sun et al., Nature 621, 493 (2023);
[2] P. Puphal et al., Phys. Rev. Lett 133, 146002 (2024);
[3] S. Abadi et al., arXiv:2402.07143

TT 52.2 Fri 9:45 H31

Theory of potential impurity scattering in pressurized superconducting $La_3Ni_2O_7$ — •Steffen Bötzel[1], Frank Lechermann[1], Takasada Shibauchi[2], and Ilya Eremin[1] — [1]Theoretische Physik III, Fakultät für Physik und Astronomie, Ruhr-Universität Bochum — [2]Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Chiba 277-8561, Japan

We study the effect of the point-like non-magnetic impurities on the superconducting state of La-327 and show that the interlayer $s_{\pm}$-wave and d-wave symmetries show a very different behavior as a function of impurity concentration, which can be studied experimentally by irradiating the La-327 samples by electrons prior applying the pressure. While d−wave superconducting state will be conventionally suppressed, the $s_{\pm}$-wave state shows more subtle behavior, depending on the asymmetry between bonding and antibonding subspaces. For the electronic structure, predicted to realize in La-327, the $s_{\pm}$−wave state will be robust against complete suppression and the transition temperature, T_c demonstrates a transition from convex to concave behavior, indicating a crossover from $s_{\pm}$-wave to s_{++}-wave symmetry as a function of impurity concentration. We further analyze the sensitivity of the obtained results with respect to the potential electronic structure modification.

TT 52.3 Fri 10:00 H31

Surface effects in infinite layer nickelates — •Leonard M. Verhoff[1], Liang Si[1,2], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]School of Physics, Northwest University, Xi'an, China

Nickelates have emerged as a compelling platform for studying high-temperature superconductivity, drawing comparisons to cuprates. Infinite layer rare-earth (R) nickelates, $RNiO_2$, consist of an alternating stacking of NiO_2 layers and rare-earth spacing layers along the crystallographic z-axis. While their bulk structure has been extensively studied computationally, the samples that exhibit superconductivity in experiments are thin nickelate films. They are synthesized through a chemical reduction process that removes apical oxygen from perovskite $RNiO_3$, often grown on substrates such as $SrTiO_3$ (001).

We explore emerging surface effects by studying the formation of various surfaces within the framework of DFT. While perfect stoichiometry favors a NiO_2-terminated surface, the presence of excess apical oxygen in the surface region – possibly a remnant of the chemical reduction process – might favor an RO-terminated surface. The atomic structures of the studied surfaces strongly influence the local electronic structure in the surface region. These surface effects indicate the absence of an electron pocket around the Γ point – even for $NdNiO_2$ surfaces, in contrast to DFT and *dynamical mean field theory* bulk calculations.

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; IWF project ID I5398.

TT 52.4 Fri 10:15 H31

Uniaxial pressure dependencies of the metal-to-metal transition in $P2_1/a$ and $Bmab$ $La_4Ni_3O_{10}$ single crystals — •Lukas Gries, Jan Arneth, Ning Yuan, Ahmed Elghandour, and Rüdiger Klingeler — Kirchhoff Institut for Physics, Heidelberg, Germany

The $n = 3$ Ruddlesden-Popper nickelate $La_4Ni_3O_{10}$ exhibits an intriguing metal-to-metal transition (MMT) accompanied by the evolution of intertwined charge and spin order [1]. We report report high-resolution capacitance dilatometry and magnetisation data on phase-pure single crystals of $P2_1/a$ and $Bmab$ $La_4Ni_3O_{10}$ grown by the high-pressure floating-zone method [2]. Our data show pronounced magnetoelastic coupling at the MMT for both phases. The extracted uniaxial pressure dependencies are negative for the *ab* plane and positive along the *c* axis. The uniaxial pressure dependencies are quantified and the relevant energy scales are investigated via Grüneisen scaling and Ehrenfest analysis.

[1] J. Zhang et al., Nat. Commun. 11, 6003 (2020)
[2] N. Yuan, et al., J Cryst. Growth 627, 127511 (2024)

TT 52.5 Fri 10:30 H31

A versatile microscope for simultaneous optical and thermodynamic investigation of $Ca_3Ru_2O_7$ — •Simli Mishra[1], Elena Gati[1], Fei Sun[1], Hilary Noad[1], Dmitry Sokolov[1], Andrew Mackenzie[1,2], and Veronika Sunko[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews, UK — [3]Department of Physics, University of California, Berkeley, California, USA

Ruddlesden-Popper-type ruthenates are well-known for hosting intriguing phenomena, including unconventional superconductivity, metal-insulator transitions, spin-orbit coupling, and strange metal behavior. Among these, the bilayer ruthenate $Ca_3Ru_2O_7$ is a polar metal that exhibits strong electronic correlations. It undergoes an antiferromagnetic transition at 56 K and a first-order structural phase transition at 48 K at ambient pressure.

In our experiments, we utilize a versatile, optics-based microscope with high spatial resolution, to investigate quantum materials. The setup has been integrated with a uniaxial pressure cell that enables pressure to be used as both a tuning parameter and a thermodynamic probe. Using this technique, we simultaneously measure the optical reflectivity and the elastocaloric effect to understand the behavior of $Ca_3Ru_2O_7$ as a function of temperature and uniaxial pressure.

TT 52.6 Fri 10:45 H31

Designed cleaving planes in ruthenium dioxide for ARPES experiments — •Marieke Visscher[1,2], Lea Richter[1], Sebastian Buchberger[2], Bruno Saika[2], Andy Mackenzie[1,2], and Phil King[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, UK

Ruthenium dioxide has a complex band structure, underpinning a variety of phenomena including superconductivity under strain and a Dirac nodal line network. It has also been proposed as a candidate altermagnet, and although recent studies suggest it lacks the requisite magnetic order, it has been shown to host unusual spin-polarised states in its band structure. These phenomena motivate the need for more detailed studies into its electronic structure. Angle-resolved photoemission spectroscopy (ARPES) would be an ideal probe for this, but the three-dimensional structure of ruthenium dioxide makes it difficult to prepare atomically clean and flat surfaces with conventional methods. We have therefore investigated a fabrication method based on Focused Ion Beam (FIB) structuring to stimulate sample cleavage along desired crystallographic planes. With this method, we were able to obtain high quality surfaces, on which we performed ARPES measurements. With this new capability to tailor the sample cleavage, we significantly improve the quality of ARPES data from this compound, opening new perspectives for studying its low-energy electronic structure.

TT 52.7 Fri 11:00 H31

Localized Ti-4s molecular orbitals and correlated 3d states in the bad metal TiO_x — •Daisuke Takegami[1,2], Anna Melendez-Sans[2], Takashi Miyoshino[1], Ryo Nakamura[1], Miguel Ferreira-Carvalho[3,2], Georg Poelchen[2], Chun-Fu Chang[2], Masato Yoshimura[4], Ku-Ding Tsuei[4], Haruka Matsumoto[5], Asuka Yanagida[5], Takuro Katsufuji[5], Liu Hao Tjeng[2], and Takashi Mizokawa[1] — [1]Department of Applied Physics, Waseda University, Japan — [2]Max Planck Institute for Chemical Physics of Solids, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]National Synchrotron Radiation Research Center, Taiwan — [5]Department of Physics, Waseda University, Japan

We have investigated the electronic structure of the rocksalt TiO_x system using polarizationdependent hard x-ray photoelectron spectroscopy. The spectra showed a vanishingly small intensity at the Fermi level, classifying TiO_x as a bad metal. With the main spectral features attributed to the Ti^{2+} 3d2 configuration, we were able to detect spectroscopically also the co-existence of both Ti and O vacancies. The presence of Ti^{3+} states were identified. It was a surprise not to find signs for Ti1+ entities. Instead a sharp occupied state of Ti 4s origin was unveiled in the valence band, which gave evidence that localized Ti-4s-based

molecular orbitals are formed around the O vacancies. Our findings suggest that a defect free and stoichiometric TiO would have been a strongly correlated a Mott-Hubbard insulator, and that the 4s is an important degree of freedom for low-valent 3d materials.

TT 53: Topology: Other Topics

Time: Friday 9:30–12:45 Location: H32

TT 53.1 Fri 9:30 H32

Quantum Geometric Tensor and Inertial Effects — •Maike Fahrensohn and Richard Matthias Geilhufe — Condensed Matter and Materials Theory Division, Department of Physics, Chalmers University of Technology, 41258 Göteborg, Sweden

The quantum geometric tensor (or Fubini-Study metric), defined on a parametrized quantum state manifold, encodes the full geometric structure of quantum space. The real part of the quantum geometric tensor, known as the quantum metric tensor, is a positive semi-definite Riemannian metric that measures the geometric distance between quantum states. This tensor has recently been shown to play a crucial role in the description of physical phenomena such as quantum transport, quantum noise, and optical conductivity. The antisymmetric part of the quantum geometric tensor, proportional to the Berry curvature, has been extensively studied and is central to the classification of topological insulators through their first Chern number.

While inertial effects have been well explored in classical mechanics, their role in quantum systems remains less understood. We build a connection between the quantum geometric tensor and inertial effects to bridge the geometric and topological properties of quantum systems to their physical response. This relationship may offer new insights into transport phenomena, stability, and collective dynamics in quantum systems.

TT 53.2 Fri 9:45 H32

Theory of Quantum Geometry in Unconventional Magnets — •Johannes Mitscherling, Jan Priessnitz, and Libor Smejkal — Max Plank Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Metals with altermagnetic spin-polarisation [1] and non-collinear spin textures [2] are emerging platforms exhibiting rich fundamental physics and spintronics applications. Remarkably, this class of materials intrinsically yields a complex interplay of at least two orbital degrees of freedom besides spin. It was recently noticed that such multiband Hamiltonians host previously overlooked geometric invariants beyond the quantum metric and Berry curvature, especially when more than two bands are involved, making altermagnetic and non-collinear magnetic systems promising candidates for novel quantum geometric responses [3]. In this talk, I will introduce a quantum geometric perspective adequate for multiband systems with both spin and orbital degrees of freedom, which helps us to determine and quantify the properties of the nontrivial Bloch states. With this systematic geometric characterization, I will elaborate on a pathway to identify the most promising observables, model parameter regimes, and tuning parameters, simplifying the search for experimental realizations.

[1] L. Smejkal, J. Sinova, T. Jungwirth, PRX 12, 031042 (2022).
[2] A. Birk Hellenes, T. Jungwirth, R. Jaeschke-Ubiergo,
A. Chakraborty, J. Sinova, L. Smejkal, arXiv:2309.01607v3.
[3] A. Avdoshkin, J. Mitscherling, J. E. Moore, arXiv:2409.16358.

TT 53.3 Fri 10:00 H32

Topological Order in the Spectral Riemann Surfaces of Non-Hermitian Systems — •Anton Montag[1,2], Alexander Felski[1], and Flore Kiki Kunst[1,2] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We show topologically ordered states in the complex-valued spectra of non-Hermitian systems. These arise when the distinctive exceptional points in the energy Riemann surfaces of such models are annihilated after threading them across the boundary of the Brillouin zone. This process results in a non-trivially closed branch cut that can be identified with a Fermi arc. Building on an analogy to Kitaev's toric code, these cut lines form non-contractible loops, which parallel the defect lines of the toric-code ground states. Their presence or absence establishes topological order for fully non-degenerate non-Hermitian systems. Excitations above these ground-state analogs are characterized by the occurrence of additional exceptional points. We illustrate the characteristics of the topologically protected states in a non-Hermitian two-band model and provide an outlook toward experimental realizations in metasurfaces and single-photon interferometry.

TT 53.4 Fri 10:15 H32

Exceptional Points of Any Order in a Generalized Hatano-Nelson Model — •Julius T. Gohsrich[1,2], Jacob Fauman[1,2], and Flore K. Kunst[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

Exceptional points (EPs) are truly non-Hermitian (NH) degeneracies where matrices become defective. The order of such an EP is given by the number of coalescing eigenvectors. On the one hand, most work focuses on studying Nth-order EPs in ($N \leq 4$)-dimensional NH Bloch Hamiltonians. On the other hand, some works have remarked on the existence of EPs of orders scaling with systems size in models exhibiting the NH skin effect.

In this talk, I introduce a new type of EP and provide a recipe on how to realize EPs of arbitrary order not scaling with system size. Therefore, I introduce a generalized version of the paradigmatic Hatano-Nelson model with longer-range hoppings. The EPs existing in this system show remarkable physical features: Their associated eigenstates have support on a subset of sites and exhibit the NH skin effect, which can be tuned to localize on the opposite end of the chain compared to all remaining states. Furthermore, the EPs are robust against generic perturbations in the hopping strengths as well as against a specific form of on-site disorder.

TT 53.5 Fri 10:30 H32

Topological Properties of the Non-Reciprocal α-Diamond Chain — Carolina Martinez-Strasser[1] and •Dario Bercioux[1,2] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, Plaza Euskadi 5 48009 Bilbao, Spain

This work explores the topological properties of a generalized non-Hermitian quasi-1D lattice, dubbed as the non-reciprocal α-diamond chain. The diamond chain is a tripartite lattice featuring three sites per unit cell, characterized by a flat band at zero energy associated with compact localized states, and topological edges edge states in the Hermitian and non-Hermitian regimes [1,2]. Building upon our previous investigations [2], we extend the analysis to a more general framework by introducing an α-parameter, quantifying the non-reciprocal hopping strength in the lower part of the diamond chain. Our generalization reveals a spectrum of non-Hermitian phenomena, including exceptional points of order 3 (EP3s) under specific parameter tuning. These EP3s, where three eigenvalues and their eigenvectors coalesce, offer valuable insights into the behavior of three-band non-Hermitian systems. The α-diamond chain thus serves as an effective 1D platform for exploring such phenomena, particularly in the presence of sublattice symmetries [3].

[1] Bercioux *et al.*, Ann. Phys. **529**, 1600262 (2017).
[2] Martinez-Strasser *et al.*, Adv.Quantum.Technol.**7**,2300225(2023).
[3] Montag and Kunst, Phys. Rev. Res. **6**, 023205 (2024).

TT 53.6 Fri 10:45 H32

Topological characterization of carbon nanotubes — •Udo Schwingenschlögl, Xiaoning Zang, and Nirpendra Singh — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

Orbital angular momentum plays a central role in quantum mechanics, from the microscopic interaction between light and matter to the macroscopic behavior of superconductors and superfluids. We show that the topology of carbon nanotubes can be characterized by winding numbers related to the orbital angular momentum. The tight-binding Hamiltonian of any carbon nanotube with C_N symmetry can be represented by N tight-binding Hamiltonians of decoupled molecular chains, for which a pseudospin formulation, characterized by specific paths in a two-dimensional auxiliary space, is developed. The quantum phases are given by the N winding numbers of these paths. The paths rotate in the auxiliary space when a magnetic field of varying strength is applied along the carbon nanotube, which gives rise to quantum phase transitions.

15 min. break

TT 53.7 Fri 11:15 H32

Non-Hermitian Quantum Fractals and Inner Non-Hermitian Skin Effects — Changan Li[1], Junsong Sun[2], Huaming Guo[2], and •Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]School of Physics, Beihang University, Beijing, 100191, China

The first quantum fractal discovered in physics is the Hofstadter butterfly. It stems from large external magnetic fields. We discover instead a class of non-Hermitian quantum fractals (NHQFs) emerging in coupled Hatano-Nelson models on a tree lattice in the absence of any fields. Based on analytic solutions, we are able to rigorously identify the self-similar recursive structures in the energy spectrum and wave functions. We prove that the complex spectrum of NHQFs bears a resemblance to the Mandelbrot set in fractal theory. We further investigate the non-Hermitian Su-Schrieffer-Heeger (SSH) model on Bethe lattice, revealing a novel localization phenomenon coined inner non-Hermitian skin effect. Our findings open another avenue for investigating quantum fractals in non-Hermitian systems.

TT 53.8 Fri 11:30 H32

Non-Hermitian Dynamics Close to Exceptional Points — •Aisel Shiralieva, Grigorii Starkov, and Björn Trauzettel — University of Würzburg, Würzburg, Germany

Exceptional points (EPs), which are degeneracies occurring in both open classical and quantum systems, play a crucial role across numerous areas of physics. This work examines the behavior of dissipative systems with N levels, with a particular emphasis on non-Hermitian qubits and qutrits. These systems are of interest due to recent experimental studies involving a driven non-Hermitian superconducting qubit embedded within a three-level structure, where the ground state serves as an "effective bath". Although significant progress have been made in understanding EPs, the precise connection between their occurrences in non-Hermitian Hamiltonians and in the Lindblad formalism remains unclear, especially if quantum jumps are treated as perturbations. Our results reveal how EPs in these two frameworks relate to each other and illustrate how perturbations can either lift the degeneracy or eliminate the EPs entirely in the Lindblad formalism.

TT 53.9 Fri 11:45 H32

Polarization-Induced Topology in Quantum Emitter Chains — •Jonathan Sturm and Adriana Pálffy — Julius-Maximilians-Universität Würzburg

Synthetic quantum matter has become a field of strongly growing interest over the past decade due to its versatility, adaptibility, and applicability in areas like quantum simulation and others. One particulary suited platform for engineered quantum systems are arrays of quantum emitters, which can be optically excited and couple by the exchange of virtual photons [1].

We theoretically study a quantum emitter implementation of the Su-Schrieffer-Heeger model. Different from earlier studies [2], we show that for certain chain geometries the topological invariant depends on the polarization of the chain, allowing us to alter the topology without altering the lattice. Moreover, we demonstrate how this mechanism can be used for a topological pumping protocol enabling controlled transport of photons through the chain.

[1] M. Reitz *et al.*, PRX Quantum **3**, 010201 (2022).
[2] B. X. Wang and C. Y. Zhao, Phys. Rev. A **98**, 023808 (2018).

TT 53.10 Fri 12:00 H32

Topological Signatures and Induced Triplet Pairing in Proximitized Quantum Hall - Superconductor Heterostructures — •Yuriko Baba, Rafael Sánchez, Alfredo Levy Yeyati, and Pablo Burset — Department of Theoretical Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

In a quantum Hall (QH) state, the proximity to a superconductor (SC) leads to the formation of hybridized electron-hole states called chiral Andreev edge states (CAES). Although the strong magnetic fields required for the QH effect are detrimental to superconductivity, recent experiments have achieved QH-SC hybrid junctions based on InAs 2DEGs [1], graphene [2], and magnetic topological insulators [3]. In this work, we theoretically study the formation of CAES in QH-SC hybrid junctions on a 2DEG. Using numerical simulations in Kwant [4], we study the formation of spin-polarized triplet Cooper pairs induced by Rashba spin-orbit coupling and Zeeman splitting [5], which may be important in 2DEG devices. We also consider the effect of the geometry of nanodevices in planar junctions [6] and in a narrow-finger configuration. In these geometries, the coupling of CAES can induce a topological band inversion and trivial localized states, both of which show particular signatures in non-local electron transport.

[1] Hatefipour et al, Nano Lett. 22, 6173 (2022);
[2] Zhao et al., Nat. Phys. 16, 862 (2020);
[3] Uday et al., Nat. Phys. 20, 1589 (2024);
[4] Groth et al., NJP. 16, 063065 (2014);
[5] Arrachea et al., arXiv:2310.13729;
[6] David at al. PRB 107, 125416 (2023).

TT 53.11 Fri 12:15 H32

Optical Hopfion quantizes inverse Faraday effect — •Emma L. Minarelli and Matthias R. Geilhufe — Chalmers University of Technology, Department of Physics, 412 96 Göteborg, Sweden

Control and manipulation of quantum materials is of paramount significance, both for fundamental characterization and for quantum technologies. Among others, light-matter interaction has recently gained traction because both optical counterpart of solid-state phenomena and emergent effects can be investigated.

We extend this paradigm to 3D topological optical quasiparticle i.e. optical Hopfion (oHop) - a knotted structure presenting robust topological protection, resolution on ultrafast time-scales, localization on nanometer-scale - as novel source to probe and regulate properties and phases of matter.

We show a first instance of OHop-matter coupling: an oHop travelling through a non-magnetic material induces a net effective magnetization, that is now promoted to be topologically quantized in virtue of the linking number (Hopf index) classifying the oHop source. By relating the induced magnetization to the Hopf index, we identify the quantum inverse Faraday effect. This quantized optical response is obtained without constraints on the material but only by introducing topological light. We conclude with a demonstration for a specific material and we give predictions about its promising application in optical protocols for communication and storage of information.

TT 53.12 Fri 12:30 H32

Network Model for Magnetic Higher-Order Topological Phases — Hui Liu[1,2], Ali G. Moghaddam[3,4,5], •Daniel Varjas[1,2,6,7], and Ion Cosma Fulga[1] — [1]IFW Dresden, Dresden, Germany — [2]Stockholm University, Stockholm, Sweden — [3]Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran — [4]Research Center for Basic Sciences and Modern Technologies (RBST), Zanjan, Iran — [5]Tampere University, Tampere, Finland — [6]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [7]Budapest University of Technology and Economics, Budapest, Hungary

We propose a network-model realization of magnetic higher-order topological phases (HOTPs) in the presence of the combined space-time symmetry $C_4\mathscr{T}$ – the product of a fourfold rotation and time-reversal symmetry. We show that the system possesses two types of HOTPs. The first type, analogous to Floquet topology, generates a total of 8 corner modes at 0 or π eigenphase, while the second type, hidden behind a weak topological phase, yields a unique phase with 8 corner modes at $\pm\pi/2$ eigenphase (after gapping out the counterpropagating edge states), arising from the product of particle-hole and phase-rotation symmetry. By using a bulk $\mathbb{Z}_4$ topological index (Q), we found both HOTPs have $Q = 2$, whereas $Q = 0$ for the trivial and the conventional weak topological phase. Together with a $\mathbb{Z}_2$ topological index associated with the reflection matrix, we are able to fully distinguish all phases. Our work suggests that such phases may find their experimental realization in coupled-ring-resonator networks.

TT 54: Correlated Electrons: Charge Order

Time: Friday 9:30–12:45 Location: H33

TT 54.1 Fri 9:30 H33

Broad-Band Noise at the Different CDW Transitions in $BaNi_2As_2$ — •Julian Beu[1], Marvin Kopp[1], Markus König[2], Amir Haghighirad[3], Matthieu Le Tacon[3], Jure Demsar[4], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]MPI CPfS, Dresden, Germany — [3]KIT, Karlsruhe, Germany — [4]Institute of Physics, JGU, Mainz

Ever since collective modes like charge (CDW) and spin density waves (SDW) have been routinely found near to or in direct competition with unconventional superconductivity in many interesting compounds, including high-T_c cuprates and iron-pnictides, the influence of these states on the superconducting phase is of interest. In this work we focus on $BaNi_2As_2$ (BNA), a structurally close analogue of the 122-type iron-based superconductors. In contrast to the iron-pnictides, no magnetic ordering was observed in BNA, and two different CDW phases, one incommensurate (I-CDW) and the other commensurate (C-CDW), replace a SDW phase. We investigate the charge carriers in samples of $BaNi_2(As_{1-3.5\%}P_{3.5\%})_2$ by analyzing the resistance and broad-band noise properties. The samples are structured by a FIB process with a meander current path in order to increase the absolute resistance by two orders of magnitude, making fluctuation spectroscopy possible. Our measurements reveal significant differences in the behavior of the electronic fluctuations at the two CDW formations, that show interesting connections to recent findings regarding the properties of the I-CDW in BNA [1] and our noise measurements performed on the conventional CDW system $K_{0.3}MoO_3$. [1] Phys. Rev. Lett. 129, 247602.

TT 54.2 Fri 9:45 H33

Visualizing p-Orbital Texture in the Charge Density Wave State of CeSbTe — Xinglu Que[1], Qingyu He[1], Lihui Zhou[1], Shiming Lei[2], Leslie Schoop[3], •Dennis Huang[1], and Hidenori Takagi[1,4,5] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Hong Kong University of Science and Technology, China — [3]Princeton University, USA — [4]University of Stuttgart, Germany — [5]University of Tokyo, Japan

The collective reorganization of electrons into a charge density wave (CDW) inside a crystal has long served as a textbook example of an ordered phase in condensed matter physics. Two-dimensional square lattices with p electrons are well-suited to the realization of CDW, due to the anisotropy of the p orbitals and the resulting one dimensionality of the electronic structure. In spite of a long history of study of CDW in square-lattice systems, few reports have recognized the existence and significance of a hidden orbital degree of freedom. The degeneracy of p_x and p_y electrons inherent to a square lattice may give rise to nontrivial orbital patterns in real space that endow the CDW with additional broken symmetries or unusual order parameters. Using scanning tunneling microscopy, we visualize signatures of p-orbital texture in the CDW state of the topological semimetal candidate CeSbTe, which contains Sb square lattices with $5p$ electrons. We image atomic-sized, anisotropic lobes of charge density with periodically modulating anisotropy, that ultimately can be mapped onto a microscopic pattern of p_x and p_y bond density waves.

TT 54.3 Fri 10:00 H33

Charge Density Wave and Phonon Softening in $EuAl_4$ — •Aleksandr Sukhanov[1], Steven Gebel[1], Artem Korshunov[2], and Marein Rahn[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 20018 San Sebastian, Spain

$EuAl_4$ is a rare earth intermetallic in which competing itinerant and/or indirect exchange mechanisms give rise to a complex magnetic phase diagram, including a centrosymmetric skyrmion lattice. These phenomena arise not in the tetragonal parent structure but in the presence of a charge density wave (CDW), which lowers the crystal symmetry and renormalizes the electronic structure. Microscopic knowledge of the corresponding atomic modulations and their driving mechanism is a prerequisite for a deeper understanding of the resulting equilibrium of electronic correlations and how it might be manipulated.

In my talk, I present inelastic x-ray scattering results, which can clarify the origin of the CDW in $EuAl_4$.

TT 54.4 Fri 10:15 H33

Charge Density Wave Quantum Critical Point under Pressure in 2H-$TaSe_2$ — •Yuliia Tymoshenko[1], Amir-Abbas Haghighirad[1], Rolf Heid[1], Gaston Garbarino[2], Luigi Paolasini[2], and Frank Weber[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]2European Synchrotron Radiation Facility, 71 avenue des Martyrs, CS 40220, Grenoble 38043, France

Suppression of the ordered state is one of the ways to increase the superconducting (SC) transition temperatures. Materials characterized by charge density waves (CDW) and SC are promising candidates for such studies, since both states can be associated with electron-phonon coupling. Transition metal dichalcogenides (TMD) are prominent examples of such coexisting phases, however, not all such materials show the expected behavior or possess additional mechanisms that complicate an unambiguous interpretation. Here, we report high-pressure X-ray diffraction (XRD) and inelastic X-ray scattering (IXS) measurements of a prototypical transition metal dichalcogenide 2H-$TaSe_2$ and determine the evolution of the CDW state and its lattice dynamics. We found that the quantum critical point (QCP) of the charge density wave is in close proximity to the reported maximum superconducting transition temperature T_{sc} = 8.2 K. Ab-initio calculations confirm that 2H-$TaSe_2$ is a typical example of enhanced superconductivity with suppressed order and can serve as a textbook example for studying superconductivity near the quantum critical point of the CDW.

TT 54.5 Fri 10:30 H33

Tunable Charge Density Wave Orders in 2H-TaS_2 — •Mihir Date[1,2], Joost Aretz[3], Enrico da Como[4], Marcin Mucha-Kruczynski[4], Malte Roesner[3], Stuart S P Parkin[1], Niels B M Schroeter[1], and Matthew D Watson[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Diamond Light Source Ltd., Didcot, UK — [3]Radboud University, Nijmegen, The Netherlands — [4]University of Bath, Bath, UK

The charge density wave (CDW) transition is an electronic instability driven by strong electron-phonon coupling, where the parent electronic band is renormalized, and shows a spectral gap. Angle-resolved photoemission spectroscopy (ARPES) has been extremely successful in identifying these spectral features, most prominently in layered van der Waals materials like 2H-$NbSe_2$ and $TaSe_2$. Surprisingly, however, until now there has not been any high-quality data reported on the 2H-TaS_2, presumably due to materials challenges. Making use of spatially resolved ARPES, we were able to overcome these challenges and measure high-quality bandstructures revealing the 3x3 commensurate charge density waves (CCDW) ground state in 2H-TaS_2. We further find variation of the stoichiometry between samples prepared by different routes, and incredibly, at a different band filling we find evidence of a new CDW order that is commensurate, but not the 3x3 reconstruction as observed in previous experiments. Our results are compared with tight-binding and ab-initio modelling which show that TaS_2 is prone to multiple instabilities that can be tuned by the band filling, with an important role played by a van Hove singularity.

TT 54.6 Fri 10:45 H33

Resistance of Vapor-Grown $NbSe_2$ Single Crystals under Strain — •Maik Golombiewski, Tianyi Xu, Simon Knudsen, Michael Paul, Sven Graus, Teslin R. Thomas, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

$NbSe_2$ shows a charge density wave (CDW) transition upon cooling below T_{CDW} = 32 K and becomes superconducting at T_c = 7.2 K. Large $NbSe_2$ single crystals were grown via chemical vapor transport with iodine as transport agent. Growth conditions, such as temperature gradient, were optimized resulting in an increase in RRR. Samples were shown to have a 1:2 stoichiometry via energy-dispersive x-ray spectroscopy and the 2H-structure was confirmed by powder x-ray diffraction measurements. Temperature-dependent resistance was measured while simultaneously straining the samples using cryogenic strain and force cells. This so-called elastoresistance exhibits a minimum around T_{CDW}. Using the force cell, large strains were applied and investigated.

We acknowledge support by the Mercator Research Center Ruhr (MERCUR), under project number Ko-2021-0027.

TT 54.7 Fri 11:00 H33

Fingerprints of a Charge Ice State in the Doped Mott Insulator Nb_3Cl_8 — •Evgeny Stepanov — CNRS, Ecole Polytechnique

Monolayer Nb_3Cl_8 is a textbook example of a Mott insulator [1,2]. However, little is known about its characteristics, particularly in doped regimes where the strong local correlations responsible for the Mott state are competing with significant spatial collective electronic fluctuations.

Our many-body calculations suggest that monolayer Nb_3Cl_8 undergoes phase separation (PS) upon doping, driven by the emergence of a charge ice state [3]. In close proximity to the PS, the charge susceptibility dramatically increases and displays a distinctive bow-tie pattern in momentum space, resembling the form of magnetic susceptibility observed in spin ice states. At the same time, the effective exchange interaction between charge densities undergoes a striking transformation, acquiring a power-law dependence in real space. This dependence is reminiscent of hydrogen bonding interactions in water and serves as a hallmark of spin ice states when applied to spin degrees of freedom. These findings allow us to associate the observed PS with a charge ice state, characterized by a remarkable power-law dependence of correlations between electronic densities in real space.

While spin ice states were first experimentally realized in 1997 by Harris et al. [4], an analogue for charge degrees of freedom has remained elusive until now. Our work not only provides a theoretical description of the charge ice state but also offers compelling evidence that this novel phase can be realized in a real material.

[1] Nano Lett. 22, 4596 (2022);
[2] PRX 13, 041049 (2023);
[3] arXiv:2405.19114;
[4] PRL 79, 2554 (1997).

15 min. break

TT 54.8 Fri 11:30 H33

Non-Thermal Cavity Control of Order in Electronic Systems — •Md Mursalin Islam[1], Michele Pini[2,1], Rafael Flores-Calderón[1], and Francesco Piazza[2,1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Augsburg, Augsburg, Germany

Cavity quantum materials have emerged as a platform to study non-thermal many-body physics with applications to the control of collective electron behavior. In an electronic system coupled to cavity photons, the superconducting gap has been predicted previously to be enhanced, due to a 'Eliashberg effect' taking place due to electromagnetic fluctuations as instead of a coherent laser source [1,2]. We extend this idea for the case of charge-density-wave order and systematically derive a generalized gap equation for the non-thermal situation using field theoretical methods. This allows us to compare the modified gap equations for superconductors and charge density waves: we find that while the two equations are exactly equivalent in thermal equilibrium, they assume different forms in non-thermal settings. Our formalism also allows us to systematically investigate the role of disorder in the non-thermal enhancement of the gap in both the cases.

[1] G. M. Eliashberg, JETP Lett. 11, 114 (1970);
[2] J. B. Curtis et. al., PRL 122, 167002 (2019).

TT 54.9 Fri 11:45 H33

Disorder in Photoexcited Charge Density Wave Systems: Insights from Stochastic Resonance in Impurity Models. — •Francesco Valiera and Martin Eckstein — Department of Physics, University of Hamburg, D-22607 Hamburg, Germany

Photoexcitation in charge density wave (CDW) systems can potentially lead to inhomogeneously disordered phases [1], where ions are displaced locally but do not achieve global ordering. In these phases, each ion moves within a local double-well potential and settles in one of the two equilibrium positions with equal probability. Similar behaviours have also been observed experimentally in VO_2 through scattering experiments [2]. A fundamental question in understanding these disordered states is identifying their signatures beyond X-ray scattering. In order to explore this, we have developed a model of a single ion embedded in a metallic host and use the semiclassical stochastic approach [3] to compute its linear response to an external probe. At low frequencies, the system exhibits a peak in the response amplitude as a function of temperature, which we attribute to stochastic resonance. The latter is typical of bistable systems that experience both periodic driving and noise and it can provide insights into the features of the local double-well potentials and the fluctuations to which the ions are subject.

[1] A. Picano et al., Phys. Rev. B 107, 245112 (2023);
[2] S. Wall et al., Science 362, 572 (2018);
[3] A. Picano et al., Phys. Rev. B 108, 035115 (2023).

TT 54.10 Fri 12:00 H33

Kinetic Magnetism and Stripe Order in the Antiferromagnetic Bosonic t-J Model — •Timothy J. Harris[1,2], Ulrich Schollwöck[1,2], Annabelle Bohrdt[1,2,3], and Fabian Grusdt[1,2] — [1]Ludwig Maximilian University of Munich, Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]University of Regensburg, Regensburg, Germany

Understanding the microscopic mechanisms governing the physics of doped quantum magnets is a central challenge in strongly correlated many-body physics. In this talk, I will present results that disentangle the role of particle statistics from the intrinsic physics of strong correlations in the antiferromagnetic (AFM) bosonic t-J model. Using large-scale density matrix renormalization group (DMRG) calculations, we map out the T=0 phase diagram on the 2D square lattice [1]. At low doping, we find evidence of partially-filled stripe structures, reminiscent of those observed in high-T_c cuprates. As doping increases, a transition occurs to a partially-polarized ferromagnetic (FM) phase, driven by formation of Nagaoka polarons as mobile holes bind to localized FM regions. At high doping or large t/J, these polarons overlap, and the system evolves into a full-polarized ferromagnet. Our findings shed new light on the role of particle statistics in strongly correlated quantum matter, revealing connections to stripe formation and the physics of kinetic ferromagnetism. I will also discuss experimental realizations of this model using state-of-the-art quantum simulators, paving the way for future studies of doped bosonic quantum magnets.

[1] T.J. Harris et al., arXiv:2410.00904 (2024).

TT 54.11 Fri 12:15 H33

SU(2) Gauge Theory for Fluctuating Stripes in the Pseudogap Regime — •Mark Henrik Müller-Groeling, Pietro Maria Bonetti, Paulo Forni, and Walter Metzner — Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

We investigate the role of charge order in a pseudogap described by an SU(2) gauge theory of fluctuating magnetic order.

The theory is based on a fractionalization of electrons into a fermionic chargon pseudospinor and a bosonic spinon, which leads to an emergent SU(2) pseudospin symmetry. In the mean-field solution of the 2D Hubbard model, which we use to describe the electrons in the copper-oxygen planes, Néel, spiral, or stripe order were observed below a density dependent transition temperature T^* [1].

Fluctuations of the spin orientation are described by a non-linear sigma model obtained from a gradient expansion of the spinon action. The spin stiffnesses are computed from a random phase approximation for the chargon susceptibility. The spinon fluctuations prevent magnetic long-range order of the electrons at any finite temperature. The phase with magnetic chargon order exhibits the most salient features characterizing the pseudogap regime in high-T_c cuprates: a strong reduction of charge carrier density, a spin gap, and Fermi arcs [2], and we set out to observe the effects of charge order in this context.

[1] R. Scholle, P. M. Bonetti, D. Vilardi, W. Metzner, PRB **108** 035139 (2023);
[2] P. M. Bonetti, W. Metzner, PRB **106**, 205152 (2022).

TT 54.12 Fri 12:30 H33

Combined Cluster and Diagrammatic Method for Symmetry Broken Phases in Correlated Electron Systems — •Félix Fossati and Evgeny Stepanov — Ecole Polytechnique

In this work, we investigate dynamical symmetry breaking in correlated electron systems. To achieve this, we refine a theoretical approach called D-TRILEX [1-3], which constructs a diagrammatic expansion based on an interacting reference system, using a cluster problem as a reference. Traditional cluster methods account for short-range correlation effects within the cluster exactly but neglect correlations beyond the cluster size. Our approach addresses this limitation by self-consistently combining the non-perturbative treatment of short-range correlations with a diagrammatic description of long-range collective electronic fluctuations. We demonstrate the effectiveness of this method by applying it to the one-dimensional Hubbard model. Our results show that the cluster extension of D-TRILEX accurately captures the transitions to the charge density wave (CDW) and bond-ordered wave (BOW) phases, which are associated with local and non-local order parameters, respectively, across various regimes of electronic interactions. This implementation provides new insights into the role of non-local interactions in dynamical symmetry breaking, establishing D-TRILEX as a promising tool for investigating complex phases in strongly correlated systems.

[1] E. A. Stepanov et al., Phys. Rev. B 100, 205115 (2019);
[2] V. Harkov et al., Phys. Rev. B 103, 245123 (2021);
[3] M. Vandelli et al., SciPost Phys. 13, 036. (2022).

TT 55: Superconducting Electronics: SQUIDs, Qubits, Circuit QED III

Time: Friday 9:30–13:00 Location: H36

TT 55.1 Fri 9:30 H36

Superconducting devices based on the NbTiN Josephson junctions — •Vasilii Sevriuk[1], Azat Gubaydullin[1], Aki Ruhtinas[2], Michael Perelshtein[1], Alexey Mironov[1], Pertti Hakonen[3], Ilari Maasilta[2], and Valerii Vinokur[1] — [1]Terra Quantum AG, Kornhausstrasse 25, 9000 St. Gallen, Switzerland — [2]Nanoscience Center, Department of Physics, University of Jyväskylä, FI-40014 Jyväskylä, Finland — [3]QTF Centre of Excellence, Department of Applied Physics, Aalto University, P.O. Box 15100, FI-00076 AALTO, Finland

Quantum devices based on superconducting circuits are a promising technology that could have a significant impact on many aspects of human life. However, the production of high-coherence circuits remains one of the key challenges. Recent results on the fabrication of NbTiN Josephson junctions using a focused helium ion beam [1] suggest that this method is well-suited for a wide range of applications in superconducting electronics, due to the excellent mechanical, electrical, and microwave properties of NbTiN. Here we present our results on the characterization of the superconducting circuits based on this technology.

[1] A. Ruhtinas, I. Maasilta, arXiv:2303.17348v2.

TT 55.2 Fri 9:45 H36

Argon milling strategies for Tantalum Transmon qubits — •Philipp Lenhard[1], Mathieu Fechant[1], Ritika Dhundhwal[1], Thomas Reisinger[1], and Ioan M. Pop[1,2,3] — [1]IQMT, Karlsruhe Institute of Technology — [2]PHI, Karlsruhe Institute of Technology — [3]1. Physikalisches Institut, University of Stuttgart

Tantalum has emerged as a promising material for enhancing the coherence time of superconducting qubits [1,2]. This study focuses on the fabrication of qubits, emphasizing the necessity of establishing a coherent contact between Ta-based structures and Al/AlO_x/Al Josephson junctions. The removal of native oxide layers via Argon milling is critical to this process. We present various approaches to achieve optimal contact through Argon milling, along with a discussion of the associated challenges and potential solutions.

[1] Place et al., Nat. Commun. 12:1779 (2021).
[2] Ganjam et al., Nat. Commun. 15:3687 (2024).

TT 55.3 Fri 10:00 H36

Simultaneous locking and operation of gradiometric fluxonium qubits — •Denis Bénâtre[1], Mathieu Féchant[1], Nicolas Gosling[1], Nicolas Zapata[1], Patrick Paluch[1], Martin Spiecker[1], and Ioan Pop[1,2,3] — [1]IQMT, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]PHI, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]PI1, Stuttgart University, 70569 Stuttgart, Germany

Gradiometric fluxoniums, introduced by Gusenkova et al. (Appl. Phys. Lett. 120, 2022), have the ability to be flux-locked at the sweet spot of operation by trapping a persistent current in their most external loop. We demonstrate the reliability of the procedure by simultaneously locking several fluxoniums sitting in the same waveguide and show that the locking in stable in time. We engineer devices with varying asymmetries and exhibit samples with close-to-zero asymmetry, allowing them to be used with little additional flux-biasing. Such devices could thus help reduce cross-talk between flux lines addressing flux qubits.

TT 55.4 Fri 10:15 H36

Low cross-talk modular flip-chip architecture for coupled superconducting qubits — •Sören Ihssen[1], Simon Geisert[1], Gabriel Jauma[2,3], Patrick Winkel[1,4,5], Martin Spiecker[1], and Ioan M. Pop[1,6,7] — [1]IQMT, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain — [3]Applied Physics Department, Salamanca University, Salamanca 37008, Spain — [4]Departments of Applied Physics and Physics, Yale University, New Haven, CT 06520, USA — [5]Yale Quantum Institute, Yale University, New Haven, CT 06520, USA — [6]PHI, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [7]Physics Institute 1, Stuttgart University, 70569 Stuttgart, Germany

We introduce a novel flip-chip architecture designed for an array of coupled superconducting qubits, where each circuit component is housed within its own microwave enclosure. Unlike traditional flip-chip designs, our approach features electrically floating qubit chips, enabling a straightforward and fully modular assembly of capacitively coupled components, including qubits, control systems, and coupling structures. This design minimizes crosstalk among components. We validate our concept using a chain of three nearest-neighbor coupled generalized flux qubits, with the central qubit functioning as a frequency-tunable coupler. Through this coupler, we achieve a transverse coupling on/off ratio of approximately 50, zz-crosstalk below 1.4 kHz between resonant qubits, and over 70 dB of isolation between the qubit enclosures.

TT 55.5 Fri 10:30 H36

Optically mediated control for superconducting qubits — •Kevin Kiener[1,2], Gleb Krylov[1,2], Florian Wallner[1,2], Max Werninghaus[1,2], Nadeem Akhlaq[2,3], Frederik Pfeiffer[1,2], Johannes Schirk[1,2], and Stefan Filipp[1,2] — [1]Walther-Meißner-Instiut, Bayerische Akademie der Wissenschaften — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics — [3]Walter Schottky Institut

In superconducting quantum computers, scaling control and readout wiring infrastructure presents significant challenges. Optical fibers offer a promising alternative to microwave cables by providing lower passive heat load, reduced footprint per channel, reduced crosstalk and the potential for multiplexing control channels. Here, we explore the conversion of microwave- to optical signals via amplitude modulation and the subsequent reconversion to microwave signals at millikelvin (mK) temperatures. Two fiber coupling strategies are experimentally evaluated in a cryogenic environment, focusing on their practicality for qubit control. We theoretically investigate methods to reduce the power dissipation of the photodiode at mK temperatures, focusing on two approaches: utilizing an impedance converter and employing high-impedance transmission lines. We investigate the validity of the signal generation for different frequencies and identify suitable frequency ranges to control different qubit architectures and coupling elements.

We acknowledge financial support from GeQCoS, MUNIQC-SC, MCQST, OpenSuperQPlus100, the Munich Quantum Valley and the Deutsche Forschungsgemeinschaft.

TT 55.6 Fri 10:45 H36

Spectroscopic characterization of noise and decoherence mechanisms in superconducting qubits — •Julian Englhardt[1,2], Emily Wright[1,2], Niklas Glaser[1,2], Leon Koch[1,2], Ivan Tsitsilin[1,2], Christian Schneider[1,2], Max Werninghaus[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften

Dynamical decoupling sequences during free evolution time have proven effective in suppressing the impact of environmental noise in superconducting qubits, thereby increasing coherence times towards the theoretical 2T1 limit. While primarily used for error suppression during quantum computation, these sequences can also serve as a diagnostic tool for noise characterization by revealing the qubit's response across specific frequency ranges. Beyond standard dynamical decoupling sequences, here we employ additional methods such as time resolved single-shot Ramsey measurements to probe low-frequency noise sources and the signature noise spectra of specific decoherence events. Specifically, we investigate charge parity jumps in superconducting Transmon qubits induced by quasiparticle tunneling across the Josephson junction. We believe that the combined toolkit for noise spectroscopy can contribute to the understanding of decoherence mechanisms in superconducting qubits.

We acknowledge financial support from GeQCoS, MUNIQC-SC, MCQST, OpenSuperQPlus100, the Munich Quantum Valley and the Deutsche Forschungsgemeinschaft.

TT 55.7 Fri 11:00 H36

Suppressing chaos with mixed superconducting qubit devices — •Ben Blain[1,2], Giampiero Marchegiani[1], Luigi Amico[1,3,4], and Gianluigi Catelani[5,1] — [1]Quantum Research Center, Technology Innovation Institute, Abu Dhabi 9639, UAE — [2]School of Physics and Astronomy, University of Kent, Canterbury CT2 7NH, United Kingdom — [3]Dipartimento di Fisica e Astronomia, Via S. Sofia 64, 95123 Catania, Italy — [4]INFN-Sezione di Catania, Via S. Sofia 64, 95127 Catania, Italy — [5]JARA Institute for Quantum Information (PGI-11),Forschungszentrum Jülich, 52425 Jülich, Germany

In quantum information processing, a tension between two different tasks occurs: while qubits' states can be preserved by isolating them, quantum gates can be realized only through qubit-qubit interactions. In arrays of qubits, weak coupling leads to states being spatially localized and strong coupling to delocalized states. Here, we study the average energy level spacing and the relative entropy of the distribution of the level spacings to analyze the crossover between localized and delocalized (chaotic) regimes in linear arrays of superconducting qubits. We consider both transmons as well as capacitively shunted flux qubits, which enables us to tune the qubit anharmonicity. Arrays with uniform anharmonicity display remarkably similar dependencies of level statistics on the coupling strength. In systems with alternating anharmonicity, the localized regime is found to be more resilient to the increase in qubit-qubit coupling strength in comparison to arrays with a single qubit type. This result supports designing devices that incorporate different qubit types to achieve higher performances.

15 min. break

TT 55.8 Fri 11:30 H36

Higher Josephson harmonics in superconducting qubits — •Abbas H. Hirkani[1,2], Giampiero Marchegiani[1], Luigi Amico[1,3,4], and Gianluigi Catelani[1,5] — [1]QRC, TII, Abu Dhabi, UAE — [2]SISSA, Trieste, Italy — [3]Dipartimento di Fisica e Astronomia, Catania, Italy — [4]INFN-Catania, Catania, Italy — [5]Forschungszentrum Jülich, Jülich, Germany

Measurements of higher-level spectra of transmon cannot be explained using the standard $I = I_0 \sin\phi$ current-phase relation, and a more accurate description of the Josephson element, with non-negligible contributions from higher harmonics, is needed [1]. Stray inductances can also lead to similar corrections to the spectrum; here we investigate the Fraunhofer effect in transmons comprising thin-film Al/AlO_x/Al junctions under parallel magnetic field [2] as a tool to discriminate between contributions from inductances and from intrinsic higher harmonics of the junctions. The magnetic field modulates each harmonic on a different field scale; this results in a field dependence of the qubit spectrum measurably different from the one due to a stray inductance alone. We also examine how the presence of a few percent higher harmonic contributions affects various qubit designs, and comment on the implications for accurate targeting of qubit parameters.

[1] D. Willsch et al., Nat. Phys. 20, 815 (2024);
[2] J. Krause et al., Phys. Rev. App. 22, 044063 (2024).

TT 55.9 Fri 11:45 H36

Impact of infrared photons on superconducting qubits — •Markus Griedel[1,2], Jonathan Huschle[2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Institut for Quanten Materials and Technologies (IQMT), Karlsruhe Institut for Technology (KIT), Karlsruhe, Germany — [2]hysikalisches Institut (PHI), Karlsruhe Institut for Technology (KIT), Karlsruhe, Germany

Low-noise superconducting quantum circuits are manipulated by microwave photons with energies below the superconducting energy gap. However, the impact of photons with much higher energies may break Cooper pairs and result in an increase in the noise level. Stray infrared (IR) radiation, e.g. transmitted through the dielectrics of coaxial cables, must be blocked by a low-pass filter to avoid this additional noise. The coherence of superconducting qubits is particularly sensitive to this influence and can be used as a detector. In the qBriqs project, we focus on studying the impact of far-infrared photons and present the results of a detailed experimental study. We propose materials to suppress the IR radiation, e.g. with an in-line filter, while maintaining good microwave properties.

TT 55.10 Fri 12:00 H36

Investigation of parasitic two-level systems in merged-element Transmon qubits — •Etienne Daum[1], Benedikt Berlitz[1], Alexey V. Ustinov[1,2], and Jürgen Lisenfeld[1] — [1]PHI, Karlsruher Institut für Technologie, 76131 Karlsruhe, Deutschland — [2]IQMT, Karlsruher Institut für Technologie, 76131 Karlsruhe, Deutschland

In conventional transmon qubits, decoherence is dominated by large numbers of parasitic two-level systems (TLS) residing at the edges of its large area coplanar shunt capacitor. Avoiding these defects by improvements in design, fabrication and materials proved to be a significant challenge that so far led to limited progress. The merged-element transmon qubit, a recently proposed paradigm shift in transmon design, attempts to address these issues by engineering the Josephson junction to act as its own parallel shunt capacitor. Incorporating an additional aluminium deposition and oxidation into the *in-situ* bandaged Niemeyer-Dolan technique, we were able to fabricate flux-tunable mergemon qubits in the low transmon regime ($E_J/E_C \approx 34$). A mean T_1 relaxation time of about $20\mu s$ ($Q \approx 5.4 \times 10^5$) has been observed over a six hour time period. TLS spectroscopy under applied strain and electric fields revealed that the majority of coherence limiting TLS (~ 60%) still reside on the interfaces of exposed qubit electrodes, despite their drastically reduced surface area. This indicates that ma-

terial and fabrication improvements, in combination with optimized electrode geometries, are still necessary before the advantages of the "mergemon" approach can be exploited.

TT 55.11 Fri 12:15 H36

Demonstration of a Solid-State Random Defect Maser — •Christian Ständer, Jan Blickberndt, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

The low temperature properties of amorphous solids are governed by atomic tunneling systems, which can be described as two-level systems (TLS) with a distribution of their energy splitting E, as assumed by the phenomenological standard tunnelling model. Recent interest in these systems due to their deteriorative effects on the performance of superconducting quantum devices lead to experimental investigations of atomic tunnelling systems.

We designed and microfabricated a superconducting LC-resonator to study the dielectric rf-response of an amorphous sample in the presence of a slowly varying electric bias field and two symetrically detuned pump tones. A novel method of applying this electrical bias field was introduced to the resonators. By shifting the energy splitting of the inverted TLS with the external bias, to match the resonators frequency we found a paramterspace of negative dielectric loss, hence gain. In this way we demonstrate that a media containing random TLS could be transformed from an inertially lossy system to a system that features no significant dielectric loss, up to a point of coherent gain.

TT 55.12 Fri 12:30 H36

Two-qubit entangling quantum gates in a 2D ring resonator architecture — •Anirban Bhattacharjee[1,2], Panya Jain[1], Jay Deshmukh[1], Srijita Das[1], Madhavi Chand[1], Meghan Patankar[1], and Rajamani Vijayaraghavan[1] — [1]Tata Institute of Fundamental Research, Mumbai, India — [2]Walther Meissner Institute, Garching b Muenchen, Germany

A novel ring resonator [1] design allows interqubit connectivity beyond nearest neighbours, which has always been a topological constraint in present state-of-art quantum architectures. In this work, we demonstrate connectivity between three fixed-frequency transmon qubits coupled to a ring resonator in a planar 2D architecture. We have also demonstrated two-qubit entangling gates between two fixed-frequency qubits in this geometry. Our results show the ability to demonstrate quantum entanglement using the ring resonator and opens up the possibility of exploring various gate implementations in this architecture.

[1] Phys. Rev. Appl. 16, 024018 (2021).

TT 55.13 Fri 12:45 H36

Study of the quarton-quarton qubits interaction — •Hossam Tohamy[1], Alex Kreuzer[1], Andras Di Giovanni[1], Thilo Krumrey[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT) — [2]Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology (KIT)

Tunable qubits are a useful resource in superconducting quantum processors to enable high-performance quantum gates. While much of the recent focus has been on the exploration of transmon multiqubit architectures, the quarton qubit [1] offers a three- to five-times higher and, in addition, positive anharmonicity. In this work, we experimentally study the interaction between two quarton qubits. We have performed spectroscopy and time-domain measurements on these qubits system, and compared the experimental results with theoretical model.

[1] F. Yan et al., arXiv:2006.04130 (2020).

TT 56: Quantum Dynamics, Decoherence, and Quantum Information (joint session DY/TT)

Time: Friday 9:30–11:15 Location: H37

TT 56.1 Fri 9:30 H37

Entanglement phase transitions in unitary circuit games with free fermions — •Raúl Morral-Yepes[1,2], Marc Langer[1,2], Adam Smith[3,4], Barbara Kraus[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences — [2]Munich Center for Quantum Science and Technology (MCQST) — [3]School of Physics and Astronomy, University of Nottingham — [4]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems

In the recently introduced framework of unitary circuit games, two competing parties an entangler and a disentangler can induce an entanglement phase transition, distinct from measurement-induced transitions. In this work, we study such games within the context of matchgate dynamics, which correspond to free fermion systems. First, we investigate the entanglement properties of fermionic Gaussian states (FGS) and explore different methods for their disentangling. We propose a representation of FGS using a minimal matchgate circuit in a standard form, and introduce algorithms for updating this representation as unitary operations are applied. Within this framework, we define a natural disentangling procedure that reduces the number of gates in the circuit, thereby decreasing the system's entanglement. We then analyze the unitary game using this gate disentangler, observing a phase transition between a volume-law and area-law entanglement phase. The nature of this transition differs depending on whether we examine Rényi-0 or other entanglement entropies.

TT 56.2 Fri 9:45 H37

Measurement Induced Entanglement Transitions in Random Qudit Clifford Circuits — •Aamod Vinayak Atre, Raúl Morral Yepes, and Frank Pollmann — Department of Physics, Technical University of Munich

Random quantum circuits with local projective measurements uncover the universal dynamical properties of generic chaotic quantum many-body systems, as their unitary evolution is independent of the microscopic features of Hamiltonians. Entanglement measures characterize these universal dynamics into volume-law and area-law regimes, which exhibit bipartite entropy scaling proportional to the system volume and system boundary respectively. This continuous entanglement scaling transition, driven by the rate of measurement, has been extensively studied in spin-1/2 (qubit) systems of various spatial geometries. In this talk, we discuss the characterization the entanglement transitions in 1D random quantum circuits of spins (qudits) with arbitrary local Hilbert-space dimension d. This work employs the generalized stabilizer formalism, taking advantage of the Clifford group which forms a unitary 2-design on the space of unitaries. We find the nature of the entanglement transition, from volume-law to area-law regimes, to be preserved for $d > 2$. The critical measurement density increases, converging to 1/2 in the limit $d \to \infty$. Lastly, we describe the stabilizer dynamics in the limit $d \to \infty$, by a dynamical classical model.

TT 56.3 Fri 10:00 H37

Entanglement phases, localization and ergodicity of monitored free fermions in 2D — •Karim Chahine and Michael Buchhold — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Monitored quantum systems, characterized by the interplay between unitary evolution and mid-circuit measurements, have recently emerged as a novel expression of quantum dynamics. Despite their inherently out-of-equilibrium nature, these systems can host robust quantum phases and display measurement-induced phase transitions (MIPT) in the entanglement entropy. Remarkably, they are also unique in providing a link between quantum dynamics in D dimensions and quantum statistical mechanics in $D + 1$ dimensions. In this talk, I will present our recent work on a new arena with a rich phenomenology: continuously monitored, $U(1)$-symmetric free fermions in 2D. I will address the emerging MIPT and its similarities and differences with Anderson-type localization transitions. Some emphasis will be put on the low-measurement regime, where intriguing features in the entanglement structure and ergodic properties emerge, revealing a richer phenomenology than previously anticipated.

TT 56.4 Fri 10:15 H37

Spectral Properties and Magic generation of T-doped Random Clifford Circuits — •Dominik Szombathy — Budapest University of Technology and Economics

We investigate the spectral properties and magic generation of T-doped random Clifford circuits. There is a direct relation between the structure of Pauli string orbits and the eigenvalue spectrum of a Clifford circuit. Operatively, we sample the closed trajectories with brick-wall circuits and determine the distribution of the eigenvalues $\lambda = e^{i\Theta}$. The autocorrelation function of the phases of the eigenvalues displays peculiar properties: extreme degeneracies as well as some level-repulsion, and features reminiscent of a fractal pattern.

To investigate the stability of orbits and head towards universal quantum computation, we introduce $\pi/4$ phase shift gates (T-gates). We find that even a single T-gate completely changes the properties of the circuit. By increasing the number of T-gates (N_T), the correlation function rapidly approaches that of the random unitary circuits. Nevertheless, some statistically significant fraction of non-trivial orbits persists at low T-gate densities (N_T/N).

We observe a similar phenomenology in the magic generation as a function of T-gate density. In particular, we find universal scaling of the maximum and mean magic as a function of N_T/N . We also highlight the structure of magic generated by these circuits. Injecting a few T-gates the distribution is discrete but becomes continuous as N_T increases. At large densities N_T/N , most of the weight is found in a sharp peak well below the theoretical maximum.

TT 56.5 Fri 10:30 H37

Magic transition in measurement-only circuits — •Poetri Sonya Tarabunga[1,2] and Emanuele Tirrito[3,4] — [1]Technical University of Munich, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 München, Germany — [3]The Abdus Salam International Centre for Theoretical Physics (ICTP), 34151 Trieste, Italy — [4]Dipartimento di Fisica "E. Pancini", Università di Napoli "Federico II", 80126 Napoli, Italy

Magic quantifies the distance of a quantum state to the set of stabilizer states, and it serves as a necessary resource for potential quantum advantage over classical computing. In this work, we study magic in a measurement-only quantum circuit with competing types of Clifford and non-Clifford measurements, where magic is injected through the non-Clifford measurements. This circuit can be mapped to a classical model that can be simulated efficiently, and the magic can be characterized using any magic measure that is additive for tensor product of single-qubit states. Leveraging this observation, we study the magic transition in this circuit in both one- and two-dimensional lattices using large-scale numerical simulations. Our results demonstrate the presence of a magic transition between two different phases with extensive magic scaling, separated by a critical point in which the mutual magic exhibits scaling behavior analogous to entanglement. We further show that these two distinct phases can be distinguished by the topological magic. In a different regime, with a vanishing rate of non-Clifford measurements, we find that the magic saturates in both phases.

TT 56.6 Fri 10:45 H37

Developing a Framework for Predicting Useful Quantum Advantage in the Calculation of Molecular NMR Spectra — •Keith Fratus, Andisheh Khedri, Juha Leppäkangas, Michael Marthaler, and Jan Reiner — HQS Quantum Simulations GmbH, Karlsruhe, Germany

Demonstrating useful quantum advantage remains a primary goal of quantum computing efforts in the NISQ era. Key to such efforts is the ability to estimate the accuracy and performance of competing classical approximation methods when exact comparisons are not available. In this talk we report on our efforts to develop and understand the behaviour of various classical approximation methods which aim to solve a specific class of chemical simulation problems. In particular, we develop classical simulation methods designed to predict molecular NMR spectra, with the aim of being able to quantify the accuracy and computational requirements of performing these simulations, even for parameter regimes which we do not directly simulate. Using such methods, we work towards a framework for predicting in which parameter regimes, system sizes, and target accuracies one can expect the failure of classical methods for this class of systems, thus allowing for the possibility of quantum advantage.

TT 56.7 Fri 11:00 H37

Linear differential equation approach to the Loschmidt amplitude — •Michael Vogl — King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

The Loschmidt amplitude is a popular quantity that allows making predictions about the stability of quantum states under time evolution. We present an approach that allows us to find a linear differential equation that can be used to compute the Loschmidt amplitude. This approach, while in essence perturbative, has the advantage that it converges at finite order. We demonstrate that the approach for generically chosen matrix Hamiltonians often offers advantages over Taylor and cumulant expansions even when we truncate at finite order. Even in low dimensional systems such as two band Hamiltonians (multi-Weyl semimetals and AB bilayer graphene) it can be used to obtain general formulas for the Loschmidt amplitude after a quench. Results readily generalize to find transmission amplitudes and specific contributions of the partition function, too. Our method can also be applied to many body spin and fermionic Hamiltonians. Here, while the approach still offers advantages, more care has to be taken than in a generic case. We also provide an estimate for a breakdown time of the approximation.

TT 57: Topology and Symmetry-protected Materials (joint session O/TT)

Time: Friday 10:30–12:15 Location: H25

TT 57.1 Fri 10:30 H25

Topological material in the III–V family: heteroepitaxial InBi on InAs — •L. Nicolaï[1], J. Minár[1], M.C. Richter[2,3], O. Heckmann[2,3], J.-M. Mariot[4], U. Djukic[2], J. Adell[5], M. Leandersson[5], J. Sadowski[6], J. Braun[7], H. Ebert[7], J.D. Denlinger[8], I. Vobornik[9], J. Fujii[9], P. Šutta[1], G.R. Bell[10], M. Gmitra[11,12], and K. Hricovini[2,3] — [1]Univiversity of West Bohemia — [2]CY Cergy-Paris Université — [3]Université Paris-Saclay — [4]Sorbonne Université — [5]Lund University — [6]Polish Academy of Sciences — [7]LMU München — [8]ALS — [9]Istituto Officina dei Materiali, CNR — [10]University of Warwick — [11]Pavol Jozef Šafárik University in Košice — [12]Slovak Academy of Sciences

InBi(001) is formed epitaxially on InAs(111)-A by depositing Bi on to an In-rich surface. ARPES measurements reveal topological electronic surface states, close to the $\overline{\mathrm{M}}$ high symmetry point. InBi surprisingly shows coexistence of Bi and In surface terminations. For the Bi termination, the study gives a consistent physical picture of the topological surface electronic structure of InBi(001) terminated by a Bi bilayer rather than a surface formed by splitting to a Bi monolayer termination. Theoretical calculations based on relativistic DFT and the one-step model of photoemission clarify the relationship between the InBi(001) surface termination and the topological surface states, supporting a predominant role of the Bi bilayer termination. Furthermore, a tight-binding model based on this Bi bilayer termination with only Bi–Bi hopping terms gives a deeper insight into the spin texture[1]. [1] Nicolaï *et al.* Phys. Rev. Research 6.4 (2024): 043116.

TT 57.2 Fri 10:45 H25

Hidden spin-texture in an inversion-symmetric Dirac crystal — Kenta Hagiwara[1,2], Peter C. Schmitz[1], Philipp Rüssmann[1], Xin Liang Tan[1,2], Ying-Jiun Chen[3], Kui-Hon Ou Yang[4], Raman Sankar[5], Chien Jing[4], Yi-Hsin Shen[4], Mahmoud Zeer[1], Dongwook Go[6], Iulia Cojocariu[1], Daniel Baranowski[1], Vitaliy Feyer[1], Minn-Tsong Lin[1,6], Stefan Blügel[1], Claus M. Schneider[1,2], Yuriy Mokrousov[1,5], and •Christian Tusche[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, — [2]Faculty of Physics, University of Duisburg-Essen — [3]Ernst Ruska-Centre, Forschungszentrum Jülich — [4]Department of Physics, National Taiwan University, Taipei, Taiwan — [5]Academia Sinica, Taipei, Taiwan — [6]Johannes-Gutenberg University Mainz

A hidden spin polarization refers to a local spin polarization caused by apparent symmetry breaking and offers new perspectives for spintronics applications. Transition metal dichalcogenides can host various topological phases depending on the symmetry of their crystal structure. Here, by means of spin-resolving momentum microscopy, we reveal the spin texture of both topologically and symmetrically distinct surface and bulk Dirac cones in the inversion symmetric Dirac semimetal $NiTe_2$. We discovered a "hidden" spin polarization the bulk Dirac cone, localized at the different Te layers of the inversion symmetric bulk unit cell, such that the overlap of the two states results in a topologically trivial Dirac cone enforced by the global crystal symmetry. This work establishes a link between topology, spin-texture, and symmetry, enabling control by external perturbations.

TT 57.3 Fri 11:00 H25

Edge spectroscopy of the quantum spin Hall insulator indenene — •Jonas Erhardt[1,2], Mattia Ianetti[3], Gianni Profeta[3], Domenico Di Sante[4], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Department of Physical and Chemical Sciences, University of L'Aquila — [4]Department of Physics and Astronomy, University of Bologna — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The non-trivial topology of the quantum spin Hall insulator indenene was recently demonstrated through bulk probes that reveal its topological band ordering [1,2]. According to the bulk-boundary correspondence, this ensures the existence of robust metallic states confined to the edge of this triangular indium monolayer. In this study, we employ scanning tunneling spectroscopy to investigate all three edge types of indenene for this correspondence. Our results demonstrate metallic edge density of states with suppressed backscattering near the bulk band gap, providing strong evidence for the existence of topologically protected edge states in indenene.

[1] M. Bauernfeind, J. Erhardt, and P. Eck *et al.*, Nat. Commun. **12**, 5396 (2021)
[2] J. Erhardt *et al.*, Phys. Rev. Lett. **132**, 196401 (2024)

TT 57.4 Fri 11:15 H25

Bismuthene at the Graphene/SiC Interface: A Protected Quantum Spin Hall Insulator — •Niclas Tilgner[1], Susanne Wolff[1], Serguei Soubatch[2], Andres D. P. Unigarro[1], Sibylle Gemming[1], F. Stefan Tautz[2], Christian Kumpf[2], Thomas Seyller[1], Fabian Göhler[1], and Philip Schädlich[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Quantum spin Hall insulators (QSHIs) hold the potential to revolutionize next-generation technologies. Kane and Mele identified 2D honeycomb structures of heavy atoms with strong spin-orbit coupling as promising candidates for these materials. To realize this potential, however, the QSHI must be shielded from environmental influences. Previous research has demonstrated the intercalation of 2D Bi layers beneath graphene on SiC, resulting in the formation of two distinct phases. Among those, the β-phase exhibits a $(\sqrt{3}\times\sqrt{3})R30^\circ$ periodicity relative

to the substrate. We identify the Bi adsorption site using x-ray standing wave imaging, a method which deterimes the element specific, 3D atomic distribution with respect to the bulk unit cell. After subsequent hydrogen intercalation, the Bi position changes significantly from hollow to top site adsorption. Further measurements with angle-resolved photoelectron spectroscopy reveal the band structure of the QSHI bismuthene with a pronounced Rashba splitting and slight p-type doping. We propose that the initial β-phase has to be considered as an electronically inactive layer of bismuthene, whose electronic structure can be established by subsequent hydrogen intercalation.

TT 57.5 Fri 11:30 H25

Probing the Electronic Structure at the Boundary of Topological Insulators in the Bi2Se3 Family by Combined STM and AFM — •Christoph S. Setescak[1], Irene Aguilera[2], Adrian Weindl[1], Matthias Kronseder[1], Andrea Donarini[1], and Franz J. Giessibl[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Amsterdam and European Theoretical Spectroscopy Facility (ETSF), Amsterdam, The Netherlands

We develop a numerical scheme for the calculation of tunneling current I and differential conductance dI/dV of metal and CO terminated STM tips on the topological insulators Bi2Se3, Bi2Te2Se and Bi2Te3 and find excellent agreement with experiment. The calculation is an application of Chen's derivative rule, whereby the Bloch functions are obtained from Wannier interpolated tightbinding Hamiltonians and maximally localized Wannier functions from first-principle DFT+GW calculations. We observe signatures of the topological boundary modes, their hybridization with bulk bands, Van Hove singularities of the bulk bands and characterize the orbital character of these electronic modes using the high spatial resolution of STM and AFM. Bare DFT calculations are insufficient to explain the experimental data, which are instead accurately reproduced by many-body corrected GW calculations.

TT 57.6 Fri 11:45 H25

Revealing higher-order topological bulk-boundary correspondence in Bi crystals with spin-helical hinge state loop and proximity superconductivity — •Dongming Zhao[1], Yang Zhong[1], Tian Yuan[1], Haitao Wang[1], Tianxing Jiang[1], Yang Qi[1], Hongjun Xiang[1,2,3], Xingao Gong[1,2,3], Donglai Feng[2,3,4], and Tong Zhang[1,2,3,4] — [1]Fudan University, Shanghai, China — [2]Collaborative Innovation Center for Advanced Microstructures, Nanjing, China — [3]Shanghai Research Center for Quantum Sciences, Shanghai, China — [4]Hefei National Laboratory, Hefei, China

Topological materials are typically characterized by gapless boundary states, known as bulk-boundary correspondence. Recently, this concept has been generalized in higher-order topological insulators (HOTIs). E.g., a 2nd-order 3D TI hosts 1D topological hinge states winding around the crystal. A complete verification of HOTI will require probing all crystal boundaries. Here we studied a promising candidate of 2nd-order TI, Bi, in the form of mesoscopic crystals grown on superconducting V3Si. Using low-temperature STM, we directly observed dispersive 1D states on various hinges. Upon introducing magnetic scatterers, new scattering channels emerged selectively on certain hinges, revealing their spin-helical nature. Combining first-principle calculation and global symmetry analysis, we find these hinge states topological and formed a closed loop encircling the crystal. This provides direct evidence on the HOTI in Bi. Moreover, proximity superconductivity is observed in the topological hinge states serving as a promising platform for realizing topological superconductivity.

TT 57.7 Fri 12:00 H25

Simultaneous Atomic-Scale Imaging and Electronic Characterization of Wet-Chemically Prepared Bi_2Se_3 Nanoplatelets — •Auke Vlasblom, Victor Wesselingh, Jara Vliem, Daniel Vanmaekelbergh, and Ingmar Swart — Utrecht University, Utrecht, The Netherlands

Colloidal semiconductor nanoparticles are of great interest for various optoelectronic applications, such as integration in displays, solar cells and electronics. For applications, the surface of nanoparticles is of critical importance. However, until now, no technique exists to simultaneously investigate the atomic structure (e.g. the presence of defects) and the electronic properties of a nanoparticle, foremost limited by the presence of ligands that prevent direct access to the surface with a local probe. Here, we present a new and widely applicable procedure that allows investigation of the surface of a nanoparticle with a local probe. Using this method, nanoparticles are transferred to an atomically clean substrate under ultra-high vacuum conditions. We demonstrate the procedure for topological two-dimensional Bi_2Se_3 nanoplatelets deposited on Au(111). We reveal the atomic and electronic structure of the surface of colloidally synthesised Bi_2Se_3 nanoplatelets with scanning tunneling microscopy and spectroscopy measurements. In this talk, I will highlight the various types of defects that occur at the (sub-)surface of Bi_2Se_3 nanoplatelets and I will show their influence on the electronic structure.

TT 58: f-Electron Systems and Heavy Fermions

Time: Friday 11:30–13:00 Location: H31

TT 58.1 Fri 11:30 H31

The in-plane magnetic anisotropy of the coupled antiferromagnetic and charge-multipolar orders in $CeRh_2As_2$ — •Konstantin Semeniuk[1], Seunghyun Khim[1], and Elena Hassinger[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Dresden University of Technology, Institute for Solid State and Materials Physics, Dresden, Germany

The heavy-fermion superconductor $CeRh_2As_2$ displays multiple intriguing electronic orders (1,2). Besides two superconducting phases, the material also hosts a state called Phase I at temperatures below $T_0 = 0.5$ K. Phase I exhibits magnetism (3), but the response of T_0 to a magnetic field H along the *ab* plane of the tetragonal lattice is incompatible with conventional magnetic orders. In particular, while $T_0(H)$ is rather stable in Phase I, at a critical field H_{cr} the material transitions into Phase II, in which T_0 rapidly increases with field.

We conducted a detailed investigation of the H-T phase diagram of $CeRh_2As_2$ for various in-plane field orientations. The behaviour of $T_0(H)$ is remarkably different for $H||[100]$ and $H||[110]$, with, respectively, suppression and enhancement of T_0 in Phase I, as well as strong anisotropy of H_{cr}. In line with recent theoretical work (4), we regard Phase I as a unique case of coupled antiferromagnetic and charge-multipolar orders, and use our results to constrain the model.

[1] S. Khim et al., Science **373**, 1012 (2021).
[2] D. Hafner et al., Phys. Rev. X **12**, 011023 (2022).
[3] S. Khim et al., arXiv:2406.16575.
[4] B. Schmidt & P. Thalmeier, Phys. Rev. B **110**, 075154 (2024).

TT 58.2 Fri 11:45 H31

Complex magnetic order from multiple Ce–sites in $CeRhSn_2$. — Petr Opletal[1], Jan Fikáček[1], Arumugam Thamizhavel[2], Zakir Hossain[3], Róbert Tarasenko[4], Vladimír Tkáč[4], and •Jeroen Custers[1] — [1]Charles University, MMF DCMP, Prague, Czech Republic — [2]DCMP & MS, Tata Institute of Fundamental Research, Mumbai, India — [3]Dept. of Physics, Indian Institute of Technology, Kanpur, India — [4]Institute of Physics, Faculty of Science, P.J. Šafárik University, Košice, Slovak Republic

Previous reports on polycrystalline $CeRhSn_2$ reveal different magnetic ground states being ferromagnetic ($T_C = 4$ K) or antiferromagnetic ($T_N = 3.5$ K). To elucidate we have grown a single crystal and conducted measurements of the magnetization (M), specific heat (C_p/T), and electrical resistivity (ρ). The compound crystallizes in the orthorhombic lattice structure with space group *Cmcm* characterized by the cell parameters $a = 4.5905(10)$Å, $b = 16.9758(5)$Å and $c = 9.5924(3)$Å. Moreover, it exhibits two crystallographic inequivalent Ce–sites with a zigzag chain of Ce–atoms running along the c–axis. Our measurements reveal an AFM phase transition at $T_{M1} = 3.6$ K manifesting by a strong decrease of the orthorhombic c–axis magnetization, while only a tiny cusp is notable along the other directions, a sharp discontinuity in C_p/T and a kink in ρ and a subsequent ferrimagnet–like (FIM) ordering at $T_{M2} = 1.7$ K visible by a λ-shape of peak in C_p/T and a sudden drop in the resistivity. We map out a B–T phase diagram for field $B \parallel b$–axis and follow the evolution of the transitions under hydrostatic pressure up to 3 GPa.

TT 58.3 Fri 12:00 H31

Anderson impurity model calculations for line shape analyses of core to valence RIXS spectra of Ce Kondo materials — •Michelangelo Tagliavini[1], Federico Mazza[2], Xinlin Yan[2], Andrey Prokofiev[2], Kurt Kummer[3], Maurits W. Haverkort[1], and Silke Paschen[2] — [1]*Institute for Theoretical Physics (ITP), Heidelberg University*, Philosophenweg 19, 69120, Heidelberg, Germany — [2]*Institute of Solid State Physics, Vienna University of Technology*, Wiedner Hauptstr. 8-10/138 A 1040 Vienna, Austria — [3]*European Synchrotron Radiation Facility*, 71 Avenue des Martyrs, CS40220, F-38043 Grenoble Cedex 9, France

In rare-earth-containing heavy-fermion compounds, the interaction of continuum electrons with 4f local moments can give rise to a Kondo screened ground state. Crystal-field excited states can be probed using Resonant Inelastic X-ray Scattering (RIXS). Interaction between localized 4f states and continuum electrons transforms the crystal-field excitations into resonances with hybridization-dependent asymmetric line shapes. In this study, we present results for two heavy-fermion compounds: $CeBa_7Au_6Si_{40}$ and $CeRu_4Sn_6$, which exhibit low (≈1 K) and high (≈ 200 K) Kondo temperatures, respectively. Using density-functional-theory-based Anderson impurity model calculations implemented in Quanty (www.Quanty.org), we link the f-f transition line shapes to the hybridiza-

tion function in these materials. Our findings reveal a direct relationship between the hybridization function, the Kondo temperature, and the crystal fields, offering new insights into the underlying physics of these complex systems.

TT 58.4 Fri 12:15 H31

Emergent in-plane anisotropic elastoresistance in $YbRh_2Si_2$ — •Soumendra Nath Panja, Jacques Gounelle-Pontanel, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

We have shown recently that the Kondo interaction in the tetragonal heavy-fermion metal $YbRh_2Si_2$ can be efficiently tuned by tensile and compressive uniaxial strain along the [100] axis [1]. Here, we present a detailed investigation of the temperature dependent elastoresistance $d\rho/d\epsilon_i$ of $YbRh_2Si_2$, for both i=[100] and [110] directions. Remarkably, elastoresistance develops a pronounced in-plane strain anisotropy at low temperatures that is analyzed with respect to the influence of uniaxial strain on the crystal electric field splitting and Kondo interaction. Furthermore, we investigate the combined impact of magnetic field and strain on the low-temperature elastoresistance behavior in $YbRh_2Si_2$.

[1] S.N. Panja, A. Jesche, N. Tang, P. Gegenwart, Phys. Rev. B **109**, 205152 (2024).

TT 58.5 Fri 12:30 H31

Anisotropic antiferromagnetic order in $EuPd_3Si_2$ — •Michelle Ocker[1], Nour Marayatta[2], Michael Merz[2], Kristin Kliemt[1], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt/Main, Germany — [2]Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

The magnetic order of a rare earth compounds is determined by the RKKY exchange interaction. In case of Eu compounds small changes in the growth method or the initial composition can potentially lead to small composition changes which than modify the physical properties [1]. For example, the compound $EuPd_3Si_2$, which crystallises in the orthorhombic space group Imma, shows a ferromagnetic transition at T_{C1} = 78 K and a spin reorientation at T_{C2} = 5 K according to Ref. [2]. Whereas our $EuPd_3Si_2$ samples show an antiferromagnetic transition at T_{N1} = 61 K and a possible reorientation at T_{N2} = 40 K. With field aligned along the three main symmetrie directions, our samples show different degrees of anisotropy, as has been observed for related compounds [3]. In this presentation, we report about the crystal growth and our evaluation of the physical properties, from which we constructed a magnetic phase diagram.

[1] K.Kliemt et al. Cryst. Growth Des. 22, 5399 (2022).
[2] S.Sharma et al. Phys. Rev. Mater. 7, 023402 (2023).
[3] K.Shigetoh et al. Phys. Rev. B 76, 184429 (2007).

TT 58.6 Fri 12:45 H31

Coherent valence dynamics in UAl_3 — •Vinicius Estevo Silva Frehse[1], Hlynur Gretarsson[2], Eric Bauer[3], Atsushi Hariki[4], Filip Ronning[3], and Marein Rahn[1] — [1]Center for Electronic Correlations and Magnetism, Augsburg, Germany — [2]P01 High Resolution Dynamics Beamline, Hamburg, Germany — [3]Institute for Materials Science, Los Alamos, USA — [4]Department of Physics and Electronics, Osaka, Japan

The interaction between itinerant and localized electrons, as proposed by the Kondo model, enables the formation of heavy fermions, and unconventional superconductivity. In f-electron intermetallics with a large Kondo temperature, the emergence of lattice-coherent valence dynamics can be resolved by resonant inelastic x-ray scattering (RIXS). In the simple cubic, strongly valence fluctuating compound UAl_3, a coherent Fermi surface of Kondo quasiparticles emerges around $T_{coh} \sim 200$ K. We study the excitations of these quasiparticles using the newly available RIXS instrumentation for the tender x-ray range. The spectra indeed reveal dispersive trends of the 5f interband excitations at low temperatures, reminiscent of the isostructural 4f compound $CePd_3$[1]. [1] M.C.Rahn, *et al.*, Nat. Comm. **13**, 6129 (2022).

TT 59: Quantum Chaos (joint session DY/TT)

Time: Friday 11:30–13:00 Location: H37

TT 59.1 Fri 11:30 H37

Semiclassical foundation of universality in many-body quantum circuits — •Maximilian Kieler[1], Felix Fritzsch[2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

For single particle systems the fundamental equivalence of quantum chaotic systems and random matrix theory is well-understood by means of semiclassical periodic orbit theory. We propose an extension to spatially local many-body systems by incorporating the concept of symmetry-breaking. Using this we show that random matrix behavior arises generically in quantum chaotic many-body systems in the form of a symmetry breaking of local time-translation symmetries. This general framework is applied to quantum circuits where an explicit correspondence to the random matrix result for the spectral form factor can be shown.

TT 59.2 Fri 11:45 H37

Distribution of resonance poles of chaotic scattering systems — •Jan Robert Schmidt, Florian Lorenz, and Roland Ketzmerick — TU Dresden, Institute of Theoretical Physics, Dresden, Germany

The distribution of resonance poles of chaotic scattering systems is investigated in the semiclassical limit at unprecedented small wavelengths. For the paradigmatic three-disk scattering system, we study the spectral gap towards the real axis, the fractal Weyl law, which counts the number of resonance poles, and the distribution of decay rates. These properties are compared to previous analytical results, e.g. from random matrix theory. In contrast to this system with full escape, systems with partial escape have significantly different properties. For the example of a dielectric cavity, we show that results from random matrix theory cannot explain the distribution of decay rates.

TT 59.3 Fri 12:00 H37

Solved after 60 years: Exact Derivation of the Ericson Transition in Quantum Chaotic Scattering — •Simon Köhnes and Thomas Guhr — University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Scattering experiments are the prime source of information on the quantum world. Scattering theory nowadays has numerous applications in various branches of physics and beyond, even including classical wave phenomena. We analyze chaotic scattering systems in the framework of Random Matrix Theory. The distribution of the scattering matrix elements is the key quantity. A strong sign of chaos in complex quantum systems is the Ericson regime of strongly overlapping resonances in which the cross sections exhibit random behavior. We apply the Supersymmetry Method. For the three Wigner-Dyson symmetry classes, we analytically calculate the transition to the Ericson regime, facilitating direct comparison with experimental results. In the course of doing so, we also gather new information on features of the underlying supersymmetric non-linear sigma model.

TT 59.4 Fri 12:15 H37

Chaotic Quantum Scattering: Exact Solutions for Systems with Spin — •Nils Gluth and Thomas Guhr — Universität Duisburg-Essen, Duisburg, Germany

Scattering experiments facilitate access to quantum systems. Scattering theory is needed to fully describe the involved experimental situations. Over the years, it became a powerful tool with applications to a large variety of different systems, such as for example compound nuclei, atoms, molecules, quantum graphs or even microwave networks and cavities. These systems are typically complex or in a broad sense chaotic, calling for statistical approaches, in particular Random Matrix Theory. Considerably extending our previous work, we calculate the distribution of scattering matrix elements and cross sections using Supersymmetry. We focus on the symplectic symmetry class which had not yet been solved, because a theoretical understanding is needed in view of recent experiments. We provide a comparison of our results with experimental data.

TT 59.5 Fri 12:30 H37

Phase-space representations and exceptional points of coupled polarized modes in cylindrical cavities — •Tom Rodemund[1], Shilong Li[2], Síle Nic Chormaic[3], and Martina Hentschel[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]College of Information Science and Electronic Engineering, Zhejiang University, Hangzhou, China — [3]Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

% Optical microcavities are often assumed to be two-dimensional (2D). This allows a convenient phase-space representation in 2D, where Poincaré surface of section for particle dynamics and the Husimi function for their wave counterpart are prominent methods. Here we extend the concept of Husimi functions for open systems [1] to three-dimensional (3D) optical microcavities of arbitrary shape. In particular we study deformed cylindrical cavities and illustrate their mode dynamics in terms of generalized Husimi functions.

The coupling between the two different polarizations (TE and TM) is a new feature in realistic 3D optical cavities that is not present in 2D. We find the interaction of polarized modes to be governed by a network of exceptional points that reflects the openness, or non-Hermiticity, of the system. The mode coupling is analyzed using the extended Husimi formalism that we find to be a comprehensive and useful way to represent the mode structure of 3D microcavities [2].

[1] Hentschel et al., Europhys. Lett. 62 636 (2003)
[2] Rodemund et al., to be submitted.

TT 59.6 Fri 12:45 H37

The classical Maldacena-Shenker-Standford bound — •Gerrit Caspari, Fabian Haneder, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Regensburg, Deutschland

The Maldacena-Shenker-Stanford (MSS) bound [1] is a condition on a system's quantum Lyapunov exponent, defined as half the growth rate of the regularised out-of-time-ordered correlator (OTOC), which states that said exponent is bounded by the system's temperature, with, e.g., black holes as characteristic systems saturating the bound.

From the perspective of classical chaos, this is surprising, since the classical Lyapunov exponent seems not to be bounded. We study chaotic quantum systems in a hyperbolic geometry with and without cusps and magnetic fields [2][3] via Selberg's Trace Formula (STF). Through this we derive bounds on the classical Lyapunov exponent from analyticity conditions in the trace formula and relate them to the MSS bound.

We report our progress in studying these bounds using the STF, which entails an investigation of the analyticity condition needed to prove the STF for the partition function of our systems and its relation to possible phase transitions.

[1] Maldacena, J., Shenker, S.H. & Stanford, J. High Energ. Phys. 2016, 106 (2016).
[2] Aurich, R., & Steiner, F. (1992)., Proceedings: Mathematical and Physical Sciences, 437(1901), 693-714
[3] Avron, J.E., Klein, M. & Pnueli, A., Phys. Rev. Lett. 69 (1992)

Working Group on Equal Opportunities
Arbeitskreis Chancengleichheit (AKC)

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Overview of Invited Talks and Sessions

(Lecture hall H2)

Invited Talks

AKC 1.1	Fri	10:45–11:15	H2	**Reshaping the History of Quantum Physics: Paths to Gender Equality** — •Andrea Reichenberger
AKC 1.2	Fri	11:15–11:45	H2	**Prevention and protection against sexual harassment, discrimination and violence (SBDG): A private matter or how much does it concern us as a university?** — •Michael Tunç

Sessions

AKC 1.1–1.2	Fri	10:45–12:15	H2	**AKC**
AKC 2	Fri	12:15–13:15	H2	**Women in Physics Lunch**

Sessions

– Invited Talks –

AKC 1: AKC

Time: Friday 10:45–12:15 Location: H2

Invited Talk AKC 1.1 Fri 10:45 H2

Reshaping the History of Quantum Physics: Paths to Gender Equality — •Andrea Reichenberger — TU Munich

We are all familiar with gender dynamics, biases, and stereotypes on the online platforms we visit, use, and co-create every day. They are ubiquitous in large language models (LLMs) and other generative AI technologies trained on large amounts of data. Their spillover effects are now well studied in scientific research. There is comparatively little research on how the history of physics is represented and practiced in today's online spaces. This talk will take you on a journey through the history of quantum physics, exploring new avenues for a gender-sensitive future of the history of physics. And it offers a critical insight into how expertise in the history of physics, science communication and public opinion influence and reinforce each other in the practice of digital history. Drawing on a series of case studies on women in the history of quantum physics, we examine the Matilda effect on online platforms and offer perspectives on how to successfully counteract this effect, which gives a name to the systematic misrecognition of women's contributions to science and technology.

Invited Talk AKC 1.2 Fri 11:15 H2

Prevention and protection against sexual harassment, discrimination and violence (SBDG): A private matter or how much does it concern us as a university? — •Michael Tunç — Katholische Hochschule für Sozialwesen, Berlin, Deutschland

Universities have the obligation to implement measures to prevent sexual harassment in the workplace according to AGG paragraph 12. But there are people reporting assaults and sexual harassment against physicists occur repeatedly.

In this lecture, participants will get brief informations how they can effectively support/protect themselves and others at universities. The lecture would like to sensitize by presenting the following basic informations:

- What is sexual harassment at the university (facts and figures)?
- What are the causes and consequences of sexual harassment for employees and the university organization?
- What are the rights of those affected and the obligations of those involved?

The topic of being/becoming a bystander includes sensitization as well as hits on concrete options for action, both for male and female participants. First ideas will be given how a complaint procedure to prosecute sexual harassment can be established. Relevant questions are:

- How can a professional protection of victims succeed?
- How do you deal with your fears of hierarchical, legal consequences?
- How can you protect dependent people from hierarchically superior people?

30 min. discussion

AKC 2: Women in Physics Lunch

Time: Friday 12:15–13:15 Location: H2

Female physicists of all career stages are cordially invited to join our meet-and-greet networking lunch or snack. Diverse and all kinds of interested colleagues are also welcome!

Working Group on Industry and Business
Arbeitskreis Industrie und Wirtschaft (AIW)

Hans-Georg Grothues
Vorsitzender des AIW
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Overview of Talks and Sessions

(Lecture halls H4)

Talks

AIW 1.1	Wed	14:10–14:30	H4	**Von Quantenwinter bis Quantensprung - Wo stehen Quantentechnologien heute?** — •Carina Kiessling
AIW 1.2	Wed	14:30–14:50	H4	**Der Weg zum praktischen Quantencomputing - Potenziale und Use-Cases** — •Nico Piatkowski
AIW 1.3	Wed	14:50–15:10	H4	**Wie verbinden wir die Quanten- mit unserer klassischen Welt?** — •Claudius Riek
AIW 2.1	Wed	16:00–16:20	H4	**Introduction to quantum cryptography and related use-cases** — •Mathieu Bozzio
AIW 2.2	Wed	16:20–16:40	H4	**Quantenkommunikation in der Raumfahrt** — •Stephan Seidel
AIW 2.3	Wed	16:40–17:00	H4	**Small is beautiful: Leading innovation in miniaturizing quantum sensors** — •Binh Tran

Sessions

AIW 1.1–1.3	Wed	14:00–15:30	H4	**Quantencomputing**
AIW 2.1–2.3	Wed	15:55–17:20	H4	**Quantenkommunikation**
AIW 3	Wed	17:20–18:30	H4	**Get Together bei Bier und Brezeln**

Sessions

– Talks –

AIW 1: Quantencomputing

Time: Wednesday 14:00–15:30 Location: H4

Willkommen und Grußwort durch AIW und AKPIK - Hans-Georg Grothues, John Kettler, Tim Ruhe

AIW 1.1 Wed 14:10 H4

Von Quantenwinter bis Quantensprung - Wo stehen Quantentechnologien heute? — •Carina Kiessling — Roland Berger

Von Quantenwinter bis Quantensprung - Wo stehen Quantentechnologien heute?", gibt einen Einblick in die Markt-Entwicklung von Quantentechnologien und in den Fortschritt kommerzieller Anwendungen. Darüber hinaus werden Zukunftspotenziale hinsichtlich Zeithorizont, Kollaboration zwischen Forschung und Wirtschaft sowie geopolitische Schwachstellen diskutiert.

AIW 1.2 Wed 14:30 H4

Der Weg zum praktischen Quantencomputing - Potenziale und Use-Cases — •Nico Piatkowski — Fraunhofer-Institut für Intelligente Analyse- und Informationssysteme

Auch wenn nahezu monatlich neue Durchbrüche berichtet werden, steckt die praktische Anwendung von Quantencomputern noch in den Kinderschuhen. Für die meisten produktiven Anwendungen sind Quantenalgorithmen nicht bekannt, und wenn doch, sind die praktischen Probleminstanzen oft zu groß für die derzeit verfügbaren Quantencomputer. Daher ist es heute wichtig, sich mit generellen Fragen der Anwendbarkeit auseinanderzusetzen. In meinem Vortrag erkläre ich, welche Berechnungsprobleme vom Quantencomputing profitieren können, und stelle drei Use-Cases aus den Bereichen Erdbeobachtung, Chipdesign und Flugplanmanagement vor. Experimentelle Ergebnisse zeigen, was heute möglich ist und wo noch Forschungsbedarf besteht.

AIW 1.3 Wed 14:50 H4

Wie verbinden wir die Quanten- mit unserer klassischen Welt? — •Claudius Riek — Zurich Instruments Germany

Die Nutzung der Quantenphysik ermöglicht Anwendungen, die über das hinausgehen, was auf der Grundlage der klassischen Physik möglich ist. Modernste Technologien wie Elektronik, Kryogenik oder Photonik erlauben es uns erst, dieses Potenzial auszuschöpfen. Zurich Instruments bietet Messtechnik und Steuerelektronik für Quantencomputer an, um Qubits zu kontrollieren, auszulesen und eine Quantenfehlerkorrektur durchzuführen und so die Quantenwelt effektiv mit unserer klassischen Welt zu verbinden. Die Umsetzung von Technologien aus dem Labor in innovative Produkte erfordert ein tiefes Verständnis der wissenschaftlichen Anwendungen. - Wie und wo Physiker auf dieser Reise ihren Beitrag leisten, ist oft nicht so offensichtlich, wie es vielleicht aussieht.

Podiumsdiskussion: Quantencomputing - Perspektiven für die Industrie

AIW 2: Quantenkommunikation

Time: Wednesday 15:55–17:20 Location: H4

Finde deinen Weg: Berufliche Orientierung und Unterstützung durch die DPG - Gabriele Becker - DPG Geschäftsstelle

AIW 2.1 Wed 16:00 H4

Introduction to quantum cryptography and related use-cases — •Mathieu Bozzio — Universität Wien

Harnessing the quantum properties of light can boost the security of communication networks by relying on physical assumptions instead of computational assumptions. This talk will provide a brief introduction to the principles of quantum cryptography and present use-cases in which its security features may be desirable such as message encryption, leader election and centralized digital payments

AIW 2.2 Wed 16:20 H4

Quantenkommunikation in der Raumfahrt — •Stephan Seidel — Airbus Defence \& Space

Das Aufkommen von Quantencomputern stellt eine Bedrohung für die derzeit verwendeten asymmetrischen Verschlüsselungsalgorithmen dar, da Quantencomputer die klassisch rechenintensiven mathematischen Probleme, auf denen diese Algorithmen basieren, in deutlich kürzerer Zeit lösen können. Dies eröffnet nicht nur die Möglichkeit Nachrichten zu entschlüsseln, die nach einer breiten Verfügbarkeit von Quantencomputern gesendet wurden, sondern auch solcher die vorher aufgezeichnet wurden.

Die Quanten-Schlüsselverteilung (Quantum Key Distribution, QKD) ist ein Mittel, um diese Bedrohung zu neutralisieren. Sie nutzt die Prinzipien der Quantenmechanik, um Schlüssel für die Verschlüsselung sicher zwischen zwei Parteien zu verteilen. Daten werden in Quantenzuständen von Licht codiert, und da jede Messung an einem Quantenzustand diesen verändert, kann ein Abfangen des Schlüssels erkannt werden. In Kombination mit symmetrischer Verschlüsselung, beispielsweise durch One-Time-Pad-Verschlüsselung, bei der jedes Bit des Schlüssels direkt ein Bit der Nachricht verschlüsselt, kann eine sichere Kommunikation hergestellt werden. Diese Kommunikation ist sowohl gegen Angriffe klassischer als auch Quantencomputer resistent.

In Zukunft könnte eine europäischen Quantenkommunikationsinfrastruktur neben terrestrische Glasfasernetzwerken ein weltraumbasiertes System umfassen, um eine vollständige Abdeckung in der EU und auf anderen Kontinenten zu gewährleisten.

Airbus arbeitet an der Entwicklung der Quanten-Schlüsselverteilung in verschiedenen nationalen und europäischen Programmen, die von der Technologieentwicklung bis hin zur Architektur einer europäischen Quantenkommunikationsinfrastruktur reichen. In dieser Präsentation geben wir einen Überblick über den aktuellen Stand der Arbeiten.

AIW 2.3 Wed 16:40 H4

Small is beautiful: Leading innovation in miniaturizing quantum sensors — •Binh Tran — Bosch Quantum Sensing

After almost ten years of research in the field of quantum sensing, Bosch is taking the next step in transforming tabletop experiments into portable sensor solutions. In this talk, I will give you an introduction into our sensor technology based on nitrogen-vacancy (NV) centers in diamond. This technology provides many advantages over conventional sensors, such as a high magnetic field sensitivity with the ability to operate at ambient conditions. Finally, I will present how these unique properties open up exciting applications ranging from detecting tiny signals in medical diagnosis to improving airplane navigation.* I joined Bosch after finishing my PhD in experimental quantum physics. As a research engineer at Bosch, I am able to readily apply knowledge from physics lectures and laboratory experience into an emerging technology.

Podiumsdiskussion: Quantenkommunikation - Chancen für globale Anwendungen

AIW 3: Get Together bei Bier und Brezeln

Time: Wednesday 17:20–18:30 Location: H4

Im Anschluss an die Sitzungen lädt der Arbeitskreis Industrie und Wirtschaft zu Bier und Brezeln ein. In diesem Rahmen kann die Diskussion mit den Referenten und weiteren anwesenden Mitgliedern des AIW im persönlichen Gespräch vertieft werden.

Working Group on Physics, Modern IT and Artificial Intelligence Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Invited Talks and Sessions

(Lecture hall H5; Poster P2)

Invited Talks

AKPIK 3.1	Tue	11:00–11:30	H5	**3D Integration Towards Autonomous Optical Neural Networks** — •Adrià Grabulosa, Anas Skalli, Daniel Brunner
AKPIK 4.1	Tue	14:00–14:30	H5	**The Scaling of Intelligence: From Transformers to Agentic AI** — •Oliver Mey
AKPIK 4.2	Tue	14:30–15:00	H5	**Inverse Design in Electromagnetics with Artificial Intelligence** — •Willie Padilla
AKPIK 4.3	Tue	15:00–15:30	H5	**Inverse design of lateral hybrid metasurfaces with machine learning** — •Rui Fang, Amir Ghasemi, Dagou Zeze, Koen Valk, Yuqing Jiao, Peter Zijlstra, Mehdi Keshavarz Hedayati

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium AI in (Bio-)Physics (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	H1	**Predicting interaction partners and generating new protein sequences using protein language models** — •Anne-Florence Bitbol
SYAI 1.2	Thu	10:00–10:30	H1	**Realizing Schrödinger's dream with AI-enabled molecular dynamics** — •Alexandre Tkatchenko
SYAI 1.3	Thu	10:30–11:00	H1	**Emergent behavior of artificial intelligence** — •Steffen Rulands
SYAI 1.4	Thu	11:15–11:45	H1	**AI in medical research - navigating complexity with AI** — •Daniel Truhn
SYAI 1.5	Thu	11:45–12:15	H1	**Computational Modelling of Morphogenesis** — •Dagmar Iber

Sessions

AKPIK 1.1–1.3	Sun	16:00–18:15	H2	**Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)**
AKPIK 2.1–2.4	Tue	9:30–10:30	H5	**Machine Learning Prediction and Optimization Tasks**
AKPIK 3.1–3.5	Tue	11:00–12:30	H5	**Research with AI: Hardware, Software, Tools**
AKPIK 4.1–4.3	Tue	14:00–15:30	H5	**Focus: Applications of Deep Neural Networks**
AKPIK 5.1–5.19	Thu	15:00–16:30	P2	**Poster**
AKPIK 6.1–6.6	Thu	16:30–18:00	H5	**AI Methods for Materials Science**

Sessions

– Invited Talks, Tutorials, Contributed Talks, and Posters –

AKPIK 1: Hands-on Tutorial: AI Fundamentals for Research (joint session BP/TUT/DY/AKPIK)

Artificial intelligence (AI) has become an essential tool in modern physics, enabling new approaches to data analysis, modeling, and prediction. This hands-on tutorial provides an accessible introduction to key AI concepts, emphasizing their practical applications in physics research.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 10.03.2025, accessible via the following options:

GitHub repository:

https://github.com/RedMechanism/DPG-SKM-2025-Tutorial-AI-Fundamentals-for-Research

ZIP file download:

https://jlubox.uni-giessen.de/getlink/fiAGRzcGTiCL3GZxk8WAjom4/

Participants are encouraged to download them ahead of time.

Organized by Jan Bürger (Aachen), Janine Graser (Duisburg), Robin Msiska (Duisburg/Ghent), and Arash Rahimi-Iman (Gießen), with support from Stefan Klumpp (Göttingen) and Tim Ruhe (Dortmund).

Time: Sunday 16:00–18:15 Location: H2

Tutorial AKPIK 1.1 Sun 16:00 H2

Introduction — Jan Bürger[1], •Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session begins with an overview of essential AI concepts, including neural networks, training methodologies, and key distinctions between AI models. Participants will gain a foundational understanding of AI principles and how these tools can be leveraged for various research challenges.

5 min. break

Tutorial AKPIK 1.2 Sun 16:40 H2

Hands-On Session 1 – Function Approximation — •Jan Bürger[1], Janine Graser[2], Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

In the first half of the interactive session, participants will work with Jupyter Notebooks to explore practical applications of machine learning. They will train simple neural networks to predict a mathematical function, gaining hands-on experience in tuning key parameters. Since neural networks can typically be considered universal function approximators, this concept is effectively illustrated using a one-dimensional function, making it easy to visualize and understand.

5 min. break

Tutorial AKPIK 1.3 Sun 17:30 H2

Hands-On Session 2 – Classification and More — Jan Bürger[1], Janine Graser[2], •Robin Msiska[2,3], and Arash Rahimi-Iman[4] — [1]ErUM-Data-Hub, RWTH Aachen University, Aachen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Department of Solid State Sciences, Ghent University, Ghent, Belgium — [4]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University Gießen, Gießen, Germany

The session demonstrates how pre-trained models can simplify tasks such as classification, making them readily applicable to research. Typical examples include recognizing handwritten digits, which showcase the power of pretrained models in solving common challenges. As a preview of advanced topics, the tutorial concludes with brief examples of large language models (LLMs) and generative AI.

AKPIK 2: Machine Learning Prediction and Optimization Tasks

Time: Tuesday 9:30–10:30 Location: H5

AKPIK 2.1 Tue 9:30 H5

Attention space geometry — •Claudius Gros — Institute for Theoretical Physics, Goethe University Frankfurt

Attention involves comparing query and key vectors in terms of a scalar product, $\mathbf{Q} \cdot \mathbf{K}$, together with a subsequent softmax normalization. Classicaly, parallel/orthogonal/anti-parallel queries and keys lead to large/intermediate/small attention weights. Here we study expressive attention (EA), which is based on $(\mathbf{Q} \cdot \mathbf{K})^2$, the squared dot product. In this case attention is enhanced when query and key are either parallel or anti-parallel, and suppressed for orthogonal configurations. For a series of auto-regressive prediction tasks, we find that EA performs at least as well as the standard mechanism, dot-product attention (DPA). Increasing task complexity, EA is observed to outperform DPA with increasing margins, which also holds for multi-task settings. For a given model size, EA manages to achieve 100% performance for a range of complexity levels not accessible to DPA.

AKPIK 2.2 Tue 9:45 H5

Global Opimization of Atomic Structures in Extra Dimensions — •Casper Larsen[1], Sami Kaappa[2], Andreas Vishart[3], Thomas Bligaard[4], and Karsten Jacobsen[5] — [1]Technical University of München — [2]Tampere University — [3]Technical University of Denmark — [4]Technical University of Denmark — [5]Technical University of Denmark

This work formulates an approach to global optimization of atomic structures by use of an atomic descriptor extending the atoms with additional nonphysical degrees of freedom. These include chemical identity coordinates, atomic existence, and hyperspatial coordinates, all of which can be energetically minimized separately or simultaneously. The minimization is performed on a surrogate potential energy surface generated by Gaussian process regression trained on DFT calculations as part of a Bayesian optimization algorithm, where it is assured that all relaxational end states and training points are physically valid. The method is shown to successfully interpolate energy and force predictions from a training set of physically valid structures to structures with nonphysical coordinates. The inclusion of extra degrees of freedom significantly improves the efficiency of optimization of both clusters and bulk materials by circumventing energy barriers encountered in the conventional potential energy surface.

AKPIK 2.3 Tue 10:00 H5

Co-orchestration of multiple instruments for automated exploration of structure-property relationships in combinatorial libraries — •Boris Slautin[1], Utkarsh Pratiush[2], Ilia Ivanov[3], Yongtao Liu[3], Rohit Pant[4],

Xiaohang Zhang[4], Ichiro Takeuchi[4], Maxim Ziatdinov[5], and Sergei Kalinin[2,5] — [1]University of Duisburg-Essen, Essen, Germany — [2]University of Tennessee, Knoxville USA — [3]Oak Ridge National Laboratory, Oak Ridge, USA — [4]University of Maryland, College Park, USA — [5]Pacific Northwest National Laboratory, Richland, USA

The advancement of combinatorial synthesis techniques has significantly accelerated the development of novel materials. However, closing the loop in materials design requires powerful approaches for characterizing the synthesized libraries. This is a non-trivial task, as characterization often involves revealing multiple methods.

We present a multimodal co-orchestration framework for autonomous combinatorial library characterization through the simultaneous coordination of various tools (e.g., Raman spectroscopy, SPM). The multimodal co-orchestration enables the real-time utilization of acquired knowledge about one property to accelerate the exploration of other properties measured by different methods. The capabilities of the proposed framework were validated by the co-orchestrating of the SPM and Raman techniques in the Sm-BiFeO3 combinatorial library. The workflow confirms its effectiveness in optimizing the exploration trajectory. The proposed framework is general and can be extended to multiple modalities and arbitrary dimensionality of signals.

AKPIK 2.4 Tue 10:15 H5

Data nexus vista: A research assistance framework for physics-informed descriptor engineering — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

In today's fast-paced world, accurate modeling and prediction of complex systems are more crucial than ever, particularly for advancing modern technologies. In energy storage, for example, the design of materials with tailored properties for sustainable, next-generation devices is a critical goal. However, the vast materials space and intricate nature of materials data poses serious challenges for experimental and computational explorations, often likened to searching for a needle in a haystack. To address this, we present "Data Nexus Vista," a flexible framework for descriptor engineering. The framework offers four core functionalities: (1) adaptive preprocessing protocols for defining physically meaningful data transformations; (2) a feature selection interface that incorporates physics-based rules for improved interpretability; (3) diverse correlation analysis tools to uncover underlying physical mechanisms; and (4) workflows for developing interpretable models that balance physical validity with statistical robustness. By enabling thorough exploration of data-physical phenomena connections, this user-guided, modular approach ensures scientific rigor while addressing uncertainties in complex systems. Moreover, its adaptable design allows seamless application across diverse domains, from energy storage, surface science to nonlinear optical properties, advancing both scientific discovery and practical innovation.

AKPIK 3: Research with AI: Hardware, Software, Tools

Time: Tuesday 11:00–12:30 Location: H5

Invited Talk AKPIK 3.1 Tue 11:00 H5

3D Integration Towards Autonomous Optical Neural Networks — •Adrià Grabulosa, Anas Skalli, and Daniel Brunner — Institute Femto-ST, Université Marie et Louis Pasteur, CNRS UMR6174, 15B Avenue des Montboucons, Besançon, France.

In the last decades, modern electronic integrated circuits has reached a fundamental limit at 2 nm feature sizes. At the same time, emerging computing concepts such as neural networks (NNs), which are already playing a major role in modern societies, further amplifying this challenge. Adopting the third dimension is a promising strategy for achieving scalability of connections over the microchip's dimensions. Here, based on additive one- (OPP) and two-photon polymerization (TPP) processes and combined with direct-laser writing (DLW) settings, a complete toolbox comprising photonic waveguides, splitters and bends towards three-dimensional (3D) photonic integration is presented. The concept CMOS is validated by printing 3D photonic waveguides onto semiconductor (GaAs) substrates and silicon-on-insulator (SOI) platforms. Finally, we show first steps towards the 3D integration of a fully autonomous NN using spatially multiplexed modes of an injection locked large area vertical cavity surface emitting laser (LA-VCSEL) capable of performing NN tasks with >98% accuracy, fully realized in hardware using off-the-shelf, low energy consumption components. Overall, these building blocks are highly appealing for realizing fully-parallel and efficient communication throughout a densely-connected network, which are pivotal concepts for future NN computing topologies.

AKPIK 3.2 Tue 11:30 H5

Brain-inspired Computing with Gold Nanoparticle Networks: A Kinetic Monte Carlo Model — •Jonas Mensing and Andreas Heuer — Institute of physical Chemistry, University of Münster, Germany

Nanoparticles interconnected by insulating organic molecules exhibit nonlinear switching behavior at low temperatures. By assembling these nonlinear switches into a network and manipulating the inner charge transport dynamics via surrounding electrodes, the network can be functionalized to approximate functions such as Boolean Logic or model dynamical systems given the temporal dependence of input data. This makes nanoparticle networks promising candidates for neuromorphic computing and eventually bring machine learning applications on hardware.

We developed a kinetic Monte Calo simulation tool that applies established principles of single-electronics to model charge transport dynamics in nanoparticle networks. We demonstrate the network*s capability to approximate functions such as Boolean logic, perform nonlinear transformation of time dependent input signals, and forecast time series. These applications are evaluated using fitness metrics, enabling the optimization of surrounding electrode voltages to train the internal charge transport for a given task. The fitness measures are further analyzed in relation to system sizes, network disorder, or temporal scales. Furthermore, newly derived metrics enable us to link these design parameters to general nonlinear properties of the network.

AKPIK 3.3 Tue 11:45 H5

Discovery of the data structure as a way for prediction accuracy improvement — •Aliaksei Mazheika — independent researcher, Berlin, DE

High prediction accuracy of machine learning (ML) models is the main figure of merit of models efficiency. Usually this is achieved by choosing an optimal ML method, discovering the hyperparameters space, augmenting the data, etc. However, if a data set contains the data subsets significantly varying in their properties, addressing such heterogeneity can be pretty challenging task. Herewith a new method is presented in which improvement of prediction accuracy is achieved by discovering the heterogeneity of the data sets. This is done using a data mining method the subgroups discovery, in which the subsets of data are generated and discovered in terms of prediction accuracy improvement of local models in comparison to the global model within certain ML formalism. The application of this method showed its efficiency for classical data sets allowing for instance to solve the XOR problem staying on the level of logistic regression. Applying developed method for building ML models for a range of perovskite materials properties (lattice vector, tolerance factor) showed improvement of prediction accuracy for up to 50% for regression tasks, and up to 10% for classification. Also the new method was found to provide improved domains of applicability for ML models compared to previously proposed ones.

AKPIK 3.4 Tue 12:00 H5

Calculating the electronic structure of GaAs using Variational Quantum Algorithms — •Ivana Miháliková[1,2], Michal Krejčí[1,2], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic

Simulating and characterizing physical systems is one of the most promising applications of quantum computing. In our research, we focused on electronic structure calculations of GaAs using quantum computer simulator. This work explores the binary crystal gallium arsenide, employing Variational Quantum Deflation (VQD) and the Subspace-Search Variational Quantum Eigensolver (SSVQE) to access the full energy spectrum. A tight-binding Hamiltonian is used to investigate the effects of optimization methods, hyperparameter tuning, and quantum circuit architecture on the performance of these variational quantum algorithms. Our findings show that higher-energy states require more iterations for accurate evaluation, with the Constrained Optimization BY Linear Approximation (COBYLA) method proving to be the most effective. Notably, SSVQE demonstrates robustness to hyperparameter settings, while VQD is highly sensitive requiring precise hyperparameter tuning for optimal performance.

AKPIK 3.5 Tue 12:15 H5

Photonics and A.I. Education Supported by Virtual Reality and Unreal Engine Contents — •Arash Rahimi-Iman — I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

3D interactive elements visualized in computer game engines combined with virtual or mixed reality (VR/XR) offer many possibilities to reach younger people. Here, we present one example of a virtual reality environment for gamification in

the field of photonics and AI, created in the Unreal Engine UE5 for own teaching and training activities.

Thanks to modern information technologies, a plethora of ways exist which allow promoting topics of interest to a wider audience - among them digital games on platforms such as PCs and phones. While modern simulation software and sophisticated 3D visualization tools from all around typically address advanced users with a much more accurate science representation, simplified exploration spaces and toy experiments can create excitement at different age levels and attract potentially new students towards natural science topics based on fun and fascination.

AKPIK 4: Focus: Applications of Deep Neural Networks

Time: Tuesday 14:00–15:30 Location: H5

Invited Talk AKPIK 4.1 Tue 14:00 H5

The Scaling of Intelligence: From Transformers to Agentic AI — •Oliver Mey — Vodafone Tech Innovation Center, Dresden, Germany

The 2024 Nobel Prize in Physics recognized fundamental contributions to artificial intelligence and highlighted its profound impact on all disciplines, including physics. Generative AI has become a central tool in science and beyond, and understanding its underlying principles, the forces driving its rapid progress, and its emerging applications opens the door to new scientific breakthroughs and transformative innovations. We trace the evolution from Moore's Law to the scaling principles that enable today's large-scale AI models. At the heart of this transformation lies the Transformer architecture, the foundation of large-scale language models (LLMs) that generate coherent, context-aware text. These models are evolving into multimodal systems that seamlessly integrate text, images and other data types, greatly expanding their capabilities. Retrieval-augmented generation (RAG) extends LLMs with dynamic memory, enabling access to external information. In parallel, new concepts for task-dependent scaling of computations allow LLMs to distribute computational effort based on task complexity, increasing their efficiency in reasoning and adaptive problem solving. These advances pave the way for AI systems that act as collaborative agents and are capable of context-aware, goal-oriented interactions. In this talk, I will provide an overview of these developments and discuss them in the context of their broader implications, setting the stage for further specialized discussions.

Invited Talk AKPIK 4.2 Tue 14:30 H5

Inverse Design in Electromagnetics with Artificial Intelligence — •Willie Padilla — Duke University, Durham, North Carolina, USA

Artificial electromagnetic materials (AEMs) have enabled exotic electromagnetic responses that are difficult or impossible to achieve with naturally occurring materials. However, as AEMs have become more complex, the relationship between their structure and resulting properties is increasingly less understood, or sometimes completely unknown. Deep neural networks (DNNs) have been shown to effectively infer the relationship between AEM geometry and their electromagnetic properties, using simulated training data. More recently, a type of DNN * termed a large language model (LLM) * has shown a remarkable ability to respond to complex prompts. This presentation explores the potential of DNNs and LLMs for the inverse design of AEMs. I present a LLM fine-tuned on simulated data that can predict electromagnetic spectra over a range of frequencies given a text prompt that only specifies the AEM geometry. In view of the great potential of deep learning for the future of AEM research, we review the status of the field, focusing on recent advances, open challenges, and future directions.

Invited Talk AKPIK 4.3 Tue 15:00 H5

Inverse design of lateral hybrid metasurfaces with machine learning — •Rui Fang[1], Amir Ghasemi[1], Dagou Zeze[1], Koen Valk[2], Yuqing Jiao[2], Peter Zijlstra[2], and Mehdi Keshavarz Hedayati[1] — [1]Durham University — [2]Eindhoven Technology University

The development of metasurface structural colour typically depends on laborious and time-consuming simulations such as Finite Element Method (FEM) or Finite-Difference Time-Domain (FDTD) simulation, along with human intuition for parameter adjustments, rendering it impractical for design optimization. In this context, we have introduced an innovative AI-assisted design process that circumvents the intricate simulations, allowing for a swift and precise correlation between metasurface parameters and colour coordinates. In this study, we have applied the model to the lateral hybrid design, a novel concept in metasurfaces proposed by our research group and demonstrated that the model can predict a structure tailored to achieve continuous colour coordinates with an accuracy of up to 97%. A noteworthy aspect of our discovery is that the model is capable of predicting the range of colours that can be generated from a single design of an active metasurface. Our deep learning approach proves to be a valuable tool in designing active metasurfaces for structural colours. This advancement contributes to the development of highly sensitive sensors, bringing tunable metamaterials closer to practical applications.

AKPIK 5: Poster

Time: Thursday 15:00–16:30 Location: P2

AKPIK 5.1 Thu 15:00 P2

Photonic Matrix-Vector Multiplication at the Quantum Limit of single photons — •Mingwei Yang[1,2], Okan Akyüz[2], Felix Kübler[2], Konrad Tschernig[1], Xavi Barcons[1,3], Enrico Stoll[2], and Janik Wolters[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Humboldt-Universität zu Berlin, Berlin, Germany.

Photonic integrated circuits (PICs) have emerged as a promising solution for performing energy-efficient matrix multiplication and addition operations (MACs) in neural networks [1]. In this work, we demonstrate a 4x4 optical matrix-vector multiplication (MVM) using a mesh of Mach-Zehnder interferometers (MZIs), operating with attenuated laser pulses at the single-photon level. Using this as an example, we analyze the quantum limit of energy consumption of optical systems for classical machine learning. [1] Wetzstein, Gordon, et al. "Inference in artificial intelligence with deep optics and photonics." Nature 588.7836 (2020): 39-47.

AKPIK 5.2 Thu 15:00 P2

Machine Learning Optimization of Chiral Photonic Nanostructures — •Davide Filippozzi[1], Nicolas Roy[2], Alexandre Mayer[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]NaXys, Namur Institute for Complex Systems, University of Namur, Belgium

Deep learning (DL) and evolutionary algorithms (EA) as part of the machine learning (ML) domain have recently been well utilized for optimization purposes, such as for nanostructure design. Particularly, unintuitive problems can benefit from the potential abstraction levels that artificial Neural Networks (NNs) can achieve based on sufficient training and proper data. Reinforcement learning approaches promise to boost inference of solutions for complicated design requirements and specific functionalities.

We present a study that discusses the nano-pattern design optimization with a combination of DL and EA for a dielectric surface's preference for single-handed circularly polarized light in reflection or transmission. Advancing our previous simulations and algorithms [O. Mey and A. Rahimi-Iman, Phys. Status Solidi RRL 2022, 16, 2100571], the optimization in chiral dichroism and reflectivity for our metasurface's design is discussed. Such ML optimization can improve desirable features of unintuitive metamaterials and photonic nanostructures, as increasingly highlighted in up-to-date literature.

AKPIK 5.3 Thu 15:00 P2

Towards an ontology-based digital twin for graphene-based conductor materials — •Fabian Teichert[1,2,3], Leonhard Niemann[4,5], Florian Fuchs[1,2,3], Jörg Schuster[1,2,3], and Martin Köhne[4] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Department of Advanced Technologies and Micro Systems, Robert Bosch GmbH, Renningen, Germany — [5]Faculty of Natural Sciences, Chemnitz University of Technology, Chemnitz, Germany

The „Platform Material Digital" (www.materialdigital.de) advances digital twins within material science, based on a semantic description using ontologies. The aim is to digitally represent (new) materials, their properties and crucial processing steps. We are actively involved in this endeavour by digitalizing graphene-based conductor materials. An ontology is created and enriched with simulation data and experimental data, covering various aspects such as model parameters, preparation processes, and measurement processes. We create the fol-

lowing demonstrator use cases with a semantic data description: (1) the integration of our simulation methods as workflows within the „Platform Material Digital", (2) an App to store, filter, and post-process our production and measurement processes and material properties of the graphene-based conductor materials.

AKPIK 5.4 Thu 15:00 P2

Machine learning to resolve the structure: Perovskites and related materials — •Ekaterina Kneschaurek, Vladimir Starostin, Valentin Munteanu, Constantin Völter, Damian Balaz, Mikhail Romodin, Maik Hylinski, Dmitry Lapkin, Ivan Zaluzhnyy, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen, Tübingen, Germany

Recent advances in synthesis of novel materials used in solar cells, such as perovskites, are supported by structural analysis, using X-rays. To unravel the complexity of such materials, we utilize both *in situ* (studying crystallization kinetics) and *ex situ* (accessing phase composition) X-ray diffraction. The high-resolution scattering patterns are recorded by large 2D detectors, resulting in enormous amounts of data, which are difficult to analyze manually [1]. In some cases, there are no crystallographic information files (.cif) for the newly synthesized materials. An initial guess, based on the composition of the studied material, can estimate ranges of expected scattering signals from distinct phases. The deep learning (DL) model can detect Bragg peaks within the diffraction pattern, while the application of clustering and 2D Gaussian fitting enables the processing of complex data to be conducted more effectively. Preliminary data analysis of 2D patterns in real time can increase the efficiency of beamtimes and provide a feedback loop to optimize the parameters of the experiment.

[1] Hinderhofer, A., Greco, A., Starostin, V., Munteanu, V., Pithan, L., Gerlach, A., Schreiber, F. (2023). J. Appl. Cryst. **56**, 3-11.

AKPIK 5.5 Thu 15:00 P2

Balancing the Cart-Pole: Deep Q-Networks vs. Echo State Networks — •Igor Polonskiy, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Balancing a pole on a moving cart by applying directional forces is a standard benchmark problem in reinforcement learning. Deep Q-Networks [1], which integrate reinforcement learning with neural networks, have been highly effective in solving this problem. However, their reliance on multiple hidden layers makes them computationally intensive and energy-demanding. Replacing these hidden layers with an Echo State Network reduces trainable parameters and energy consumption. In this study, we compare the performance of Deep Q-Networks and Echo State Networks on the Cart-Pole problem. We show that an Echo State Network-Q-Network combination, with sufficient size and runtime, can not only match but also surpass Deep Q-Networks in cumulative rewards and control success rates.

[1] V. Mnih et al., Nature 518, 529 (2015)

AKPIK 5.6 Thu 15:00 P2

Latent Measures of Memory and Stochasticity in Dynamical Systems: Murphy's Law of Tumbling Toast — •Janine Graser, Atreya Majumdar, Kübra Kalkan, Ross Knapman, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of DuisburgEssen, 47057 Duisburg, Germany

Murphy's Law, which suggests that "anything that can go wrong will go wrong," is often exemplified by toast landing butter-side down. In reality, a toast falling from a table can be described by Newtonian mechanics and is bound to fall on the butter side under standard conditions [1]. Here, the fall is modelled through its seemingly hidden aspects (table height and toast asymmetry because of the butter).

We revisit the tumbling toast problem using the data-driven machine learning tools - latent entropy and latent dimension -introduced by Horenko et al. [2]. We develop a Python-based implementation that characterizes the fall using these latent measures. This approach has broader applications in other dynamical systems, such as predicting and optimizing magnetic material properties.

[1] R. A. J. Matthews, Eur. J. Phys. 16 172 (1995)
[2] I. Horenko et al., Commun. Appl. Math. Comput. Sci. 16 267-297 (2021).

AKPIK 5.7 Thu 15:00 P2

Measurement of thermal conductivity and thermal diffusivity through spatial and temporal temperature gradients — •Junsheng Zhuo[2] and Stephanie Lippmann[1,2] — [1]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Thuringia, 07745, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Thuringia, 07743, Germany

To address the challenges of measuring thermal properties of metal, a new device is being developed to measure both thermal conductivity and thermal diffusivity quickly and accurately. The sample is heated directly using an electromagnetic induction furnace, avoiding thermal resistance issues. High-resolution infrared cameras capture temperature distribution with ultra-short time and space intervals, allowing for precise thermal conductivity and diffusivity measurements. Mineral oil is used for cooling, enabling rapid heat transfer. This device calculates temperature-dependent thermal conductivity using spatial temperature gradients and heat flow, based on Fourier's law assisted by fitting, statistics, and machine learning, while thermal diffusivity is derived from real-time transient temperature gradients using the inverse method. Specific heat capacity is then calculated from these two values.

AKPIK 5.8 Thu 15:00 P2

Deterministic Model of Multi-Agent Boltzmann Q-Learning: Transient Dynamics, Feedback Loops, and Non-Convergence — •David Goll[1], Jobst Heitzig[2], and Wolfram Barfuss[3] — [1]Humboldt University of Berlin — [2]Potsdam Institute of Climate Impact Research — [3]University of Bonn

Multi-Agent Reinforcement Learning involves interacting agents whose learning processes are indirectly coupled through their shared environment, giving rise to emergent, collective dynamics that are sensitive to initial conditions and parameter variations. A Complex Systems approach, which examines dynamic interactions in multi-component systems, can uncover the underlying dynamics by constructing deterministic, approximate models of stochastic algorithms. In this work, we show that even in the simplest case of independent Q-learning with a Boltzmann exploration policy, previous models fail to capture actual learning behaviour. Specifically, the dynamics of the Q-space—representing agents' state-action value estimates—cannot be directly reduced to the lower-dimensional policy space representing their strategies, as assumed in earlier models. By explicitly incorporating agents' update frequencies, we propose a new discrete-time model that captures the observed behaviours and uncovers a fundamentally more complex dynamical landscape. We demonstrate the utility of this approach by applying it to the Prisoner's Dilemma, where our model distinguishes transient states, which might be mistaken for equilibria, from true equilibria. Furthermore, we show that varying hyperparameters, such as the discount factor, can prevent convergence to a joint policy.

AKPIK 5.9 Thu 15:00 P2

Noisy quantum computing of electronic structure of crystals — •Vojtěch Vašina[1,2], Ivana Miháliková[1], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Brno University of Technology, Brno, Czech Republic

Quantum computing is currently emerging as a useful paradigm for solving highly complex computational problems. Current quantum computers are unfortunately too noisy to provide sufficient accuracy, and quantum-classical hybrid algorithms emerged as a solution. Variational Quantum Eigensolver (VQE) has gained significant attention for addressing challenges in quantum chemistry, material science, etc. VQEs typically use multiple optimization methods, and the correct choice of optimization method can significantly impact performance. In our study, we focused on the comparison of multiple optimization methods used in VQE when applied to the electronic structure of crystals. The quantum part of VQE ran on a classical simulator with imported noise models from real quantum computers from the IBM Quantum Platform.

AKPIK 5.10 Thu 15:00 P2

Advancing Digital Transformation in Research on Universe and Matter in Germany — Martin Erdmann[1], •Jan M. Bürger[1], Banjamin Fischer[1], Stefan Fröse[2], Judith Steinfeld[1], and Angela Warkentin[1] — [1]RWTH Aachen University — [2]TU Dortmund University

Research on Universe and Matter (ErUM) at major infrastructures such as CERN or large observatories, jointly conducted with university groups, is an important driver for the digital transformation. In Germany, about 20,000 scientists are working on ErUM-related sciences and can benefit from actual methods of artificial intelligence. The central networking and transfer office ErUM-Data-Hub provides support by designing, organizing and performing schools and workshops for young and expert scientists in the areas of big data, machine learning, sustainable computing and many more. We present the actual achievements of the ErUM-Data-Hub in the German ErUM community.

AKPIK 5.11 Thu 15:00 P2

The graphene resonant metasurface substrate in near-zero refractive index regime to control the surface plasmon-polariton propagation length — •Zoya Eremenko — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Deutschland

The study goal is to identify and investigate conditions for controlling the propagation length of graphene surface plasmon-polaritons (SPP) through the utilization of hybrid graphene-dielectric metasurfaces. We study the spectral characteristics of resonant multipole modes in all-dielectric metasurface using the photonic crystal approach, metasurface unit cell modelling approach and implement these approaches by the commercial software Comsol Multiphysics 6.2. For controlling the propagation length of graphene SPPs we used all-dielectric metasurface as a substrate of graphene layer in a near-zero refractive index regime. The determined the parameters of the near-zero refractive index regime for the studied metasurface, which is crucial for achieving the main project goal of con-

trolling SPP propagation length in the graphene layer. Knowing the effective refractive index of the metasurface unit cell in the near-zero regime, these values are used in Comsol modeling the hybrid metasurface as a graphene layer substrate to calculate the SPP propagation length.

AKPIK 5.12 Thu 15:00 P2

Development of a Parametric Design Program for Building Construction Elements using Artificial Intelligence — •Artem Burdin — Moscow, Russia

Thesis: The aim of this research is to develop a parametric design program for building construction elements using artificial intelligence, focusing on the application of modern IT and artificial intelligence in physics-based modeling and simulation. The program will enable the creation of complex building structures, such as bridges, tunnels, and high-rise buildings, with increased accuracy and efficiency. Key objectives: * Analyze the current state of parametric design in building construction * Develop a parametric design program using artificial intelligence and machine learning algorithms * Implement the program using a suitable programming language and software * Test and validate the program using real-world examples * Evaluate the program's performance and potential applications in the construction industry Expected outcomes: * A parametric design program capable of generating complex building structures with increased accuracy and efficiency * A comprehensive analysis of the current state of parametric design in building construction * A detailed evaluation of the program's performance and potential applications in the construction industry * Contributions to the development of artificial intelligence and modern IT in physics-based modeling and simulation Keywords: parametric design, building construction, artificial intelligence, machine learning, physics-based modeling, simulation, computer-aided design (CAD), construction industry.

AKPIK 5.13 Thu 15:00 P2

Working group on physics, modern Information technologies and artificial Intelligence — •Adam Barakhoev — Moscow, Russia

Artificial intelligence and modern computer infrastructure are changing the approach to physics, combining powerful computational methods with experiments. These innovations help scientists process large amounts of data, automate complex tasks, and make accurate predictions. One of the important achievements is the use of artificial intelligence to improve physical experiments, especially in quantum mechanics and optical systems. Machine learning algorithms can predict results based on incomplete data and help set up experiments in real time, which significantly increases their efficiency and accuracy. Also, modern OT technologies, such as cloud services and high-performance computing, are important for managing the large-scale modeling needed in modern physics research.

AKPIK 5.14 Thu 15:00 P2

Autonomous Vehicles: Technologies and Challenges — •Nikita Timoshin — Moscow, Russia

Autonomous vehicles are transforming transportation with technologies such as artificial intelligence (AI), machine learning, and advanced sensor systems like LiDAR, radar, and cameras. These vehicles rely on AI to make real-time decisions, using data from various sensors through sensor fusion for accurate environmental perception. Communication networks like V2X (Vehicle-to-Everything) and 5G enable vehicles to interact with infrastructure and other vehicles.

The benefits include enhanced safety by reducing human error, improved traffic efficiency, and increased mobility for people with disabilities. However, challenges such as sensor limitations in adverse conditions, high computational demands, and ethical dilemmas about decision-making in critical situations remain. Additionally, regulatory and privacy concerns need to be addressed. As autonomous vehicles integrate with smart cities, they could significantly reshape urban mobility.

AKPIK 5.15 Thu 15:00 P2

Experimental examination of the validity of the Turing test for considering Artificial Intelligence as having subjectivity — •Lev Gelbart and Alexey Iakovlev — Moscow, Russia

The speed of development of Artificial Intelligence (AI) raises questions about its subjectivity and thinking. Alan Turing, who set the criteria for thinking, did not consider subjectivity. There are sharp discussions on this topic, for example, Doctor of Law Valery Zorkin, professor at MSU, opposes endowing AI with subjectivity, emphasising humanism.

It should also be taken into account that the Turing test may be invalid if we consider people, who are not capable of passing it. For example, a study by Alan Ropper (2010) showed that patients in a vegetative state can demonstrate brain activity, but are clearly unable to pass the Turing test, which does not detract from their human value.

We have considered, whether a machine can pass a test designed for humans. Machines are thought to not be able to adequately mimic emotions, so we tested three chatbots (Lily, AI Chat, ChatGPT) for emotional intelligence using the IDRlabs test. All chatbots performed above the average of humans (77.27%, 68.87%, 64.6%), but this, obviously, does not make them subjects of law.

Conclusion: the Turing test is not valid for assessing the subjectivity of AI.

AKPIK 5.16 Thu 15:00 P2

Unmanned transportation in the field of cargo transportation and its contribution to industry. — •Alexey Platonov — Moscow, Russia

In recent years, the transportation industry has witnessed a transformative shift towards automation and innovation, with unmanned transportation systems emerging as a pivotal force in cargo logistics.

Unmanned transportation significantly improves safety in cargo movement. By reducing the reliance on human drivers, the industry can mitigate the risks associated with human error, a leading cause of accidents in transportation.

The integration of LiDAR into cargo transportation also opens up new avenues for delivery services.

It is worth considering that the active introduction of unmanned vehicles in cargo transportation is beginning. Several test shipments of real orders were made on KamAZ-5490 trucks without direct driver control. There was only a mechanic controller in the cockpit, who checked the performance of the systems.

By enhancing efficiency, improving safety, and fostering innovation, these technologies are set to revolutionize the logistics landscape, proving that the future of transportation is indeed unmanned.

AKPIK 5.17 Thu 15:00 P2

Crawler-motor grader — •Vyacheslav Kharchevnikov — Moscow, Russia

An overview of the relevance and necessity of developing a crawler-mounted motor grader. A description of the problems that this equipment solves in the construction and road sector. An analysis of existing models of motor graders, including wheeled and tracked versions, their advantages and disadvantages. Defining the main goal of the project - to create an effective crawler-mounted motor grader. Setting the tasks necessary to achieve the goal, such as improving the cross-country ability and stability of the equipment. A detailed description of the design of a crawler-mounted motor grader, including the features of the chassis, control system and attachments.

An analysis of the economic feasibility of introducing a crawler-mounted motor grader, a comparison with traditional models, an assessment of production and operating costs. An assessment of the environmental impact of using a crawler-mounted motor grader, measures to reduce emissions and reduce noise. Summarizing the research, assessing the results achieved and prospects for further development and implementation of a crawler-mounted motor grader.

AKPIK 5.18 Thu 15:00 P2

Development of a design solution for automating a set of tasks in the production preparation subsystem of an automated control system for a small construction company — •Tikhon Shabrov — Moscow, Russia

automation of processes for small companies use of new technologies

AKPIK 5.19 Thu 15:00 P2

Acceleration of crystal structure relaxation with Deep Reinforcement Learning — •Elena Trukhan, Efim Mazhnik, and Artem R. Oganov — Moscow, Russia

We introduce a Deep Reinforcement Learning (DRL) model for the structure relaxation of crystal materials and compare different types of neural network architectures and reinforcement learning algorithms for this purpose. Experiments are conducted on Al-Fe structures, with potential energy surfaces generated using EAM potentials. We examine the influence of hyperparameter settings on model performance and benchmark the best-performing models against classical optimization algorithms. Additionally, the model's capacity to generalize learned interaction patterns from smaller atomic systems to more complex systems is assessed. The results demonstrate the potential of DRL models to enhance the efficiency of structure relaxation compared to traditional methods.

AKPIK 6: AI Methods for Materials Science

Time: Thursday 16:30–18:00 Location: H5

AKPIK 6.1 Thu 16:30 H5

Bayesian Optimization for High-Resolution Transmission Electron Microscopy — •Xiankang Tang[1], Lei Jin[2], Yixuan Zhang[1], Rafal Dunin-Borkowski[2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Ernst Ruska-Centrum für Mikroskopie und Spectroskopie mit Elektronen, FZ Jülich, 52428 Jülich, Germany

Advances in machine learning technologies make it possible to automatize material characterizations, indispensable for the near-future implementation of autonomous experimentation for solid-state materials. High-resolution transmission electron microscopy (HRTEM) allows the study of the atomic structure of solid materials with sub-Angstrom resolution. By matching experimental and simulated images, unknown experimental parameters and crystal structures can be determined. However, this process entails strong domain expertise and can be time-consuming. In this work, we implement a Bayesian optimization-based approach to automatize the image analysis processes. Combined with some prior information, such as the experimentally measured aberration, the 3D crystal structure of the specimen can be reconstructed from a single HRTEM image. Specifically, by defining the mean square error(MSE) of pixel intensity values between experimental and simulated images, our method effectively captures both global and local image features. This approach not only achieves an exact match in absolute image contrast but also identifies unknown experimental parameters, optimizes atomic positions, and reveals surface morphology at atomic resolution.

AKPIK 6.2 Thu 16:45 H5

Synthetic Data Generation for Enhanced Segmentation of Electron Microscopy Images — •Amir Omidvarnia[1], Ali Ghaznavi[2], Junbeom Park[1], Shibabrata Basak[1], and Simone Köcher[1] — [1]Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

Monitoring structural changes in materials via operando electron microscopy (EM) is crucial for understanding the material's changes under operating conditions, which directly impacts its durability and performance. However, accurate segmentation of features such as cracks or pores in EM time-series data requires extensive labeled datasets, which are challenging to produce due to the labor-intensive, subjective nature of manual annotation. Our research addresses this limitation by exploring different synthetic data generation techniques that can effectively supplement scarce annotated data and improve segmentation outcomes. We evaluate multiple synthetic image generation approaches to enhance the training dataset for U-Net models aimed at segmenting EM time-series data: (1) deep convolutional generative adversarial networks (DCGAN) to produce realistic textures; (2) time-varying image synthesis that mimics the temporal development of features and introduces artificial features to simulate structural imperfections; and (3) standard data augmentation methods. These methods are evaluated in generating training data for EM image segmentation from a limited set of EM images.

AKPIK 6.3 Thu 17:00 H5

Neural Networks in Surface Crystallography: A New Paradigm for GIWAXS Analysis — •Erwin Pfeiler[1], Vladimir Starostin[3], Alexander Hinderhofer[3], Roland Resel[2], Frank Schreiber[3], and Stefan Kowarik[1] — [1]University of Graz, Austria — [2]TU Graz, Austria — [3]University of Tübingen, Germany

Thin film materials are essential to modern technology, with grazing incidence X-ray diffraction (GIWAXS) being the primary method for resolving their crystal structure. However, the current data analysis process is often slow and labor-intensive, frequently requiring more time and resources than the GIWAXS measurements themselves. Accelerating this bottleneck is critical for enabling automated materials discovery.

In this work, we present an AI-driven approach utilizing neural networks to streamline and enhance GIWAXS analysis. Our model predicts unit cell dimensions (a, b, c) and angles (α, β, γ) directly from the positions of Laue reflections. Additionally, it identifies the Miller indices of the contact plane, providing insights into the film texture.

Using both simulated GIWAXS data and real-world examples, we demonstrate the neural network's potential to significantly accelerate the analysis process, delivering accurate structural predictions with sub 0.01 Å precision.

AKPIK 6.4 Thu 17:15 H5

Reflectivity Analysis with AI: The LISA Data Pipeline at P08/DESY — •Julia Kobus[1,2], Lukas Petersdorf[1,2], Svenja Hövelmann[1,2], Alexander Hinderhofer[3], Vladimir Starostin[3], Chen Shen[4], Florian Bertram[4], Linus Pithan[4], Frank Schreiber[3], and Bridget Murphy[1,2,4] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel, Germany — [2]Ruprecht-Haensel Laboratory, Olshausenstr. 40, 24098 Kiel, Germany — [3]University of Tübingen, 72076 Tübingen, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

We present a data analysis pipeline that is under development within TA3 of DAPHNE4NFDI for the LISA instrument at the P08 beamline at DESY. This pipeline is adapted from the development on solid surface XRR AI analysis to be used for liquid surfaces and interfaces. The pipeline aims at performing data reduction and subsequent analysis for reflectivity measurements using AI-based models. This approach increases measurement efficiency by processing data in real time, allowing flexible adjustments during the experiment and providing immediate insights. This will help users make better-informed decisions for subsequent measurements. The pipeline also will make advanced data analysis accessible to less experienced users. Our work will demonstrate the potential of AI to transform experimental workflows and data interpretation, and provides a blueprint for similar developments in the scientific community.

AKPIK 6.5 Thu 17:30 H5

Prediction of Infrared Spectra of organic molecules with Active Learning — •Gusein Bedirkhanov[1], Nitik Bhatia[1], Ondrej Krejci[2], and Patrick Rinke[1,2] — [1]Department of Physics, Technical University of Munich, Germany — [2]Department of Applied Physics, Aalto University, Finland

Infrared (IR) spectroscopy is a valuable tool for understanding catalytic processes, but interpreting experimental spectra is challenging due to the strong influence of the species environment. Ab initio molecular dynamics (AIMD) offers accurate theoretical spectra, accounting for anharmonic effects, but at a high computational cost. Machine-learned interatomic potentials (MLIPs), such as MACE [1], provide an alternative to AIMD, enabling accurate and fast IR spectra predictions. To reduce the amount of training data, we have established the active learning method PALIRS [2] (a Python-based active learning code for infrared spectroscopy). PALIRS predicts IR spectra of organic molecules essential in catalytic processes accurately, with peak positions matching experiment within 20cm^{-1}. We aim to further improve the efficiency of PALIRS, using only a hundredth of DFT data in comparison with AIMD, through optimization of MACE training strategies. We will inspect various combinations of transfer learning and conventional iterative training to find the ideal match between training time and final MLIP accuracy.

[1] I. Batatia *et al.*, Adv. Neural inf. Process. Syst. (2022).

[2] N. Bhatia *et al.*, GitHub (2024), `gitlab.com/cest-group/PALIRS`

AKPIK 6.6 Thu 17:45 H5

Towards AI-assisted high-throughput thin film research workflow — •Dmitry Lapkin, Roody Nasro, Constantin Völter, Valentin Munteanu, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen

The compositional optimization of new materials necessitates the high-throughput screening of a multitude of compositions, which must be investigated to elucidate the non-linear and non-monotonic structure-property-composition dependencies. In this regard, data-driven material science enables researchers to accelerate the identification of new materials with desired properties for specific applications by efficiently exploring vast material spaces. Such high-throughput data-driven studies comprise two key elements: the combinatorial preparation of suitable sample libraries spanning wide compositional ranges, and the high-throughput screening of the structure and properties of the synthesized samples.

In this work, we present a complete workflow for high-throughput studies of thin films. A specially designed vacuum deposition chamber enables the production of gradient thin films suitable for high-throughput screening. Surface-sensitive X-ray scattering methods available at modern X-ray sources comprise a convenient tool for resolving the thin film structure with ultimate resolution and high speed, while the developed AI-based approaches provide on-the-fly analysis of the collected X-ray scattering data.

A. Chalke, Bhagyashree .... MA 31.31
A. Curcio, Christine ..... BP 17.17
A Fiete, Gregory ..... MA 5.5, TT 1.5
A. Habib, Shaimaa ..... •MM 9.16
A. Heuver, Jeroen ..... MA 15.40
A. L. Marques, Miguel ..... MM 27.2
A. Miwa, Jill ..... O 88.1
a. s. júnior, sebastião ..... TT 37.42
A. Tsirlin, A. ..... MA 40.5
A. Tulapurkar, Ashwin ..... MA 31.31
A. Weber, Christoph ..... BP 17.69
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Abdelbaki, Ihab .....•CPP 32.30
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Abdelghaffar, Yasmin .....•BP 17.2
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Abd-El-Latif, Abdelaziz A. .. KFM 13.1
Abdelwahab, Anas ..... •TT 4.9
Abdeslam, Saad .....CPP 15.54
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Abdoli, Iman .....•DY 9.1
Abdou Ahmed, Marwan ..... HL 7.2
Abdullah Khan, Muhammad HL 29.60, HL 29.61
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Abegg, Lukas ..... •BP 17.67
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Abuawwad, Nihad •DY 33.11, •MA 3.7
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Adhikari, Yuwaraj .....MA 34.2
Adhyapak, Tapan Chandra .. BP 31.3, CPP 42.3, DY 43.3
Adibi, Elaheh .....•TT 37.49
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Aeschlimann, Martin ..... MA 9.8, MA 26.6, O 23.19, O 23.21, O 46.5, O 46.6, O 46.7, O 69.7, O 71.4, O 72.9
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Agnieszka, Paszuk .....HL 20.8
Agrawal, Aditi ... MA 40.2, •MA 40.6, MM 6.3, MM 6.4, MM 6.9
Agterberg, Daniel F. MA 9.3, MA 13.13
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Ahmad, Arshid .....•CPP 45.3
Ahmad, Ather .....•HL 46.10
Ahmad, Izzi A. ..... MM 9.53
Ahmadi, Gelavizh ..... O 15.1, TT 6.1
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Aikkila, Paula .....•BP 26.1
Ajdari, Mohsen ..... •O 46.1
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Albert, Nico ..... •DY 31.10
Albino, Andrea .... •TUT 2.3, •DS 2.4, •O 1.3
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Albrecht, Jan .....•BP 10.4, •DY 14.4, DY 28.7
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Albrecht, Martin .....DS 2.4
Albrecht, Theresa .....•MA 31.18
Alcalde, Daniel .....TT 26.12
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Ali, Zayan Ahsan •MA 34.1, MA 41.27
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Allakulyyeva, Malika .....•DY 28.3
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Álvarez-Garrido, Fabián ..... BP 17.9, •DY 18.2
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Amaseder, Markus .....•HL 20.1
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Amelio, Ivan .....•HL 2.6
Amersdorffer, Ines ..... HL 39.9
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An, Yun ..... •MM 8.5
Anabaraonye, Chinwendu Nancy •CPP 32.20
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Anchutkin, Gordei •BP 28.3, CPP 25.7, •CPP 35.3, DY 23.7, •DY 36.3
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Ando, Yoichi ..... DS 13.16, HL 29.82, TT 4.3, TT 35.2
Andorfer, Fabian . •MM 4.6, MM 9.13, MM 9.28
Andres, Beatrice .....DS 15.7
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Anhäuser, Sebastian .....•HL 16.3, HL 54.5
Aniés, Filip .....CPP 3.4
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Antunes, Gonçalo .....•BP 28.6, •CPP 35.6, •DY 36.6
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Arlego, Marcelo .....•MA 15.46
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Arndt, Hans-Dieter .....BP 17.21
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Arneth, J. .....•MA 41.25
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Arpavate, Witchitaya .....KFM 18.5
Arrachea, Liliana .....TT 11.18
Arregi, Jon Ander .....MA 26.12
Arrell, Christopher ..... DY 31.7
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Arshad, Atiqa .....DS 10.1
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Artyukhin, Sergey •KFM 8.4, MA 40.7, MA 43.2, MA 45.11
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Arztmann, Manuela ..... •MM 21.3
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Asa Rajan, Sruthy .....•CPP 15.43
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Aslam, Nabeel ....•SYMS 1.3, DS 3.1, DS 7.7, DS 13.13
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Aslyamov, Timur ..... DY 9.6, •DY 9.7
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Ayari, Jihed ..... KFM 13.1
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Ayuso, David ..... MA 5.3, TT 1.3
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Azevedo, Tamara ..... •MA 3.11
Azhar, M. ..... MA 6.11
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Bär, Macus ..... O 73.3
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Bauer, Wolfgang .. •BP 10.6, •DY 14.6
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Baumann, Tim R. ..... •BP 28.9, •CPP 35.9, •DY 36.9
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Becker, Maximilian T. ..... •BP 8.1, •CPP 9.1
Becker, Petra ..... KFM 9.3, MA 13.8
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Blanco-Rey, María ..•MA 46.4, O 15.8, TT 6.8
Blänsdorf, Jan Luca ..... •HL 32.3
Blanter, Yaroslav M. ..... TT 16.10
Blasco, Eva ..... CPP 26.2
Bläßer, Jonathan ..... •MA 18.5
Bläsing, Jürgen ..... HL 52.2
Blason, Andrea ..... TT 4.13
Blatnik, Matthias ..... O 13.10
Blazevic, Luka ..... •HL 1.4
Blecker, Veronika ..... O 37.1
Bleher, Sonja ..... O 24.10
Bleibaum, Anton .... •TT 11.1, TT 44.3
Bleyer, Ulrich ..... PSV VI
Blick, Robert ..... MA 15.11
Blick, Robert H. ..... TT 49.3
Blickberndt, Jan . •TT 11.47, TT 11.48, TT 55.11
Bligaard, Thomas . O 85.7, AKPIK 2.2
Blinov, Lara ..... •HL 29.6
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Blödorn, Felix ..... O 7.3, O 7.8
Blok, Machiel ..... TT 11.39
Blonski, Markus .... HL 33.7, HL 39.1
Blonski, Markus A. ..... •HL 33.1
Bloomfield-Gadêlha, Hermes BP 32.8
Blue, Brandon ..... •O 98.8
Blügel, Stefan ..... •PLV VI, MA 6.5, MA 9.6, MA 28.5, MA 32.1, MA 32.2, MA 33.13, O 30.7, O 36.1, O 85.4, O 92.8, O 101.2, TT 5.3, TT 11.22, TT 40.1, TT 40.2, TT 57.2
Bluhm, Hendrik ..... HL 29.54
Blum, Jonas ..... HL 53.5
Blüm, Michael ..... MM 9.55
Blümler, Peter ..... MA 38.6
Bo, Yifan ..... CPP 22.5
Boariu, Florin ..... MA 31.16
Boban, Honey . DS 4.8, O 51.2, O 88.6
Bobu Cimpoi, Emma ..... •BP 12.6, •CPP 18.6
Bobzien, Laric ..... O 5.6, •O 5.7
Bocchini, Adriana . •KFM 18.2, O 73.7
Bochow, Nils ..... DY 28.5
Bock, Thomas ..... O 66.2
Bockhorn, Lina .... HL 29.3, •HL 30.2
Bockstedte, Michel ..... TT 7.5
Bocquet, François C. O 33.11, O 33.16, O 62.1, O 79.5, O 80.6
Bode, Matthias ... MA 46.1, MA 46.2, O 24.1
Bode, Simeon ..... O 33.9, •O 33.17
Bodea, Marius-Aurel ..... TT 16.5
Bodermann, Bernd ..... •DS 9.2
Boeckmann-Clemens, Hannes O 48.2
Boeglin, Alex ..... O 20.7, O 43.4
Boehme, Christoph ..... •SYMS 1.1

Boekhoven, Job ..... BP 26.8
Boer, Lotte ..... MA 43.4
Boeri, Lilia ..... •SYES 1.1
Boesenberg, Ulrike ..... O 23.7
Boesler, Dorothee ..... O 28.1
Bogdanoff, Nils ..... O 5.5, O 20.2
Bogdanov, Sergei ..... O 26.9
Bögle, Klara-Maria ..... •CPP 15.15, HL 16.7
Bogner, Christina CPP 25.14, DY 23.14
Bogoeva, Stefani ..... •DS 13.41
Bogucki, Aleksander ..... •O 24.4
Bohamud, Tamam ..... O 8.4
Bohaty, Ladislav .. KFM 9.3, MA 13.8, TT 37.22
Bohlemann, Chris ..... KFM 14.4
Bohlemann, Chris Y. ..... •CPP 32.31, HL 20.8
Bohlemann, Chris Yannic ..... O 86.7
Böhler, Annika ..... TT 17.5, •TT 17.6
Böhlke, Thomas ..... MM 4.5
Böhlmann, Winfried ..... TT 4.2
Böhm, Maite ..... •O 35.2
Böhme, Florian . •BP 31.2, •CPP 42.2, •DY 43.2
Böhmer, Anna ..... MM 6.7, TT 9.10, TT 37.26
Böhmer, Anna E. .... TT 3.10, TT 3.11, TT 3.12, TT 5.11, TT 37.32, TT 37.33, TT 54.6
Böhmer, Jan ..... •HL 6.7, HL 29.42
Böhmer, Michael ..... CPP 3.1
Bohmhammel, Klaus ..... KFM 14.16
Bohnen, Tim ..... •CPP 15.37
Böhnke, Jan ..... DS 15.7, •O 40.2
Bohorquez, Laura Teresa Corredor TT 26.3
Bohrdt, Annabelle .. DY 28.1, TT 16.9, TT 17.5, TT 17.6, TT 17.7, TT 37.34, TT 43.5, TT 54.10
Boie, Larissa ..... DS 15.7, DY 31.7
Boigner, Sandra ..... O 63.4
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Bokemeyer, Paul ..... •HL 9.6
Boll, Torben ..... MM 4.6, MM 9.13
Bolle, Frederik ..... •TT 5.6, TT 11.4, TT 11.5
Bollmers, Laura ..... KFM 18.7
Boltz, Horst-Holger ..... DY 22.10
Bölükbaşi, Ismail ..... HL 29.72
Bomers, Mario ..... PSV II
Bonafé, Franco O 43.7, •O 87.2, O 96.1
Bonafé, Franco P. ..... O 85.9
Bonanni, Alberta ..... HL 2.8
Bonanni, Valentina ..... HL 29.88
Bondzio, Laila .. CPP 15.31, DS 13.20, MM 9.57
Bonell, Frédéric ..... MA 19.5
Bonetti, Pietro ..... TT 3.1, TT 17.12, TT 43.4
Bonetti, Pietro Maria ..... TT 54.11
Bonilla, Mauricio Rincón ..... MM 4.9
Bonitz, Michael ..... DY 29.2, O 61.6, TT 29.6
Bonkhoff, Martin ..... TT 43.11
Bonmassar, Nicolas ..... •DS 2.1
Bonnet, Nicéphore ..... O 58.6
Bontke, Florian ..... O 60.1
Boras, Dominik .. KFM 5.4, •KFM 5.6, •KFM 5.7
Borchers, Christopher .... •HL 29.76, HL 29.80
Borchert, Juliane ..... HL 1.6
Bordács, Sándor ... MA 4.4, MA 28.8, MA 43.13, MA 43.14
Bordes, Romain ..... CPP 31.5
Borges Gomes Lima, Yuri ... MM 11.7
Boric, Tina ..... •BP 17.48
Borin Barin, Gabriela ..... O 12.8
Borisenko, Sergey ..... O 67.9
Borisov, Andrei ..... O 20.7
Borisov, Vladislav ..... •MA 43.8
Bork, Peer ..... BP 29.6, DY 38.6
Bork, Sophie ..... MA 31.14, MA 41.7
Borne, Vincent ..... BP 25.8
Bornhake, Thomas ... O 85.4, •O 92.8
Bornholdt, Stefan ..... SOE 4.4
Bornschein, Beate ..... DY 22.21
Bornschein, Lutz ..... DY 22.21
Bornscheuer, Uwe T. ..... MA 15.11
Borodin, Dmitriy ..... O 22.6, O 45.5, O 59.1, •O 90.4
Borondics, Ferenc ..... CPP 15.19
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Borras, Vicent ..... MA 18.3
Borrego-Varillas, Rocio ..... HL 54.6
Borrelli, Raffaele ..... O 42.4
Borysenko, Yelyzaveta ..... •MA 10.4, •TT 13.4
Bosche, Jonas ..... BP 11.2
Böse, Olaf ..... KFM 13.1
Bossini, Davide .... HL 61.4, MA 26.2, MA 48.2
Bostwick, Aaron ..... O 61.7, TT 29.7
Botana, Antia S. ..... MA 40.4
Botello-Méndez, Andrés ..... TT 32.2
Bothe, Lucas ..... DS 11.3, DS 13.24, •DS 13.26, DS 13.64
Bothe, Marc ..... •O 33.5
Bothner, Daniel .... TT 11.56, TT 50.9
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Böttcher, Jan ..... HL 12.1, TT 12.1
Böttcher, Lukas ..... •O 52.1
Böttger, Ole ..... •O 18.5
Böttger, Simon ..... HL 16.9
Botti, S. ..... MM 18.10, MM 31.7
Botti, Silvana ..... BP 29.5, DY 38.5, HL 1.11, HL 3.1, O 64.6, O 89.7
Bottinelli Montadon, Tecla . CPP 10.2
Bottomley, Adam ..... O 98.8
Bötzel, Steffen ..... •TT 52.2
Bouard, Chloé ..... MA 11.7, TT 14.7
Bouaziz, Juba ..... •MA 45.9, O 15.6, TT 6.6
Bouchenoire, Laurence ..... DS 13.35
Boudjenane, Meriem N. .. •CPP 32.23
Boudouvis, Andreas ..... DY 27.12
Bougeard, Dominique ..... HL 6.10, TT 11.18, TT 38.1
Bouleimen, Azza ..... •SOE 10.3
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Bourgeois, Laure ..... •MM 19.1
Bournel, Fabrice ..... O 32.4
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Bouss, Peter ..... SOE 7.8, •SOE 7.9
Bouzid, Mehdi ..... BP 8.5, CPP 9.5
Bovensiepen, U. ..... O 67.5
Bovensiepen, Uwe . PSV II, KFM 15.7, •O 18.7, O 23.1, O 23.11, O 30.5, O 67.1, O 97.4, O 99.6
Bovkun, Leonid .... HL 12.1, •HL 13.6, HL 13.7, TT 12.1
Bovornratanaraks, Thiti .... MM 9.35
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Boydas, E. ..... MM 18.10, MM 31.7
Boydas, Esma ..... BP 29.5, DY 38.5
Bozhko, Dmytro ..... MA 3.4
Bozhko, Dmytro A. ..... MA 3.5
Bozzio, Mathieu ..... •AIW 2.1
Braak, Daniel ..... TT 50.8
Brabec, Christoph ..... CPP 15.49
Brabec, Christoph J. ..... CPP 24.4, MM 9.68
Braden, Markus ... MA 13.8, MA 31.2, TT 16.2, TT 37.30
Bradford, Jonathan ..... O 88.7
Bradley, A. Louise ..... KFM 15.5
Braemer, Adrian ..... TT 43.9
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Brajović, Vladan ..... HL 51.1, TT 46.1
Brameyer, Sophie ..... BP 4.6
Brancolini, Giorgia ..... CPP 15.63
Brand, Christian ..... O 37.5, O 61.1, •O 99.6, O 99.8, TT 29.1
Brand, Hauke ..... HL 6.13
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Brandstetter, Dominik ..... O 69.8
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Bratschitsch, Rudolf ..... CPP 15.61, CPP 40.1, HL 20.24, HL 29.16, HL 29.25, HL 29.28, MA 15.22, MA 20.14, MA 31.39, MA 41.11, O 83.7, TT 45.7
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Braun, Dieter ..... BP 14.20, BP 26.1, BP 26.2, BP 26.7
Braun, Franziska ..... CPP 6.3
Braun, Frederic ..... •O 49.9, O 52.4, O 52.5
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Braun, J. ..... O 101.1, TT 57.1
Braun, J.R. ..... •DY 22.22
Braun, James ..... O 22.1, O 73.1
Braun, Larissa ..... PRV III
Braunecker, Bernd ..... TT 51.5
Brauns, Fridtjof .... •BP 6.2, •CPP 7.2, •DY 7.2
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Braunschweig, Björn ..... BP 12.4, CPP 18.4, CPP 20.5, CPP 32.7, CPP 38.3, O 34.5
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Bräutigam, Patrick ..... CPP 44.1
Bredow, Jorrit Marius ..... •DS 5.4
Brehm, Lucas ..... BP 31.4, CPP 42.4, DY 43.4
Brehm, Martin ..... HL 20.5
Brehm, Moritz ..... HL 15.6
Brehm, Verena ..... •MA 45.2
Breiholz, Benjamin ..... HL 57.12
Breitbach, David . MA 20.9, MA 31.30
Breiten, Tobias ..... HL 36.3
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Brem, Samuel ..... O 7.6, O 57.9
Bremer, Lara ..... •TT 37.61
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Brems, Maarten ..... MA 29.7
Brems, Maarten A. ..... MA 29.8, MA 41.34, MA 41.40
Brenig, Wolfram .. •TT 27.2, TT 37.17
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Brennfleck, Ellen ..... •O 72.9
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Brian Winkler, Thomas ..... MA 41.3, MA 41.35
Briganti, Matteo ..... MA 34.7, O 59.7
Brill, Lorenz ..... •O 50.1
Brink, Tobias ..... MM 11.3, •MM 21.5
Brinker, Theresa ..... MA 15.11
Brinkmann, Kai-Thomas .... HL 46.10
Brinkop, Achim T. . BP 29.11, DY 38.11
Brinkop, Achim Theo ..... •BP 17.77, BP 18.6
Brison, J. P. ..... TT 24.2
Brito, Hermi Felinto ..... BP 22.9
Brito, Mariano ..... CPP 1.3
Brixner, Tobias .. HL 29.89, HL 29.90, O 60.6
Brizolla, Gusthavo ..... •MA 8.4
Brockers, Vincent ..... •SOE 10.2
Brockmann, Dirk ... BP 21.9, DY 27.3, SOE 8.9
Brockner, Florian ..... O 49.9
Brödner, Kerstin ..... CPP 27.6
Broekhoven, Rik ..... O 45.12, O 90.8
Brommer, Peter ..... MM 28.1
Bronsch, Wibke .. •DS 15.7, MA 31.25, O 40.3
Brookes, Nicholas B. O 29.9, TT 20.9
Brosda, Nico ..... •HL 39.2
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Brösigke, Georg ..... O 21.1, O 21.2
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Brovang, Bertram ..... HL 44.2
Browne, George ..... •MA 41.10
bruchal, kamil .. CPP 25.15, DY 23.15
Brücher, Eva ..... MA 28.4
Brückel, Thomas ..... MA 39.3
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Bruckmeier, L. ..... O 26.6
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Brückner, Leon ..... O 26.5
Brückner, Max ..... TT 3.12, •TT 5.11
Brückner, Maximilian ..... •CPP 20.4
Brückner, Sebastian ..... DS 2.4
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Bruder, Enrico ..... MA 7.3
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Brunner, Philipp ..... MM 23.4
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Bruns, Hendrik ..... BP 30.7
Brusnikin, Mikhail ..... •MM 9.72
Brütting, Fabian .. HL 20.22, •HL 61.1
Brütting, Wolfgang ..... CPP 15.38, CPP 22.1, CPP 32.40, HL 16.6
Bryzgalov, Aleksandr ..... •SOE 5.3
Buba, Jonas .... •CPP 25.9, •DY 23.9
Büble, Joschua ..... DS 13.11
Bublikova, Anastassiya ... CPP 15.18
Buchberger, Sebastian ..... TT 52.6
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Buchhold, Michael .. DY 13.7, DY 41.3, TT 19.7, TT 56.3
Buchholz, D. Bruce ..... HL 11.6
Buchinger, Quirin .. HL 36.11, HL 57.11
Büchner, B. ..... MA 33.1
Büchner, Bernd ..... MA 37.5, O 67.9, TT 9.9, TT 10.3, TT 11.15, TT 16.2, TT 24.8, TT 26.3, TT 35.3, TT 37.14, TT 37.31, TT 49.13
Buchta, Maximilian •DS 11.3, DS 13.26
Buck, Jens ..... O 29.6, TT 20.6
Bučko, Tomáš ..... HL 20.1, MM 12.7
Büddefeld, Jan ..... DY 6.1
Budker, Dmitry ..... MA 41.15
Bud'ko, S. L. ..... MA 15.30, TT 37.18
Bud'ko, Sergey L. ..... TT 37.1
Budniak, Adam K. ..... DS 4.8
Budnyk, Andriy ..... CPP 30.8
Bueno Villoro, Ruben ..... MM 15.1
Buffler, Raphael ..... •HL 39.23
Bugase, Jonas ..... •MA 15.15
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Bukov, Marin ..... DY 20.13, TT 28.13
Bülbüloğlu, Burak ..... •TT 11.57
Bulut, Nebahat . MM 9.33, •MM 9.50, MM 36.2
Bulut, Yusuf ..... CPP 8.2, CPP 15.19, DS 13.32
Bunch, David ..... TT 11.32
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Bünte, Judith .. •CPP 15.31, DS 13.20, MA 13.10, MA 22.7
Bunz, Uwe H. F. ..... CPP 27.6
Buonaiuto, Luciana ..... CPP 20.5
Burdin, Artem ..... •AKPIK 5.12
Burekovic, Sumeja ..... •BP 13.1, •CPP 19.1, •DY 15.1
Bürger, Jan TUT 1.1, •TUT 1.2, TUT 1.3, BP 1.1, •BP 1.2, BP 1.3, AKPIK 1.1, •AKPIK 1.2, AKPIK 1.3
Bürger, Jan M. ..... •AKPIK 5.10
Bürger, Julius ..... DS 1.6, DS 1.7
Burger, Ludwig •BP 31.12, •CPP 42.12, •DY 43.12
Burghard, Marko ..... MA 41.5
Burgholzer, Katharina ..... HL 2.8
Bürgler, Daniel ..... MA 48.6
Bürgler, Daniel E. ..... •O 80.1
Burgwal, Roel ..... •O 20.11
Burkard, Ruben ... •MA 21.5, MA 21.6
Burke, John H. ..... HL 11.6
Burkert, Katrin ... •TT 11.58, TT 11.59, TT 47.11
Burkmann, Konrad ..... KFM 14.16
Burla, Aditya ..... •MM 35.1
Burnet, Anton Francis ..... •BP 25.2
Burr, David ..... BP 27.1, O 91.1
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Burri, Florence ..... HL 11.2
Burriel, Mónica ..... TT 37.35
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Burwitz, Vassily V. ..... KFM 14.13
Burwitz, Vassily Vadimovitch •MM 32.8
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Busch, Michael ..... •O 27.2
Busch, Oliver .... •MA 26.5, MA 31.18
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Busch, Sebastian . CPP 37.3, MM 4.7, MM 12.10
Buschbaum, Peter Müller .. DS 13.32
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Bushev, Pavel ..... TT 11.5
Busiello, Daniel Maria ..... DY 9.11
Businski, Artjom ..... CPP 32.11
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Bustamante Lopez, Daniel . •MA 10.3, •TT 13.3
Bustorff, Nuno ..... BP 30.6
Butcher, Tim .... MA 15.19, MA 41.39,

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Butler, Paul ..... •DS 2.3
Butté, Raphaël ..... HL 24.1
Buttenschön, Sönke ..... O 27.6
Butterling, Maik ... DS 2.5, KFM 14.8, MM 32.8
Büttgen, Norbert .... MA 2.7, MA 21.3
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Büttner, Felix ... MA 15.39, MA 31.12, MA 43.10, MA 43.12
Büttner, Ludwig ..... CPP 44.1
Büttner, Simon ..... HL 29.90
Butz, Vera ..... •TT 37.53
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Buyan-Arivjikh, Altantulga .. CPP 5.2, CPP 11.1, •CPP 11.3, CPP 24.3
Bykov, E. ..... •MA 22.6, MA 31.6
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C. Palekar, Chirag ..... HL 15.4
C. Peets, Darren ..... MA 40.3
C. R. Souza, Alan ..... O 14.3
Cadar, Oana ..... CPP 15.17
Caffrey, Nuala M ..... O 38.4
Caglieris, F. ..... TT 16.3
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Cahen, D. ..... HL 46.4
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Cai, Lei ..... CPP 24.1
Cakaj, Albin ... CPP 15.38, •CPP 22.1
Cakan, Asli ..... HL 6.5
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Calandra, Matteo . HL 11.5, HL 39.25, HL 46.7, MA 4.1, TT 7.1
Caldentey, Llorenc Albons .... O 42.2
Caldevilla-Asenjo, David .... •TT 32.5
Caldwell, Joshua D. . HL 18.4, O 84.3, O 96.7
Calleja, Fabián ..... O 15.2, TT 6.2
Calligaris, Guilherme ..... TT 10.1
Callsen, Gordon ... •HL 24.1, HL 24.2, HL 24.3, HL 52.6
Caltzidis, Ioannis . HL 29.21, •HL 36.6
Calugaru, Dumitru ... TT 18.1, TT 39.1
Calupitan, Jan Patrick ..... O 17.1
Calvanese, Francesco ..... BP 20.10, DY 25.10
Calvo, Reyes ..... HL 8.4
Calvo-Fernandez, Aitor O 15.8, TT 6.8
Camacho Ibarra, Oscar ..... •HL 6.11
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Camilli, Luca ..... •O 8.2, O 32.4
Campbell, Aidan Flynn ..... •HL 32.5, O 26.2
Campbell, Richard A. ..... CPP 32.7
Campen, R. Kramer ... O 40.6, O 49.3
Campi, Gustavo ..... O 8.8
Campidelli, Stéphane ..... O 68.2
Canalias, Carlota ..... •KFM 18.1
Candia, Adriana ..... O 30.6
Candolfi, Fabio ..... •HL 29.50
Canfield, P. C. .... MA 15.30, TT 37.18
Canfield, Paul C. ..... TT 37.1
Cangi, Attila ..... O 88.9
Cangialosi, Daniele ..... MM 9.52
Cannizzaro, Francesco ..... •MM 3.5, O 84.4
Cano, Andrés ..... KFM 8.3
Cano, Jennifer ..... TT 49.9
Canola, Sofia ..... O 20.7, O 43.4
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Canova, Fillippo Federici ..... O 16.4
Cantele, Giovanni ..... DS 3.2
Canton-Vitoria, Ruben ..... O 68.7
Cao, Derang ..... MA 48.6
Cao, Lei ..... MA 39.3
Cao, Nan ..... •MA 41.26
Cao, Pengfei ..... KFM 14.20
Cao, Xin ..... HL 42.5
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Caprara, Sergio ..... MM 32.10
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Carbogno, Christian ..... DY 33.12, MM 9.44, MM 12.1, MM 12.2, O 96.8
Carbone, Amedeo ..... •HL 62.3
Cardenas-Gamboa, Jorge .. •MA 45.8
Cardoso, Claudia . •HL 40.7, MM 34.7
Caretta, Antonio ..... HL 29.88
Carini, Giulia ..... HL 18.4, O 96.8
Carley, R. ..... O 67.5
Carlin, Jean-François ..... HL 24.1
Carlos Lippmann, Otto .... •DS 13.35
Carlstroem, Stefanos . MA 5.3, TT 1.3
Carolina Oliveira, Calisa ..... O 76.1
Caron, Luana ..... MA 22.7, MA 31.8, MA 41.30
Carpeggiani, Paolo ..... O 7.8
Carpeggiani, Paolo A. ..... O 7.3
Carrano, Vincenzo ..... HL 29.86
Carrasco, Daniel ..... HL 46.9
Carrascosa-Tejedor, Javier . CPP 32.7
Carreño, Vanessa ..... O 8.8
Carrete, Jesús ..... HL 51.2, KFM 8.7, TT 46.2
Carrillo-Cabrera, Wilder ..... TT 5.12
Carstens, F.L. ..... •MA 15.8
Carter, Ross ..... TT 11.8
Cartoceti, Alice ..... •O 69.10
caruso, fabio . O 83.5, O 99.5, TT 45.5
Carva, Karel ..... MA 48.3
Casari, Carlo Spartaco ..... O 69.10
Casarin, Barbara ..... HL 29.88
Caspari, Gerrit .... •DY 45.6, •TT 59.6
Caspari, Verena ..... O 45.10
Cassabois, Guillaume ..... O 88.7
Cassol, Francesco .... TT 7.6, •TT 7.7
Castellano, Claudio ..... SOE 10.1
Castellanos Gomez, Andres .. HL 8.4
Castellanos-Gomez, Andres .HL 17.11
Castrillo, Rodrigo ..... MA 46.4
Castro, Jose Martinez ..... O 16.7
Castro, Túlio de ..... MA 31.20
Casu, Maria Benedetta ..... O 97.1
Casula, Michele .. CPP 33.4, MM 6.2, MM 7.5, TT 7.6, TT 7.7
Catalan, Gustau . KFM 4.2, KFM 14.17
Catalan, Rodrigo ... BP 17.1, BP 17.30
Catalan, Rodrigo E. ..... •BP 17.29
Catalano, Sara ..... TT 32.5
Catelani, Gianluigi .. TT 55.7, TT 55.8
Cates, Michael E. .. BP 13.1, CPP 19.1, DY 15.1
Cattaneo, Pietro ..... TT 32.5
Caulfield, Lachlan ..... •O 63.5
Cavanaugh, Kate ..... BP 18.10
Cavar, Lukas ..... MA 33.8
Cavar, Lukas D ..... •MA 33.7
Caviezel, Andrin ..... •MA 31.17
Cavignac, Théo ..... HL 3.3, MM 27.2
Cayao, Jorge ..... TT 18.9, TT 25.11, TT 48.3
Ceccatto, Alisson ..... •O 8.8
Čechal, Jan ..... O 8.5, O 8.6, O 13.1, O 13.10
Çelik, Hüseyin ..... O 89.6
Çelik, Mustafa ..... MM 14.3
Cemin, Giovanni •DY 20.13, •TT 28.13
Cen, Yu-Jie ..... DY 22.9, HL 51.2, •HL 51.3, TT 46.2, •TT 46.3
Ceratti, Davide ..... HL 11.9
Cerbino, Roberto ..... BP 17.7
Cerchez, Mihai ..... HL 29.83
Ceriotti, Michele ... MM 3.2, MM 3.3, MM 9.62, MM 31.4
Cerisola, Federico ..... DY 31.6
Čermák, Petr ..... MA 13.1
Černá, Lenka ..... O 8.6
Cerna, Verena ..... •CPP 15.5
Cerqueira, Tiago ..... HL 3.1
Cerqueira, Tiago F. T. ..... HL 3.3
Cerreta, Andrea . CPP 40.7, MA 37.10
Čerstvý, Radomír ..... O 49.2
Cerullo, Giulio ..... CPP 30.6
Cervellera, Luca .... DY 6.1, •TT 37.37
Cetin, Fatih ..... TT 5.11
Çeven, Kadir ..... •TT 37.58
Chaabani, Montassar ..... HL 39.19
Chagas, Thais •O 14.3, O 83.3, O 89.9, TT 45.3
Chahar, Preeti ..... O 13.4
Chahib, Outhmane ... O 45.13, O 90.9
Chahine, Karim ... •DY 41.3, •TT 56.3
Chailloleau, Pierre ..... TT 37.24
Chainani, Ashish ..... O 11.6, •O 86.4
Chakkingal, Aswathi M. ..... MA 21.7
Chakrabartty, Dola ..... MA 43.9
Chakraborti, Subhadip ..... •BP 17.6
Chakraborty, Arijit ..... •HL 20.13, HL 29.78, HL 42.5
Chakraborty, Atasi . MA 16.5, MA 47.5
Chakraborty, Debamitra .... MA 48.6
Chakraborty, Koushik ..... •MA 40.2, MA 40.6, MM 6.3, MM 6.4, MM 6.9
Chakraborty, Poulami ..... MM 4.9, •MM 13.5
Chakraborty, Suman ..... O 88.1
Chan, Julia ..... TT 3.8
Chan, Yu-Te ..... •KFM 13.7, MM 8.4
Chand, Madhavi ..... TT 55.12
Chandola, Sandhya ..... •DS 8.1
chandra, manabendra ..... DS 15.3
Chandrashekhar, Prathibha •MM 9.69
Chandratre, Chinmay ..... •DY 22.8
Chang, C.F. ..... MA 40.5
Chang, Chun-Fu ..... TT 52.7
Chang, Li-Wei ..... •TT 11.41
Chang, Seo Hyoung ..... DS 13.49
Chang, Weiche .. •MM 28.5, MM 36.8
Chang, Young Jun ..... DS 13.49
chao kao, ming ..... O 39.2
Chaou, Adam Yanis ..... TT 35.6
Chapelier, Claude ..... TT 42.2
Chapman, Richard T. ..... O 23.12
Charras, Guillaume ..... BP 17.76
Chatterjee, Anasua ..... HL 44.2
Chatterjee, Banhi ... •MA 5.7, •TT 1.7
Chatterjee, Sangam ..... HL 17.2, HL 20.23, HL 40.11, HL 45.12, HL 45.13, HL 51.4, TT 46.4
Chatterjee, Swarnajit •BP 2.3, BP 2.4, •CPP 2.3, CPP 2.4, •DY 3.3, DY 3.4
Chattopadhyay, Manthan .. •DY 22.27
Chatzichrysafis, Dimos ..... •MA 5.6, •TT 1.6
Chatzieleftheriou, Maria .... •TT 43.6
Chatzigiannakis, Georgios ... •DS 4.9
Chatzittofi, Michalis ..... DY 24.9
Chaudhary, Swati ... •MA 5.5, •TT 1.5
Chauhan, Amit ..... •TT 37.50
Chauhan, Keerti ..... •CPP 17.5
Chaulagain, Narendra ..... CPP 1.2
Chava, Phanish ..... HL 23.4, TT 21.4
Chavez, Tanny ... CPP 30.1, CPP 30.3
Chawla, Aashna ..... •CPP 43.11, •DY 44.11
Cheenikundil, Rajgowrav .... MA 12.2
Chekhonin, Paul ... DS 10.1, KFM 15.6
Chen, Bin ..... MA 31.8
Chen, Chen ..... DS 3.8
Chen, Daqiang ..... O 99.2
Chen, Enze ..... MM 13.2
Chen, Eugene ..... CPP 32.28
Chen, Famin ..... O 67.8
Chen, Feng ..... O 82.4
Chen, Fenghua ..... MA 31.8
Chen, Hao ..... •MM 32.9, TT 7.2
Chen, Jinghao ..... O 30.5
Chen, Jingyi ..... MA 6.3
Chen, Li ..... •CPP 44.3
Chen, Limei ..... HL 46.10
Chen, Peng ..... HL 1.1, MM 18.3
Chen, Qifan ..... •O 9.7
Chen, Qing ..... O 99.2
Chen, Shouzheng ..... •CPP 15.26, CPP 24.1
Chen, Shuang ..... •O 21.7, O 39.6
Chen, Xi ..... •BP 10.5, •DY 14.5
Chen, Xiaobing ..... MA 13.9
Chen, Xin ..... DS 3.4
Chen, Xinren ..... MA 37.4, MM 9.8, MM 9.10
Chen, Xinxiang ... •BP 9.2, •CPP 12.2
Chen, Yang ..... •HL 20.2, •HL 20.15
Chen, Yingfan ..... O 87.9
Chen, Ying-Jiun .. MA 15.6, •MA 32.2, O 101.2, •TT 40.2, TT 57.2
Chen, Yingzhen ..... O 4.5
Chen, Yong P. ..... O 88.2
Chen, Yo-Xun ..... O 86.4
Chen, Yunan ..... CPP 15.44
Chen, Zekai ..... •TT 37.5
Chen, Zheqi ..... CPP 15.53
Cheng, E. ..... MA 33.1
Cheng, Jing ..... MA 48.6
Cheng, Lyuyang ..... •CPP 32.21, CPP 32.22
Cheng, Shangjun ..... •BP 17.21
Cheng, Shiwang ..... CPP 20.4
Cheng, Tin S. ..... O 88.7
Cheng, Xinxin ..... O 40.6
Cheng, Ya-jun ... CPP 16.4, CPP 16.6, CPP 32.18, CPP 32.19, CPP 32.21
cheng, yu ..... •HL 6.2
Cheng, Zhiyuan ..... •TT 3.8
Chennur, Madhuri .. DS 3.5, •HL 29.31
Cherasse, Marie ..... HL 45.5
Cherepanov, Vasily ..... HL 40.4
Cherkasskii, M. ..... MA 10.6, TT 13.6
Cherkasskii, Mikhail ..... MA 10.12, TT 13.12
Chernenko, Kirill ..... O 36.8
Chernikov, Alexey .. HL 40.11, HL 63.5
Cherniukh, Ihor ..... HL 29.76
Chernov, S. ..... O 26.6
Chernov, S.V. ..... MM 6.5
Chernov, Sergii ..... KFM 5.2
Chernov, Serhii V. ..... MA 8.3
Cherubini, Marco ..... •MM 6.2
Cheruvary, Karthik ..... DY 22.11
Chervanyov, Alexander .... •CPP 33.5
Chettab, Meriem ..... •KFM 1.6
Chhajed, Kartik ..... SYED 1.1
Chi, Lifeng ..... O 62.6
Chiang, Tse-Min ..... CPP 15.12
Chiatti, Olivio ..... •HL 29.85, TT 5.1
Chien, Jing ..... MA 32.2, TT 40.2
Chigrin, Dmitry ..... O 87.9
Chioncel, Liviu ..... MA 4.5, MA 28.3, •TT 37.39, •TT 47.8
Chirala, Rajesh ..... •HL 32.6
Chirita Mihaila, Marius Constantin O 26.4
Chiu, Wei-Hsun ..... •HL 1.1
Chiu, Wei-Sheng ..... •MA 15.6
Chiuzbaian, G. S. ..... O 67.5
Chlouba, Tomas ..... O 26.5
Chmeruk, Artem ..... •MA 4.5
Cho, Doohee .. O 61.5, O 83.1, O 83.8, TT 29.5, TT 43.2, TT 45.1, TT 45.8
Cho, Hyeyeon ..... •KFM 14.7
Cho, Hyun Kyong ... HL 33.1, HL 39.1, HL 39.4
Chobanyan, Ani ..... MA 34.12
Chochos, Christos ..... CPP 29.2
Choi, Chang Hyuck ..... O 84.1
Choi, Dasom ..... O 30.8, O 90.3
Choi, Jeehye ..... SOE 4.5
Choi, Kwang-Yong .. MA 7.2, MA 21.2, TT 26.1
Choi, Young-Gwan ..... •MA 43.4, MM 6.10
Cholsuk, Chanaprom ..... •HL 6.5
Chong, Yan Meng ..... •KFM 4.4
Chorkendorff, Ib ..... O 32.6, O 81.3
Chou, Fang-Cheng ..... TT 9.11
Choubey, Peayush ..... TT 34.12
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Choudhary, Monika ..... •DS 13.10
Choudhary, muhammad Iqbal KFM 14.2
Choudhary, Shraddha ..... •MA 31.31, MA 31.39
Chowdhury, Sourav ..... •MA 41.39
Christ, Bernadette ..... •HL 29.38
Christ, Simon ..... BP 29.3, •BP 29.8, BP 29.10, DY 38.3, •DY 38.8, DY 38.10
Christen, J. ..... HL 58.2, HL 58.3
Christen, Jürgen ..... HL 32.2
Christensen, Oliver ..... O 32.6
Christianen, Ruben ..... O 59.6
Christiani, Georg ..... DS 2.1
Christiansen, Dominik ..... O 10.5
Christiansen, Hanno ..... •O 71.3
Christiansen, Henrik ..... CPP 23.2
Christiansen, Silke ..... CPP 10.1
Christis, Maximilian ..... O 21.8
Chryssos, Leon .. MM 9.30, MM 9.67
Chshiev, Mairbeck . MA 32.6, TT 40.6
Chu, Hao ..... TT 16.7
Chu, Hyunwon ..... MM 12.8
Chu, Liansong ..... •CPP 15.40
Chuang, Chien-Wen ... •O 11.6, O 86.4
Chuang, Feng-Chuan ..... MA 15.6
Chudzinski, Piotr ..... SYES 1.3
Chulliparambil Shaju, Sandra MA 33.2, •MA 41.31
Chumak, Andrii ... MA 3.2, MA 20.10, MA 31.38, MA 45.10
Chumak, Andrii V. .. MA 3.5, MA 20.1
Chumakov, Andrei ..... •MA 41.2
Chung, Jae-Ho ..... MA 21.2
Chyzhykova, Anastasiia ... •TT 42.13
Ci, Xiaojing ..... CPP 11.1, CPP 11.3, CPP 32.35, •CPP 32.36
Ciancio, Regina ..... HL 29.88
Cichos, Frank ..... BP 7.5, BP 14.2, BP 14.4, BP 28.2, BP 28.3, •CPP 25.7, CPP 25.15, CPP 35.2, CPP 35.3, •DY 23.7, DY 23.15, DY 36.2, DY 36.3, DY 39.5, O 72.10
Cicuta, Pietro ..... BP 19.5
Ciesielski, Richard ..... O 96.3
Cigarini, Luigi ..... •MM 32.7
Cihan, Ebru ..... O 17.8, •O 31.5
Cilento, Federico ..... O 40.3
Cimalla, Volker ..... HL 36.10
Cimander, Moritz .. HL 61.4, MA 26.2

Cinchetti, Mirko . . MA 31.14, MA 41.7, O 7.5, O 29.4, O 33.21, O 64.6, O 79.1, TT 20.4
Čípek, Petr . . . . . MA 30.4, •MM 34.4
Cirera, Borja . . . . . O 20.9
Cirillo, Carla . . . . . TT 24.6
Ciroth, Nils . . . . . HL 36.3
Cisternas, M.A. . . . . BP 5.3
Cisternas, Marcelo A. . . . . BP 14.22, O 21.5, O 50.4
Citro, Roberta . . . . . MA 47.3
Ciuchi, Sergio . . . . . TT 34.2, TT 43.1
Civaia, Federico . . •MM 8.2, MM 32.2
Civas, Ege N. . . . . HL 32.6
Ciwan, Mokessh Kannah . . . . . DS 3.1, •DS 13.13
Cizek, Rebecca . . . . . •DS 13.37
Claes, Joshua . . . . . •HL 41.1
Claessen, R. . . . . MM 6.5
Claessen, Ralph . . . . . DS 5.5, DS 9.8, O 55.3, O 61.7, O 74.7, O 86.2, O 86.10, O 101.3, TT 29.7, TT 57.3
Claeys, Pieter W. . . . DY 13.8, DY 13.9, DY 20.2, TT 19.8, TT 19.9, TT 28.2
Claro Rodriguez, Juan Nicolas •HL 20.3
Claro Rodriguez, Nicolas . . . HL 57.11
Claro-Rodríguez, Nicolás . . HL 29.67, HL 36.6
Classen, Laura . . . . . TT 10.5, •TT 18.2, TT 37.12
Claus, Ralf . . . . . •TT 33.5
Claussen, Jens Christian . . . •DY 18.6, SOE 3.7, SOE 5.2
Clerc, Marcel . . . . . DY 18.3
Clever, Guido . . . . . O 17.3
Cobet, Christoph . . . . . DS 9.4
Cocchi, Caterina CPP 13.1, CPP 15.50, HL 16.3, HL 54.5, HL 62.5, MM 22.3, O 79.8, O 80.3, O 92.1, O 92.11
Cochran, Tyler A. . . . . TT 2.11
Coen, Sebastian . . . . . •CPP 15.44
Coffey, Aidan . . . . . CPP 30.3
Cohen, Galit . . . . . O 79.3
Coin, Irene . . . . . DS 7.6
Cojocariu, Iulia . . . . . MA 32.2, O 14.9, O 101.2, TT 40.2, TT 57.2
Coker, Helena . . . . . BP 22.4
Colazzo, Lucinao . . . . . O 30.8
Cole, Jacqueline . . . . . •SYFD 1.4
Coletti, Camilla . . . . . O 33.20, O 67.11
Colin, Xavier . . . . . CPP 21.5
Colinet, Hélène A. . . . . •DY 4.10
Colla, Alessandra . . . . . TT 15.10
Collard, Johann . . . TT 37.7, •TT 37.46
Colling, Maurice . •MA 29.5, MA 43.11
Combe, Nicolas . . . . . MM 11.1
Concepción, Omar . . . . . MA 39.3
Confalone, Tommaso . . . . . TT 50.3
Conradi, Maximilian . . . . . •CPP 23.2
Conrads, Lukas . . . DS 13.24, HL 63.1, •O 60.1, O 60.4, O 71.1, O 71.2, O 72.11, O 87.9
Consiglio, Armando . . . . . O 86.2
Constantinou, Anna P. . . . . CPP 31.6
Conti, Andrea . . MM 9.70, O 6.7, O 6.9
Contreras, Diego . . . . . TT 11.38
Contreras, Max . . . . . •SOE 3.8
Contreras, Sebastian . . . . . SOE 7.2
Cook, Ashley . . . . . TT 4.7, •TT 31.1
Cook, Ashley M. . HL 29.81, MA 41.41, TT 4.5, TT 10.6
Coppersmith, Susan N. . . . . O 16.3
Corbel, Catherine . . . . . HL 1.9
Corbett, Brian . . . . . KFM 15.5
Corley-Wiciak, Agnieszka Anna HL 15.6
Corominas-Murtra, Bernat . . SYED 1.2
Coronado, Eugenio . . . . . MA 7.4
Coronica, Piero . . . . . MM 18.2
Corradini, Andrea . . . . . •HL 39.25
Corredor Bohorquez, Laura Teresa MA 15.27
Corsaletti Filho, José Claudio •MA 15.12, MA 43.5
Corso, Martina O 17.1, •O 64.2, O 68.4
Cortes, Emiliano . . . . . DS 4.5, O 79.7
Cortes-Huerto, Robinson . •CPP 34.3, DY 5.4
Corts, Wieland . . . . . O 89.3
Cosinschi, Mihaela . . . . . •DY 33.13, MM 35.3
Costa, Andreas . . . . TT 25.1, •TT 25.2, TT 42.3, TT 42.12
Costa, António . . . . . •MA 9.5, •O 64.4
Costa, Fábio J. R. . . . . O 88.7
Costa, Natanael C. . . . . •MA 4.7
Costinas, Codrut . BP 12.6, CPP 15.17, CPP 18.6, •CPP 32.14
Cotelli, Giacomo . . . . . •HL 13.3
Cotet, Liviu Cosmin . . . . . CPP 32.14
Coto, Pedro B. . . . . CPP 13.3
Courtois, Hervé . . . . . TT 42.2
Courtois, Theo . . . . . TT 5.10
Covaci, Lucian . . . . . HL 29.69
Covre Da Silva, Saimon Filipe HL 57.11
Crassous, Jeanne . . . . . O 97.5
Cremer, Julian . . . . . MM 18.11
Crépel, Valentin . . . . . TT 39.5
Cresser, James . . . . . DY 31.6
Creutzburg, Carl Nelson . . . •HL 29.66
creutzburg, marcus . . . . . O 39.2
Crippa, Lorenzo . . . . •TT 39.1, TT 43.1
Croitori, Dorina . . . . . •MA 31.47
Croy, Alexander CPP 15.69, CPP 44.3
Cruz Hidalgo, Rau'l . . . . . DY 21.7
Cruz-León, Sergio . . . . . •BP 32.5
Csire, Gábor . . . . . SYES 1.2
Csizmadia, Tamás . . . . . O 7.8
Csontos, Miklos . . . . . HL 54.3
Cuba Supanta, Gustavo . . . . MM 9.54
Cubitt, Robert . . . . . CPP 1.2, CPP 31.2
Cuccu, Marzia . . . . . HL 40.11
Cucinotta, Clotilde . . . . . O 58.9
Cudazzo, Pier Luigi . . HL 46.7, MA 4.1
Cudazzo, Pierluigi . . . . . HL 11.5
Cuevas, Carlos . . . . . TT 42.9
Cuevas, Juan Carlos . . . . . O 45.17
Cui, Kai . . . . . CPP 25.6, DY 23.6
Cui, Mengnan . . . . . •MM 31.6
Culum, Nina . . . . . O 98.8
Cuniberti, Gianaurelio . . . . . BP 32.10, CPP 15.69, CPP 44.3, MM 18.11, MM 36.3
Cupak, Christian . . . . . O 89.4
Curcio, Davide . . . . . O 79.6, O 89.8
Currle, Marc . . . . . TT 18.4
Curticean, Ronald . . . . . CPP 26.2
Custers, Jeroen . . . . . •TT 58.2
Cvetko, Dean . . . . . O 68.7
Cygorek, Moritz . . . SYIS 1.5, •HL 30.4
Cyran, Jenee D. . . . . O 4.7
Czajka, Titus . . . . . •BP 30.7
Czap, Gregory . . . . . MA 15.10
Czasch, Benjamin . . . . . O 10.8, O 18.4
Czekelius, Contanstin . . O 15.1, TT 6.1
Czerner, Michael . . . HL 39.5, HL 58.1, MM 9.45, MM 9.71
Czibula, Caterina . . . . . KFM 5.5
D. Bapat, Rudheer . . . . . MA 31.31
D. Wieck, Andreas . . . . . HL 29.79
da Como, Enrico . . . . . TT 54.5
da Silva, Thalis H. B. . . . . HL 3.3
Daddi-Moussa-Ider, Abdallah . DY 5.7, DY 22.2
Dadgar, A. . . . . HL 58.3
Dadgar, Armin . . . . . HL 32.2
Dadhich, Priyal . . . . . •HL 29.41
Daelman, N. . . . . MM 18.10, •MM 31.7
Daelman, Nathan . •TUT 2.2, BP 29.5, DY 38.5, •O 1.2
Daghofer, Maria . . •MA 47.6, TT 35.7, TT 37.9, TT 37.10
D'Agosta, Paolo . . . . . O 69.10
Dahdoul, Remah . . . . . SOE 4.7
Dahiya, Sunil . . . . . O 99.5
Dahler, Katharina . . . . . •HL 39.24
Dahmann, Christian . . . . . BP 17.79
Dahmen, David . . . . SOE 7.4, SOE 7.5, SOE 7.8
Dahmen, Karin . . . . . MA 6.2
Dähn, Christoph . . . . . •MM 12.1
Dähne, Mario . . . . . O 13.4, O 89.6
Dai, Dinghe . . . . . O 96.3
Dai, Haitao . . . . . HL 39.6
Dai, Mian DY 33.7, •MM 3.7, •MM 18.3
Dake, Jules M. . . . . MM 4.6, MM 9.13, MM 21.8
Dakovski, G. . . . . O 26.6
Dalacu, Dan . . . . . HL 29.30
Daligou, Gérard . . . . . HL 29.55
Dalton, Benjamin . . . BP 34.4, DY 46.4
Dalzell, James . . . . . •KFM 4.1
Damerow, Sarah . . . . . •TT 2.5
Damm, Josha . . . . . HL 45.11
Dammer, Katharina . . . . . •MM 29.3
Dammermann, Alexander . . . BP 16.3, DY 17.3
Dan, Minjiang . . . . . HL 29.33
Dan, Shachar . . . CPP 15.6, •CPP 15.7, CPP 30.2
Dan, Yaping . . . . . HL 29.32
Danailov, Miltcho . . . . . HL 29.88
Dänekamp, Felix T. . . . . •BP 26.7
Danel, Zoriana . . . . . •CPP 23.6
D'Angelo, Giovanna . . . . . MM 9.20
Dani, Olfa . . . . . •HL 23.5, •TT 21.5
D'Anjou, Benjamin . . . . . TT 11.39
Danneau, Romain . . . . . TT 11.20
Dannegger, Tobias . . . . . •MA 9.10
Dannenberg, Simon . . . . . BP 3.11
Danner, Lukas . . . . . •TT 42.11
Danon, Jeroen . . . . . HL 44.2, TT 25.4
Dany, Leonie-C. . . MA 29.8, MA 41.40
Dany, Leonie-Charlotte . . . . . •MA 6.7
Danziger, Jakob Boris Günther CPP 4.6
Dao, Radek . . . . . O 14.2
Daoulas, Kostas . . . . . CPP 17.5
Daoust, Patrick . . . . . •HL 29.55
Darby, Matthew . . . . . O 58.9
Dargel, Carina . . . . . •BP 19.4
Darmawan, Andri . MA 8.3, •MA 10.11, •TT 13.11
Darvishi Kamachali, Reza . . MM 30.5
Das, Ankita . . . . O 13.4, O 17.5, O 41.5
Das, Arkaprava . . . . . •O 97.1
Das, Bikram Kumar . . . . . •MM 4.9
Das, Chandan K. . . . . •BP 32.3
Das, Debankur . . . . . DY 22.6
Das, Debashish . . . . . HL 59.5
Das, Ipsita . . . . . TT 18.4
Das, Mowpriya . . . . . O 13.4
Das, P. . . . . MA 15.30, TT 37.18
Das, Pragna . . . . . •DY 29.5
Das, Risov . . . . . MM 12.1
Das, Sayar . . . . . •MA 38.8
Das, Shibananda . . •BP 6.6, •CPP 7.6, •DY 7.6
Das, Shuvankar . . . . . O 89.11
Das, Srijita . . . . . TT 55.12
Das, Sujit . . . . . MA 41.39
Dasanna, Anil Kumar . . . . . BP 5.6
Dasari, Durga . . . . . TT 11.55
Dash, Soumyaranjan . . . . . MA 41.39
Dašić, Miljan . . CPP 15.30, •CPP 23.5
Dasol, Kim . . . . . HL 20.17
Date, Mihir . . . . . •TT 54.5
Datta, Agniva . . . . . BP 31.5, CPP 42.5, DY 37.7, DY 43.5
Datta, Sawani . . . . . O 33.2, •O 33.8
Dattani, Umang A . . . . . •BP 13.10, •CPP 19.10, •DY 15.10
Daum, Etienne . . . . . •TT 55.10
Daum, Winfried . . . . . O 50.9
Dauwe, Tim . . . . . HL 63.4, •TT 8.8
Davazoglou, Dimitris . . . . . DS 15.6
David, C. . . . . O 67.5
David, Céline . . . . . BP 22.7
Davídková, Kristýna . . . . . MA 3.2, •MA 20.10
Daviet, Romain . . . . . DY 31.9
Davis, Tim . . . . . O 87.3
Davis, Timothy J. . . . . O 7.7, O 60.7
Davoudiniya, Masoumeh . . MA 11.14, TT 14.14
Day, Graeme . . . . . KFM 8.7
Day, Matthew . . . . . O 57.5
De Angelis, Francesco . . . . . HL 1.1
de Beer, Sissi . . . . . CPP 20.5
De, Binoy Krishna . . . . . MM 6.4
de Campos Ferreira, Rodrigo Cezar •O 20.9, O 46.10
de Castro, Tulio . . . . . O 99.3
de Coene, Yovan . . . . BP 8.5, CPP 9.5
de Coster, George . . . . . O 11.12
De Donno, Marcello . . . . . •KFM 15.10
De Feyter, Steven . . . . . O 97.5
de Juan, Fernando . . . . . TT 5.2
de la Higuera Domingo, Marina Isabel •O 32.1
de la Torre, Bruno . . BP 33.6, •O 68.6, O 100.6
de Liberato, Simone . . . . . O 96.7
De Los Rios, Paolo . . . . . DY 9.11
De Luca, Filippo . . . BP 13.1, CPP 19.1, DY 15.1
De Marzo, Giordano . . . . . •SOE 10.1, SOE 10.3, SOE 10.5
de' Medici, Luca . . . . . TT 39.1
De Ninno, Giovanni . . . . . HL 29.88
de Oliveira Mann, Carina C. . . . BP 3.4
de Oliveira Petrocchi Ribas, Lucas BP 18.11
De Oliveira, Thales . . . . . TT 16.7
de Oteyza, Dimas G. . . . . •O 68.4
De Paciani, Gaia . . . . . •TT 33.7
De Santis, Duilio . . . . . DY 31.2
de Siervo, Abner . . . . . O 8.8
De Sio, Antonietta . CPP 30.6, HL 11.7, HL 11.8, HL 11.9, HL 54.1, HL 54.5
De Souza, Roger . . . . . •MM 2.1
De Vita, Alessandro •O 29.9, •TT 20.9
de Vos, Erik . . . . . TT 37.5
de Vos, Erik Willem . . . . . •HL 11.2
de Vries, Insa F. . . . . •MM 9.39
De'Ath, Clare . . . . . BP 30.10
Deb, Marwan . . . . . MA 26.10
Deb, Swarup . . . . . DS 3.7, HL 29.4, HL 29.12
Debertolis, Maxime . DY 20.6, TT 28.6
Debnath, Tanwi . . . . . •BP 19.10
Dec, Jan . . . . . KFM 18.6
Decleva, Piero . . . . . MA 5.3, TT 1.3
Decurtins, Silvio . . . . . O 90.9
Dedkov, Yuriy . . . . . MA 15.2
Dedroog, Lens . . . . . BP 8.5, CPP 9.5
Deeb, Mahmood . . . . . MA 28.2
Deepman, Airton . . . . . SOE 4.2
deere, christophe . . . . . HL 8.1
Degen, Christian L. . . . . KFM 11.2
Degerman, David . . . . . •O 81.4
Deguchi, Kazuhiko . . . . . KFM 1.3
Degutis, Giedrius . . . . . HL 1.1
Dehm, Gerhard . . . . MM 7.1, MM 9.10, MM 21.5
Dehnen, Stefanie . . . . . CPP 15.4
Dehnert, Martin . . •BP 17.72, BP 17.74
Dehning, Jonas . . . . . SOE 10.11
Deibel, Carsten . . . . . CPP 15.41
Deilmann, Thorsten . . . . . HL 20.24, •HL 59.1, HL 60.5, O 61.4, TT 29.4
Deinert, Jan-Christoph . . . . . DS 10.1, TT 16.7
Deisenhofer, Joachim MA 2.5, MA 4.4
Deissenbeck, Florian . . . . . MM 9.21
Deka, Jitul . . . . . MA 18.1
del Pino, Javier . . . . . SYQS 1.4
Del Vecchio, Patrick . . . . . HL 29.55
Delby, Niklas . . . . . KFM 15.12
Delcea, Mihaela . . . . . MA 15.11
Deleporte, Emmanuelle . . . . . HL 45.5
Delgado, Frederico . •HL 1.10, HL 52.1
Delgado-Buscalioni, Rafael . . BP 19.8
Delic, Selma . . . . . HL 20.7, •HL 29.51, HL 29.52
Delin, Anna . . . . . MA 43.8
Dellago, Christoph . . . . . MM 36.9
Demange, Gilles . . . . . MM 11.7
DeManuel-Gonzalez, Victor . . . O 87.5
Dembecki, Marco . . . . . DS 3.10
Dembski-Villalta, Michał . . . . . MA 2.4
Demidov, Vladislav . . . . . MA 20.14
Demidov, Vladislav E. . . . . MA 31.39
Demidovich, Alexander . . . . HL 29.88
Demir, Johannes . MA 11.5, MA 31.26, TT 14.5
Demir, Merve . . . . . HL 45.1, HL 45.3
Demler, Eugene . . . . DY 31.2, TT 37.34
Demmer, Angus . . . . . KFM 14.16
Demokritov, Sergej O. . . . . MA 31.39
Demokritov, Sergey . . . . . MA 20.14
Dempewolf, A. . . . . HL 58.2, HL 58.3
Demsar, J. . . . . MM 6.5
Demsar, Jure . . . . . DY 31.7, O 23.10, TT 54.1
Deng, Yunpei . . . . . DY 31.7
Deng, Zhi- Yuan . . . . . O 23.4
Denizer, Florian . . . . . O 18.7
Denk, Mariella . . . . . DS 8.3
Denker, Christian . . MA 6.2, MA 15.11
Denlinger, J.D. . . . . O 101.1, TT 57.1
Denneulin, Thibaud . . . . . MA 8.9
Deparis, Christiane . . . . . HL 11.6
Derendorf, Pascal . . . . . •TT 34.12
Derla, Mishael . . . . . DY 27.13
Derlet, Peter . . . . . •MM 16.1
Derzhko, Oleg . . . . . MA 15.33
Desaules, Jean-Yves . . . . . •DY 13.3, •TT 19.3
Deschaume, Olivier . . BP 8.5, CPP 9.5
Deshmukh, Dhruv . . . . . •DY 20.10, •TT 28.10
Deshmukh, Jay . . . . . TT 55.12
Desplat, Louise . . . . . MA 46.6
Detavernier, Christophe . . . . . HL 1.1
Dethloff, Christiane HL 39.14, HL 52.8
Dette, Ulrike . . . . . •MM 36.6
Deutsch, Andreas . . . BP 2.7, CPP 2.7, DY 3.7
Deutsch, Dennis . . . . . HL 20.3
Devolder, Thibaut . . MA 3.1, MA 20.13
dey, jyotirban . . . . . DS 15.3
Dey, Manoj . . . . . •HL 17.4
Dey, Sourav . . . . . •MA 46.11
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Di Mascio, Paolo ..... BP 22.9
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Di Miceli, Daniele .. TT 35.8, •TT 51.4
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Di Palo, Nicola ..... HL 54.6
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Di Sante, Domenico . DS 9.8, O 101.3, TT 57.3
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Dick, Daniel ..... •HL 51.8, •TT 46.8
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Dieball, Cai ..... •DY 37.2, DY 42.5
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Diederich, Jonathan ..... DS 13.50
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Diekmann, Jan ..... •CPP 14.2
Diercks, Alexander ..... HL 1.3
Dierke, Tobias ..... DS 3.4, •DS 9.9, HL 62.4
Diesen, Elias ..... •O 4.2
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Dietrich, C. ..... HL 29.29
Dietzek-Ivanšić, Benjamin .. CPP 44.1
Dietzel, Dirk ..... TT 8.6
Diez, Stefan ..... BP 11.2
Díez-Carlón, Andrés ..... DS 13.15
Diezemann, Gregor ..... •DY 9.9
Dijkstra, Alain ..... HL 60.8, TT 18.5
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Dilling, J. ..... O 26.6
Dimic, Vjeko ..... TT 11.18, •TT 11.36
Dimitriev, Grigory ..... HL 41.3
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Dinca, Paul ..... MM 35.3
Ding, Fei ..... HL 20.13, HL 29.73, HL 29.74, HL 29.76, HL 29.77, HL 29.78, HL 29.80, HL 36.9, HL 42.1, HL 42.5, •HL 47.2, HL 57.5
Ding, Hui ..... •MM 13.2, MM 35.6
ding, shilei ..... •MA 11.2, •TT 14.2
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Dinh, Thao ..... TT 25.3
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Dirnberger, F. ..... HL 60.6
Dirnberger, Florian ..... HL 29.34, HL 29.35, HL 63.5
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Dittler, Michael ..... MM 9.4
Dittloff, Johannes .. HL 32.3, HL 33.3
Dittmann, Regina .... MA 39.3, O 12.7
Dittmann, Tobias . •HL 39.11, HL 57.8
Dittmar, Marco .. MA 41.46, •MA 47.1
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Diwan, Parisha ..... •MM 12.9
Dix, Melvin ..... •BP 10.8, •DY 14.8
Dixit, Saurabh ..... HL 18.4
Djukic, U. ..... O 101.1, TT 57.1
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Dlamini, Thembelihle ..... •HL 29.43
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Dobie, Jack ..... KFM 15.5
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Dockhorn, Ron ..... CPP 23.4
Doerr, M. ..... MA 33.1
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Dogahe, Badrosadat Ojaghi .. HL 17.2
Dogariu, Aristide ..... CPP 31.6
Dohi, Takaaki ..... MA 29.13
Döhn, Johannes ..... •KFM 12.3
Dolai, Pritha ..... •BP 20.7, •DY 25.7
Dolak, Tomas ..... HL 20.20
Doležal, Jiří .. O 20.9, O 46.12, O 97.3
Doll, Sven ..... HL 13.2
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Dolso, Gian Luca ..... HL 54.6
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Dolynchuk, Oleksandr ..... CPP 4.1, •CPP 4.2, CPP 4.6
Domack, Moritz ..... •KFM 14.26
Domann, Stephan ..... •MM 16.7
Dombi, Péter ..... O 7.8
Dömer, Niklas •KFM 14.11, KFM 14.21
Domínguez Arca, Vicente .. •BP 32.12
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Dominik, Lüthi ..... •O 12.8
Dominik, Nikolas ..... •DS 4.6, O 38.2
Domröse, Till ..... O 10.7, •O 26.8
Donarini, Andrea ..... O 45.4, O 101.5, TT 32.6, TT 57.5
Donath, Markus ..... O 11.1, O 11.10, O 11.11, O 14.8, O 29.8, O 86.6, O 89.5, TT 20.8
Donati, Fabio ..... O 30.8, •O 90.3
Dong, Chengye ..... O 23.4
Dong, Shuo ... O 10.5, O 29.7, TT 20.7
Dong, Yulian ..... KFM 13.5
Donges, Jonathan F. ..... DY 28.5
Donnelly, C. ..... MA 12.1, MA 30.3
Donnelly, Claire . MA 15.12, MA 15.13, MA 15.16, MA 33.12, MA 43.4, MA 43.5, MM 6.10, TT 5.12
Donner, Reik V. ..... •DY 34.5
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Dopita, Milan ..... MA 2.9
Dorenkamp, Yvonne ..... O 9.4
Dörfler, Magdalena ..... •HL 16.1
Dörflinger, Patrick ..... HL 29.44
Dorfner, Maximilian ..... HL 16.2
Dorfner, Maximilian F.X. .. •CPP 36.2, DS 13.2
Döring, Allan ..... •MA 22.8
Döring, F. ..... O 67.5
Dormann, Kay-Robert ..... •BP 5.1, CPP 25.5, DY 23.5, DY 24.11
Dormenev, Valera ..... HL 46.10
Dorn, Anton ..... •BP 14.7
Dornich, Kay ..... O 52.2
Dornseifer, Jan Luka .. DS 6.3, DS 6.4
Dorokhin, Mikhail ..... HL 41.3
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Dörstel, Tobias .... •DY 13.7, •TT 19.7
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dos Santos Dias, Manuel .. •TUT 4.2, •MA 13.1, •O 2.2
Döschl, Fabian ..... •TT 17.7
Dösinger, Christoph ..... •MM 13.3
Doumy, Gilles ..... HL 11.6
Douveas, Iason-Konstantinos •MA 15.13
Drabbels, Marcel ..... BP 30.9
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Drašar, Čestmír ..... O 13.10
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Drautz, Ralf ..... TUT 5.1, •SYMD 1.2, MM 1.1, MM 7.4, MM 11.2, MM 18.8, MM 23.2, MM 36.5
Drawer, Jens-Christian ..... •HL 2.10, HL 62.1
Drawner, J. ..... HL 46.4
Draxl, C. ..... MM 18.10, MM 31.7
Draxl, Claudia ..... •SYIS 1.1, BP 29.5, DY 38.5, HL 11.6, MM 31.5, O 38.1, O 53.1, O 53.2, O 57.6
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Drechsler, Felix ..... •MM 9.7
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Dreißigacker, Christoph ..... CPP 3.1
Drescher, Emilia ..... HL 57.8
Drescher, Knut ..... •BP 4.1
Drescher, Lauren ..... •HL 54.2
Dreßler, Christian ..... CPP 15.2, CPP 15.66, CPP 15.67, •MM 27.3, O 22.2, O 22.3
Dressel, Martin ..... MA 10.1, TT 5.6, TT 11.4, TT 11.5, TT 11.7, TT 11.26, TT 13.1, TT 37.21, TT 37.41, TT 50.2
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Drevelow, Tim ... MA 46.8, •MA 46.9, O 30.1
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Dreyer, Niklas ..... •HL 58.2
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Driouech, Mustapha ..... •CPP 13.1
Drossel, Barbara ..... DY 5.1, DY 32.6
Drost, Robert ..... O 64.5, •O 88.5
Drouard, Marc ..... MA 11.7, TT 14.7
Drozdowski, Oliver M ..... BP 11.5
Dsouza, Raynol ..... •MM 6.6
D'Souza, Sunil ..... TT 41.10
Dsouza, Sunil W ..... O 51.5
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Du, Lanlin ..... •O 15.7, •TT 6.7
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Duan, Juanmei ..... HL 40.12, O 72.8, O 96.2
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Dufresne, Eric R. .... BP 8.4, CPP 9.4
Duine, Rembert ..... MA 3.9
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Duppel, Viola ..... KFM 13.7
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Durgun, Abdullatif ..... MA 30.2
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Dyakonov, Vladimir ..... CPP 15.14, CPP 15.15, HL 6.3, HL 6.12, HL 16.7, HL 29.44, HL 29.45, HL 29.46, HL 29.47
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Dye, Natalie ..... SYED 1.1
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E. Ali, Shehab ..... MM 9.16
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E. Gruner, Markus . MA 10.11, O 99.10, TT 13.11
Ebbecke, Jens ..... HL 6.3
Ebeling, Daniel ..... •BP 27.5, O 8.7, O 16.11, O 31.9, O 35.4, •O 91.5
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Eberhard, Eike .. BP 31.12, CPP 42.12, DY 43.12
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Ebert, Adrian ..... •O 80.2
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Folland, Thomas G. ..... HL 18.4
Folz, Frederic ..... •BP 21.1, •SOE 8.1
Fomin, Mykola ..... BP 14.17
Fomin, Vladimir M. ..... TT 5.12
Fondell, Mattis ..... HL 11.6
Fong, Kin Chung ..... DS 13.15
Fonin, Mikhail ..... •MA 34.7
Foppa, Lucas ..... MM 3.6, MM 3.10, TT 34.13
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Forero-Martinez, Nancy C. . CPP 34.3
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Forschner, Lukas ..... •O 12.3
Forslund, Axel ... MM 17.6, •MM 17.7
Forster, Robin P. ..... •O 51.2
Förster, S. ..... HL 45.9
Förster, Stefan ..... O 6.1, O 14.1
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Forti, Mariano ..... •MM 18.8
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Fowley, Ciaran ..... MA 41.13
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Fragkos, Sotirios ..... O 99.4
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Franchini, Cesare . HL 1.13, HL 20.20, KFM 4.5, TT 5.8
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Franck, Max ..... DS 13.10
Franco-Oñate, María-José . •BP 18.10
Frank, Andreas ..... HL 6.9
Frank, Bettina .. O 7.7, O 82.8, O 96.4, O 96.5
Frank, Jonathan .... DS 9.5, DS 13.59
Frank, Julia ..... MM 9.55
Frank, Marcus ..... BP 17.22
Frank, Otakar ..... DS 4.7, O 14.8
Franke, Christian ..... BP 17.25
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Frankenfeld, Katrin .. BP 8.2, CPP 9.2
Frankerl, Moritz ..... •O 43.6
Fransson, Erik ..... •MM 6.1
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Franz, Evanie ..... O 65.11
Franz, Marcel ..... TT 34.10
Franz, Martin ..... O 13.4, O 89.6
Franz, Torsten ..... HL 29.89
Franze, Kristian .. BP 17.48, BP 17.78, BP 25.3
Franzka, Steffen ..... O 33.15, O 37.4, O 37.5
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Fraser, Marie-Louise ..... •O 13.4
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Fratus, Keith ..... •DY 41.6, •TT 56.6
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Fregin, Bob ..... BP 17.36, BP 17.37, •BP 17.38
Frehse, Vinicius Estevo Silva . TT 10.1
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Frenzel, Maximilian HL 45.5, MA 10.7, TT 8.5, TT 13.7
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Frey, Maximilian ..... •MM 16.2
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Freysoldt, Christoph ..... MM 32.9, MM 37.2, O 27.3, •TT 7.2
Friák, Martin ..... •MA 30.4, MA 38.7, MM 9.51, MM 34.4, AKPIK 3.4, AKPIK 5.9
Fricker, Jascha ..... CPP 11.3
Friebel, Janna X. ..... •DS 1.7
Friederich, Pascal ..... •HL 3.4
Friedlander, Tamar •BP 20.3, •DY 25.3
Friedrich, Benjamin M. ..... BP 17.80, BP 18.11, BP 18.12
Friedrich, Christoph ..... MA 9.6
Friedrich, Dennis ..... DS 13.50
Friedrich, Florentine ..... •HL 2.9, HL 29.26
Friedrich, Johannes ..... MA 29.4, •TT 11.40
Friedrich, Lena .. •MM 9.25, MM 9.55
Friedrich, Niklas ..... •O 5.4
Friedrich, Rico ... •HL 30.5, MM 9.37, O 36.1, O 64.8, O 88.10
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Frischmann, Michael ..... BP 17.77, •BP 29.11, •DY 38.11
Fritsch, Daniel ..... •HL 52.3
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Fritz, Jonas H. ..... •DY 42.4
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Fritzsch, Felix ..... •DY 20.2, DY 45.1, •TT 28.2, TT 59.1
Fritzsche, Alexander ..... HL 6.13
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Fröhlich, Simon .... MA 6.7, MA 29.7
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Frömter, Robert ..... MA 6.6, MA 6.7, MA 29.13, MA 41.35
Fröse, Stefan ..... AKPIK 5.10
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Fu, Linhui . BP 13.4, CPP 19.4, DY 15.4
Fu, Pei-Hao ..... TT 25.11
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Fuchs, Alexander ..... •MM 31.8
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Fuchs, Lorenz ..... TT 25.1
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Fuhrberg, Andreas .. DS 5.1, DS 13.48, •KFM 5.2
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Fuhrmann, Felix . MA 11.4, •MA 15.24, TT 14.4
Fuhrmann, Jürgen ... HL 36.3, O 21.1
Fuhrmann, Sindy ... MM 9.3, MM 9.9
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Fukuda, Akihisa ..... BP 18.3
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Füllgraf, Merlin .... •DY 16.3, •TT 22.3
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Fürst, Maximilian ..... •TT 31.4
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Füßer, Bastian ..... •DY 22.24
Fyta, Maria ..... BP 14.6, BP 32.3
G. Allis, Damian ..... O 98.8
G. Calatayud, David ..... CPP 32.32
G. de Oteyza, Dimas ..... O 17.1
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Gabbrielli, Ruggero ..... KFM 15.4
Gabel, Konstantin ..... DS 7.4
Gabriel, Jan Philipp ..... CPP 15.60, DY 21.6
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Gaiardoni, Irene ..... MA 47.3
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Gaimann, Mario U. .. BP 2.8, CPP 2.8, DY 3.8, •DY 31.8
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Galazka, Zbignew ..... KFM 15.12
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Galíndez Ruales, Edgar ..... MA 11.3, TT 14.3
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Gamiz Hernandez, Ana ..... BP 29.9, DY 38.9
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Ganss, Fabian .... DS 10.1, KFM 15.6, MA 12.4
Ganster, Friederike ..... •CPP 32.1, CPP 32.12, CPP 32.23
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García de Abajo, F. Javier .... HL 18.7
García de Viedma, Dolores . HL 29.80
García, Martín ..... BP 14.14, HL 54.4, O 48.1
García Valenzuela, Aurelio ... •DS 3.5
Garcia-Baucells, Júlia ..... BP 16.3, DY 17.3
Garcia-Diez, Raul ..... MM 21.3
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Gardner, Geoff ..... TT 25.1
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Gareis, Frederik . •CPP 43.3, •DY 27.1, •DY 44.3
Garg, Manish ..... •O 78.1
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Garst, Markus ..... MA 2.4, MA 46.6
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Gary, Dominik ..... BP 8.2, CPP 9.2
Gass, Sebastian ..... MA 15.27
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Gelbart, Lev ..... •AKPIK 5.15
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Ginga, Victoria ..... •TT 9.1
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Gingras, Michel ..... TT 33.1
Gingras, Olivier ..... TT 24.11
Ginot, Felix ..... CPP 31.1
Giordano, Nico ..... TT 9.1
Giordano, Silvia ..... SOE 10.3
Giorgi, Giacomo ..... O 32.4
Gioria, Esteban ..... O 32.3
Girard, M. ..... MM 18.10, MM 31.7
Girard, Martin ..... BP 29.5, •BP 30.4, BP 32.1, BP 32.4, DY 38.5
Girella, Alessandro ..... MM 4.7
Giri, Sajal Kumar ..... CPP 15.12
Girot, Antoine ..... BP 17.29
Gisti, Martina ..... •DY 20.6, •TT 28.6
Gisy, Johannes ..... MM 4.5
Gittinger, Moritz ... CPP 30.6, HL 11.7
Giuli, Samuele ..... TT 3.9
Giunta, Giovanni BP 31.12, CPP 42.12, DY 43.12
Giustino, Feliciano ..... •SYIS 1.3
Gkekas, Ioannis .. •BP 14.13, BP 28.9, CPP 35.9, DY 36.9
Glamsch, Stephan MA 15.47, MA 45.7
Glaser, Niklas ..... TT 55.6
Glaser, Theresa ..... O 67.6
Glaser, Timo ..... O 98.4
Glatz, Fabian ..... •HL 29.33
Glatzel, Thilo ..... MM 21.10, O 45.13
Glaum, Julia .... KFM 9.3, KFM 14.17
Glawe, Henning .... BP 29.7, DY 38.7
Glazov, Mikhail M. ..... HL 40.2
Glerean, Filippo ..... TT 2.3
Glezakou, Vanda ..... MM 17.1
Glikman, Dana ..... •CPP 38.3
Glöckl, Katharina ..... •O 43.7
Glorius, Frank .. O 13.4, O 17.5, O 41.5
Gloskovskii, A. ..... MM 6.5
Gloskovskii, Andrei ..... DS 13.48, KFM 11.4, •MA 31.43
Gloter, A. ..... DS 6.5
Glunz, Stefan W. ..... HL 1.6
Gluth, Nils ..... •DY 45.4, •TT 59.4
Gmitra, M. ..... O 101.1, TT 57.1
Gmitra, Martin ..... DS 4.10, •DS 4.11, DS 13.9
Gnandt, Christian ..... TT 11.38
Gnecco, Enrico ..... O 31.5
Gnewkow, Richard ..... HL 11.6
Go, Dongwook .... MA 11.4, MA 32.1, MA 32.2, O 101.2, TT 14.4, TT 40.1, TT 40.2, TT 57.2
Göbel, Börge ..... MA 11.1, •MA 11.10, MA 26.5, MA 29.12, MA 31.18, TT 14.1, •TT 14.10
Göbel, Christoph ..... MM 12.6
Göbel, Sophie ..... O 73.9, •O 98.4
Gödde, Jonas ..... •O 46.7, O 69.7
Göddenhenrich, Thomas ..... O 35.4
Godec, Aljaz . BP 20.5, DY 4.3, DY 5.2, DY 9.8, DY 16.6, DY 25.5, DY 32.5, DY 37.2, DY 42.5, TT 22.6
Gödecke, Gilles ... •MA 29.6, TT 35.1
Godfrey, Alan ..... O 98.8
Godlewski, Szymon ..... •O 62.5
Godoy, Guillermo ..... •HL 39.7
Goedecker, Stefan CPP 15.64, O 85.2
Goennenwein, S.T.B. MA 10.6, TT 13.6
Goennenwein, Sebastian T.B. MA 3.10, MA 9.12, MA 10.12, MA 11.12, MA 15.18, MA 15.25, MA 15.38, •MA 23.1, MA 32.5, TT 13.12, TT 14.12, TT 40.5
Goering, Eberhard ..... MA 41.5

Goerlitz, Sarah L. ..... TT 37.7
Goerzen, Moritz A. ..... MA 6.8
Goerzen, Moritz Alexander . MA 46.3
Goetz, Anika ..... MA 4.7
Göhler, Fabian ..... O 33.14, O 33.16, O 101.4, TT 57.4
Göhmann, Frank .. •DY 20.8, •TT 28.8
Gohsrich, Julius T. ..... •TT 53.4
Golan, Ohad ..... •DS 13.39
Goldhahn, Rüdiger .. HL 32.1, HL 52.2
Göldl, Michael ..... HL 29.53
Goldman, A. I. ... MA 15.30, TT 37.18
Goldman, Nathan ..... TT 48.5
Goldmann, Wolfgang ..... CPP 10.1
Goldobin, Edward ... TT 11.8, TT 16.5, •TT 25.7
Goldoni, Andrea ..... O 68.7
Golestanian, Ramin . BP 6.3, CPP 7.3, CPP 25.1, DY 7.3, DY 23.1, DY 24.9
Golez, D. ..... O 67.5
Golež, Denis ..... TT 2.10
Golias, Evangelos . MA 18.5, MA 33.7, MA 33.8
Goll, David ..... •AKPIK 5.8
Gollnick, Jörg ..... •MM 30.1
Golombiewski, Maik MM 6.7, TT 3.11, TT 5.11, TT 37.32, TT 37.33, •TT 54.6
Golovin, Anastasia SOE 3.4, SOE 10.8, •SOE 10.9
Gölz, Thorsten ..... O 96.5
Gölzhäuser, Armin CPP 15.59, O 88.11
Gomez Melo, Santiago ..... •CPP 6.4
Gómez, Santiago ..... •MM 9.32
Gómez-Rodrigo, Lucía ..... O 68.8
Gómez-Vierling, Nancy ..... •BP 5.3, BP 14.22, O 50.4
Gomonay, Olena .. MA 33.7, MA 33.8
Gompf, Bruno ..... TT 37.41
Gompper, Gerhard ... BP 5.6, BP 18.2, BP 19.10, BP 31.9, BP 31.11, BP 32.9, CPP 42.9, CPP 42.11, DY 24.8, DY 43.9, DY 43.11
Gonçalves Pereira, Rodrigo . TT 43.12
Gondolf, Jannik ..... •MA 9.3
Gong, Xingao ..... O 101.6, TT 57.6
Gong, Yuanyuan ..... MA 31.8
Goniakowski, Jacek ..... O 6.2, O 6.5
Gönnheimer, Nils ..... •MM 3.4
Gonzales-Hernandez, Rafael MA 13.4
González, José ..... TT 7.8, TT 39.2
González Lastre, Manuel .... •O 16.11
Gonzàlez, Marcelo ..... HL 6.6
Gonzalez Oliva, Ignacio ..... O 57.6
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Gonzalez-Orellana, Carmen .. O 30.6, O 64.2
Goodge, Berit ..... TT 50.3, TT 50.4
Goodner, Stephen ..... DS 6.7
Goodson III, Theodore .... CPP 15.12
Goosen, Neill ..... O 58.4
gopakumar, thiruvancheril g. DS 15.3, O 98.7
Göpfrich, Kerstin ..... BP 17.45
Gopi, Ajesh K ..... TT 11.19
Gorbachev, Roman ..... MA 15.2
Gørbitz, Carl H ..... KFM 8.7
Gördes, Jendrik .. MA 17.1, •MA 26.7, MA 31.15
Gordeyeva, Korneliya ..... BP 12.1, CPP 18.1
Gorenflot, Julien ... CPP 3.2, CPP 3.4
Gorfer, Alexander ..... •MM 36.9
Gorini, Cosimo ..... HL 11.10
Görling, Andreas ..... O 13.8, O 69.6
Görlitz, Sarah L. ..... •TT 37.40
Gort, R. ..... O 67.5
Gosar, Žiga ..... O 30.3
Göser, J. ..... HL 29.13
Gößler, Markus ..... DS 7.6, MA 31.11, MA 31.46, •MA 39.1
Gosling, Nicolas ..... TT 55.3
Gossen, Kai ..... •BP 9.3, •CPP 12.3
Gossing, Florian .. MA 6.2, •MA 41.18
Goswami, Amrita ..... •CPP 15.71
Goswami, Kaustav ..... BP 17.77
Goth, Florian ... •BP 29.10, •DY 38.10
Gottardi, Stefano ..... HL 13.3
Götte, Michael ..... SYFD 1.2
Gottfried, J. Michael ... O 6.8, O 17.11, O 31.9, O 62.1, O 62.2, O 62.8, O 62.9, O 68.1
Gottfried, Knut ..... O 52.2
Gotthold, Fläschner ..... O 16.1
Gottschall, T. ..... MA 22.5, MA 22.6, •MA 31.6, MA 31.7
Gottschall, Tino ..... KFM 14.19
Gottwald, Alexander .. DS 9.4, DS 9.6
Gouder, Andreas ..... KFM 13.7
Gouder, Thomas ..... O 32.7
Gough, Zara ..... •BP 4.6
Gounelle-Pontanel, Jacques . TT 58.4
govendir, matt ..... BP 11.3
Goyal, Kshitij V ..... HL 46.11
Göz, Manuel ..... •BP 17.62
Gozlinski, Thomas ... O 12.1, TT 16.10
Graalmann, Jan-Hauke ..... •O 83.7, •TT 45.7
Grabarics, Marko ... BP 33.6, O 24.2, O 75.1, O 100.6
Grabowski, Blazej . MM 4.8, MM 9.36, MM 17.6, MM 17.7, MM 37.3
Grabs, Richard ..... HL 6.9
Grabulosa, Adrià ..... •AKPIK 3.1
Gradauskaite, Elzbieta ..... •KFM 1.1, KFM 11.2
Gradhand, Martin . MA 11.11, TT 14.11
Gradl, Johannes ... O 33.20, •O 67.11
Gradwohl, Kevin ..... KFM 5.2
Graf, David ..... TT 9.3
Graf, Isabella ..... •BP 10.1, •DY 14.1
Gräf, Stephan ..... O 31.5
Graf, Thomas ..... HL 7.2
Grafe, H.-J. ..... MA 15.8
Grafe, Hans-Joachim ..... TT 49.13
Gräfensteiner, Phillip ..... CPP 33.2
Gräff, Kevin ..... •BP 12.5, •CPP 18.5, CPP 38.2
Graff, Peter Severin ..... SOE 3.10
Graml, Maximilian .... O 5.10, O 85.3, •O 92.4
Grammer, Matthias ..... •MA 17.4, MA 32.5, TT 38.4, TT 40.5
Grams, Christoph ..... KFM 9.3
Granados, Katja D. ..... HL 18.4
Granas, Oscar ..... MA 15.41
Granberg Cauchi, Sabastian •TT 37.19
Grandel, Jonas ..... •MM 9.60
grandidier, bruno ..... HL 8.1
Grandjean, Nicolas ..... HL 24.1
Graniero, Paolo ..... SYFD 1.2
Grankin, Andrey ..... O 87.6
Granovsky, S. ..... MA 33.1
Granovsky, Sergey ..... MA 15.27, MA 21.8, MA 28.2, MA 40.3, TT 3.4
Granwehr, Josef ..... DY 28.6
Granz, Leon F. ..... MM 20.5
Graper, Erik ..... •HL 32.1
Grapin-Botton, Anne ..... •SYED 1.4
Graser, Janine ..... •TUT 1.1, TUT 1.2, TUT 1.3, •BP 1.1, BP 1.2, BP 1.3, MA 41.16, •AKPIK 1.1, AKPIK 1.2, AKPIK 1.3, •AKPIK 5.6
Gräßer, Timo .... MA 15.5, •MA 15.21
Gräßler, N. ..... MA 15.8
Gräter, Frauke ..... •PLV VIII
Graupeter, Sarina .. HL 33.2, •HL 33.5
Graus, Sven ..... •TT 3.10, TT 3.11, TT 3.12, TT 5.11, TT 54.6
Grawert, Tanja ..... BP 22.2
Gray, Gabriel ..... •MA 12.4
Graziotto, Lorenzo ... HL 2.1, HL 31.4
Greb, Christian ..... MA 48.6
Grebener, Lars ..... HL 29.8
Greczmiel, Luca ..... •HL 58.3
Grefe, Julius ..... MA 29.6, TT 35.1
Gregg, John ..... MA 3.12
Gregg, John F. ..... MA 31.41
Gregg, Marty ..... KFM 4.1, KFM 9.1
Gregor, Ingo ..... BP 7.2
Greilich, Alex ..... •HL 31.1, •HL 46.1
Greißel, Phillip ..... CPP 22.5
Greiter, Martin ..... HL 6.13
Grelier, Mathis ..... •CPP 15.23
Grenzer, Patrick ..... HL 29.90
Gresista, Lasse ..... •MA 21.9
Gretarsson, Hlynur ..... TT 58.6
Greten, David ..... •MM 9.64
Greten, Lara .... •HL 29.36, HL 29.37, HL 40.11
Greto, Eric ..... BP 20.8, DY 25.8
Gretz, Oliver ..... O 31.2
Greule, Paul ... O 24.7, O 24.8, O 45.1, O 68.10, •O 90.2
Greve, Christopher ..... CPP 13.4
Greve, Daniel ..... •DY 18.1
Grey, Clare ..... MM 22.1
Grieb, Tim ..... HL 8.2, HL 20.6
Griedel, Markus ... TT 11.50, •TT 55.9
Gries, Lukas ..... •TT 52.4
Griesinger, Andreas ..... MM 9.41
Griesser, Christoph ..... O 65.4
Griffin, Sinéad ..... MA 8.2
Grifoni, Milena ..... TT 11.1, TT 32.6, TT 44.3, •TT 50.7
Grigoletto, Massimo ..... HL 33.2, HL 33.4, HL 33.7, HL 39.3, HL 39.4
Grigorieva, Irina ..... •PLV IV
Grill, Leonhard BP 17.13, O 5.3, O 31.4, O 42.3, O 46.4, O 47.3, O 62.7, O 73.2
Grilli, Marco ..... MM 32.10
Grimm, Tobias ..... MM 9.55
Grinenko, V. ..... TT 16.3
Grinenko, Vadim ..... TT 11.15
Grisan Qiu, Yan Yan ..... O 69.8
Grisk, Holger ..... •MA 48.1
Gritsch, Andreas ..... •HL 6.14
Gröbmeyer, Franz ..... DS 4.5
Gröbmeyer, Johannes ..... HL 11.1
Groenenboom, Gerrit ..... O 49.8
Groenhagen, Mathis ..... •DY 22.7
Groh, Henrik ..... •BP 17.64
Groh, Jordan Dieter ..... •BP 17.35
Gromova, Polina ..... DS 9.3
Gronin, Sergei ..... TT 25.1
Gröning, Oliver ..... O 8.1
Gronwald, Imke ..... HL 63.3
Groome, Ryan ..... O 98.3, O 98.8
Groß, Axel KFM 12.3, KFM 12.4, O 9.2
Gros, Claudius ... BP 26.3, •SOE 7.10, •AKPIK 2.1
Groß, Petra ..... O 72.8
Groß, Vincent ..... DY 39.2
Großerhode, Paul Luca .... •HL 29.25
Größle, R. ..... DY 22.22
Größle, Robin ..... DY 22.21, O 22.1, O 66.8, O 73.1, O 77.3
Großmann, Max .... HL 3.5, MM 27.3, MM 31.10, •O 86.7
Großmann, Robert . BP 10.4, BP 31.5, CPP 42.5, DY 14.4, DY 28.7, •DY 37.7, DY 43.5
Gross, Axel ..... KFM 12.2, O 4.3, AKPIK 2.4
Gross, Leo ... •O 31.8, O 62.4, O 62.7, O 68.5, O 68.8
Gross, Miela ..... MA 33.7, MA 33.8
Gross, R. ..... MA 10.6, TT 13.6
Gross, Rudolf ..... MA 32.5, MA 37.3, TT 8.4, TT 11.52, TT 11.54, TT 11.57, TT 15.8, TT 15.9, TT 40.5, TT 50.12
Gross, Thilo ..... BP 21.3, DY 5.3, •SOE 3.6, •SOE 7.7, SOE 8.3
Grossmann, Lukas ..... •O 12.9
Grossmann, Max ... DY 22.4, HL 20.8
Grósz, Tímea ..... O 7.3, O 7.8
Grote, Linus P. ..... •TT 5.1
Grothues, Hans-Georg ..... PSV V
Grötzner, Gabriel ... HL 32.3, HL 33.3
Grover, Catherine ..... O 14.3, •O 89.9
Gruber, Manuel ..... O 23.1, O 24.11, O 46.3, O 47.4
Gruber, Markus ..... TT 5.10
Gruber, Raphael . •MA 29.7, MA 41.40
Gruenewald, Marco ... O 13.3, O 49.6, O 50.2, •O 50.3, O 79.1, O 97.2
Gruenhaupt, Lukas ..... TT 11.41
Grüger, Benedikt ..... •DY 34.4
Gruhl, Robert ..... MA 29.1, TT 41.3
Grumbach, J. ..... MA 33.1
Grumbach, Justus ..... •MA 28.2, MA 40.3, TT 3.4
Grumet, Manuel ... HL 20.1, MM 12.7, MM 12.8
Grumm, Jonas ..... O 72.12, •O 96.9
Grumser, Melvin ..... •O 45.10
Grund, Nicolai ..... MM 26.2
Grundmann, Jana ..... DS 9.2
Grundmann, Marius .. DS 5.4, HL 9.2, HL 9.3, HL 9.4, HL 9.6, HL 20.2, HL 20.14, HL 20.15, HL 29.40, HL 39.14, HL 39.15, HL 46.8, HL 52.7, HL 52.8
Grünebohm, Anna ..... KFM 8.2, KFM 14.24
Grüneis, Andreas ..... O 85.8
Gruner, Markus ..... MA 22.3, O 18.7
Grunert, Malte ..... DY 22.4, •HL 3.5, MM 27.3, MM 31.10, O 22.2
Grünewald, Marco ..... HL 39.22
Grünewald, Mona ..... BP 11.2
Grünhagen, Marvin ..... MA 19.4
Grünhaupt, Lukas . TT 11.25, TT 11.37, TT 38.2, TT 38.3
Grüning, Myrta .... •SYES 1.3, DS 4.7, MM 34.2
Gruschwitz, Markus . •O 28.5, O 33.1, O 33.2, O 33.5, O 33.9
Grusdt, Fabian ..... TT 16.9, TT 17.7, TT 33.7, TT 37.34, TT 43.5, TT 48.5, TT 54.10
Grützmacher, Detlev ..... HL 20.7, HL 29.51, HL 29.52, HL 51.1, TT 4.1, TT 42.8, TT 46.1, TT 51.1
Gruverman, Alexei ..... KFM 1.2
Grytsiuk, Sergii .... MA 32.2, TT 40.2
Grzeszczyk, Magdalena ..... O 24.4
Gschwandtner, Peter ..... •HL 36.11
Gu, Genda ..... TT 16.10
Gu, Mingqiang ..... MA 13.9
Gu, Mong-Wen ..... •O 17.2
gu, yanwei ..... O 84.5
Gu, Yujia ..... •CPP 32.6
Guan, Mengxue ..... O 67.8, O 99.2
Guarcello, Claudio ..... MA 47.3
Guardascione, Marcello ..... TT 11.5
Guardi, Giorgia .... •MM 4.2, MM 9.17
Guatieri, Francesco ..... MM 9.67
Gubanov, Kirill ..... •CPP 22.5, DS 6.7
Gubaydullin, Azat ..... TT 55.1
Gubbin, Christopher R. ..... O 96.7
Gubler, Moritz .. CPP 15.64, MM 9.73, O 85.2
Guccini, Valentina ..... •CPP 34.1
Guck, Jochen .... BP 17.43, BP 17.51, BP 25.12
Gückelhorn, Janine MA 32.5, TT 40.5
Güdde, Jens ... O 10.6, O 57.1, O 57.8
Gude, Maik ..... MM 36.2
Gudovannyy, Alexey ..... •CPP 29.4
Gueckstock, Oliver ..... •MA 48.5
Guerra Santillan, Karla Yanin •BP 17.79
Guerrero, Jorginho Villar ..... TT 8.2
Guerrini, Michele ..... CPP 13.1, CPP 15.50, HL 54.5, O 79.8
Guhr, Thomas ..... DY 45.3, DY 45.4, SOE 1.2, SOE 1.3, TT 59.3, TT 59.4
Guijarro, Albert ..... O 97.5
Guillet, Alexandre ..... •BP 26.4
Guimarães, José ..... TT 5.9
Guizar-Sicairos, M. ..... MA 30.3
Gul, Iram ..... •HL 29.60, •HL 29.61
Gulczynski, Vivian Maria ... BP 17.28
Güldenpfennig, Tim ..... •O 33.9
Gulder, Tanja ..... DS 7.3
Guldi, Dirk M. ..... CPP 22.5
Güler, Günnur ..... BP 17.57
Güleryüz, Oktay ..... O 76.2
Gulomov, Jasurbek ... •HL 1.8, HL 1.9
Gulyás Oldal, Lénárd ..... O 7.8
Gumeniuk, Roman MA 21.8, MA 21.11, MA 40.3
Gumerov, Rustam A. ..... CPP 26.3
Günay Ramovic, Bensu ..... •O 73.2
Güneş, Nurhan ..... DS 6.1
Gunkel, Felix ..... MA 39.3, O 12.7
Günkel, Robin HL 8.5, •HL 17.2, O 6.8, O 83.6, TT 45.6
Gunsenheimer, Ute ..... •SYFD 1.3
Günthel, Michael ..... HL 1.6
Günther, Florian .... DS 13.3, DS 13.6, •DS 13.7, O 28.3
Günther, Florian S. ..... O 33.19
Günthert, Marina S. ..... •MM 9.68
Günzing, D. ..... MA 30.3
Günzing, Damian ..... MA 28.9
Guo, Cong ..... •O 17.11
Guo, Fei ..... •O 29.2, •TT 20.2
Guo, Haojie ..... TT 5.2, TT 16.1
Guo, Hua ..... O 22.6
Guo, Huaming ..... TT 53.7
Guo, Jiadong ..... O 43.1, •O 77.1
Guo, Si Yue ..... O 98.3
Guo, Yingjian ..... •CPP 15.19
Guo, Yong ..... •MA 31.8
Guo, Zisu Emily ..... •TT 50.9
Gupta, Ajay ..... CPP 30.7, DS 13.32
Gupta, Akash ..... •O 86.1
Gupta, Deeksha ..... MA 31.20
Gupta, Mayanak Kumar ..... MM 6.4
Gupta, Rahul ..... MA 11.4, MA 11.7, TT 14.4, TT 14.7
Gurbuz, Emel ..... •MM 16.4
Gurevich, Svetlana ... •DY 8.1, DY 8.2
Gurevich, Svetlana V. ..... DY 8.3
Gurieva, Tatiana ..... MA 2.6
Gurlek, Burak ..... O 96.1
Gurunarayanan, Vinithra ..... O 98.7
Gurung, Sabina ..... DY 31.7
Guse, Julia ..... HL 30.1, •O 33.18
Guskova, Olga .. •CPP 36.1, CPP 41.3
Gutbrod, Karolína ..... MM 21.8
Gutfleisch, O. ..... MA 30.3
Gutfleisch, Oliver .. DS 13.61, MA 7.3, MA 22.3, MA 22.4, MA 22.8, MA 30.2, MA 30.5, MA 31.3, MA 37.4, MA 38.2, MA 38.8, MM 9.8

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Gutierrez, Rafael ..... CPP 44.3
Gutnikov, David .. MA 31.14, •MA 41.7
Gutowski, Olof ..... O 81.1
Guttmann, Dominic ..... •O 41.1
Guttmann, Martin .. HL 33.4, HL 46.5
Gutzeit, Mara ..... MA 46.8
Gvindzhiliia, Georgii ..... CPP 26.4
Gyulavári, Tamás BP 12.6, CPP 15.17, CPP 18.6
H. B. da Silva, Thalis ..... MM 27.2
H. Christensen, Morten ..... •TT 41.4
H. Heenen, Hendrik ..... O 58.8
H. McDonald, Allan ..... HL 40.7
H. Moleiro, Lara ..... BP 19.4
Ha, Yookyung ..... O 24.3
Haag, Justus ..... DS 13.51
Haag, Luca ..... MA 9.8, MA 26.13
Haag, Luca Felipe ..... •MA 9.7
Haag, Philipp ..... O 22.1, O 73.1
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Haag, Tim ..... •MM 9.56
Haags, Anja ..... O 98.2
Haas, Benedikt ..... KFM 15.12
Haas, Michael ..... •TT 38.5
Haas, Pierre A. ..... BP 18.8, •BP 18.9
Haase, Jürgen ..... DS 3.1, DS 13.13
Haase, Markus ..... KFM 14.25
Habben, Christian ..... HL 8.2
Habel, Jonas ..... •MA 21.12
Habenschaden, Christopher •MA 37.10
Haberkamm, Hannes ..... MA 41.46, MA 47.1
Haberkern, Sebastian ..... HL 39.21
Habermann, Franziska .... KFM 14.16
Habermann, Melanie ..... •BP 21.3, •SOE 8.3
Hache, Toni ..... MA 15.11, MA 37.9
Haciosmanoglu, Selcuk Kaan •CPP 15.20
Hadad, Yorgo ..... TT 11.6
Hadilou, Naby ..... •HL 54.5
Hadjadj, Sebastien E. •O 30.6, O 88.3
Hadjadj, Sebastien Elie ..... MA 17.1
Hadjimichael, Yiannis ..... HL 13.4
Hadjivasiliou, Zena SYED 1.2, BP 16.2, DY 17.2
Hadmojo, Wisnu ..... CPP 3.4
Haehner, Jonathan ..... O 87.3
Haenel, Rafael ..... TT 11.14
Haertl, Patrick ..... MA 46.2
Haeussler, Ellen ..... MA 15.27
Hafermann, Martin ..... DS 13.56, HL 29.10
Hafez, Hassan .. KFM 14.10, MA 15.3
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Hagara, Jakub ..... CPP 8.3
Hagedorn, Sylvia ... HL 33.1, HL 33.2, HL 33.5, HL 39.1, HL 39.4
Hägele, Daniel ..... HL 23.6, HL 23.7, TT 21.6, TT 21.7
Hagenow, Alexander ..... MA 34.8
Hager, Martin ..... CPP 44.1
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Haghighirad, Amir-Abbas . MA 41.39, TT 54.4
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Hamarat, Berken ..... •BP 17.57
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Hameed, Sadeed ..... •MA 41.6
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Hampshire, Peter A. E. ..... •BP 2.10, •CPP 2.10, •DY 3.10
Hamrle, Jaroslav . MA 15.4, MA 23.2, MA 23.8, •MA 32.3, MM 9.34, •TT 40.3
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Hankiewicz, Ewelina M. ..... HL 12.1, TT 12.1
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Hartmann, Carsten ..... HL 33.2
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Hauer, Jürgen ..... CPP 36.2
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Häusler, Wolfgang ..... MA 29.9
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Hecht, Lukas ..... CPP 25.5, DY 23.5
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Hecker, Fabian ..... BP 17.61
Hecker, Katrin ..... HL 17.6
Hecker, Tim K. ..... •MM 35.2
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Heine, Johanna ..... CPP 15.8
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Heinig, Peter .... •MA 31.9, MA 31.42
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Heinritz, Christina ..... BP 17.30
Heins, Christopher •MA 3.1, MA 20.13
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Held, Tobias ..... MA 26.9, O 23.18, O 23.20, •O 42.5, O 67.10
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Hemaid, Mustafa ..... DS 3.7
Hemann, Tom-Hannes .... CPP 25.7, DY 23.7
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Henkel, Christopher ..... •CPP 14.4
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Henkel, Malte ..... DY 22.15
Henkel, Pascal ..... •HL 1.2
Henkelmann, Gideon ..... •MM 21.1
Henkes, Laila ..... •DY 9.2
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Hennig, Joshua ..... •HL 61.2
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Henning, Pia ..... DS 13.22, DS 13.23, DS 13.25, •DS 13.28, MM 9.15
Henninger, Robert ..... O 45.18
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Henriques, Clarisse ..... •CPP 15.38
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Henß, Anja ..... DS 10.2
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Herges, Rainer .. CPP 32.11, MA 19.4, O 59.2
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Hermann, Sophie ..... •DY 5.6
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Heyen, Hauke ..... MA 15.11
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Höche, Hannah ..... CPP 1.6
Hocker, Stephen ..... •MM 9.5
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Hoecht, Jonas ..... TT 37.40
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Jin, Haolin ..... TT 50.3, •TT 50.4
Jin, Haonan .....MA 6.3
Jin, K. .....O 38.5
Jin, Keda .... O 50.7, •O 83.2, O 88.6, •TT 45.2
Jin, Lei .....AKPIK 6.1
Jin, Limei .....•DY 28.6
Jin, Xuelin ..... HL 20.7, HL 29.51, •HL 29.52
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Jin, Youn Un ..... KFM 18.5
Jin, Zhaonan . CPP 15.39, •CPP 32.35
Jindal, Vishwas ..... HL 53.8
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Jobst, Bernhard ..... •TT 2.11
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Joens, Klaus ..... HL 20.3
Johánek, Viktor ..... O 65.11, O 81.7
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Johansson, Mats K. G. .... CPP 15.26
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John, Karin ..... BP 4.2
John, Marco . •DS 2.2, O 66.4, O 66.5, O 66.9
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John, Philipp ..... KFM 15.8
John, Thomas ... BP 17.16, BP 17.20, •BP 25.9, BP 25.10
Johnson, Agaya ..... •BP 14.12
Johnson, David C. ..... TT 5.1
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Jordt, Philipp ..... DS 13.34, DS 13.35
Jörns, Arne ..... •HL 20.14
Jose Palliyan, Annarose ... •TT 37.15
Joseph, Darin ..... •KFM 4.5
Joseph, Jerelle A. ..... CPP 45.4
Joshi, Abhishek ..... DY 4.5
Joshi, Aprajita ..... •TT 9.12
Joshi, Yug ..... MM 14.2, MM 30.4, MM 32.1, MM 32.4
Josse, Pierre ..... O 12.10, O 30.8
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Jugovac, Matteo ... HL 29.88, O 14.9, O 30.7
Jülicher, Frank ... •SYED 1.1, BP 19.11, BP 26.4
Juluri, Raghavendra . HL 51.1, TT 46.1
Jun Cha, Byeong ..... O 84.1
Jung, Erik ..... HL 57.10
Jung, Hyein ..... •MA 31.20, O 61.8, O 99.7, TT 29.8
Jung, Hyunwook ..... •O 41.4
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Jung, Jong Hyun ..... MM 17.7
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Jungmann, Ralf ..... •BP 22.1
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Kainbacher, Nina ..... •O 80.5
Kaiser, David ..... BP 8.2, CPP 9.2, •CPP 44.1
Kaiser, Julian ..... TT 26.2
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Kaiser, Marius M. ..... •BP 17.9
Kaiser, Ruth ..... TT 37.7, •TT 37.44
Kaiser, Sebastian ..... CPP 22.3, •CPP 30.4
Kaiser, Stefan ..... TT 11.13, TT 11.60, TT 16.7
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Kalinin, Sergei ..... KFM 18.6, O 41.3, AKPIK 2.3
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Kallappara, Shashank ..... •DY 28.2
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Kamra, Akashdeep ..... •HL 60.3, MA 3.10, MA 10.2, MA 10.8, MA 15.14, MA 32.5, TT 13.2, TT 13.8, TT 40.5
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Kanduč, Matej ..... BP 5.1
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Käs, Josef ..... •BP 15.1
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Käseberg, Tim ..... DS 9.2
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Keller, Ursula ..... HL 11.2
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Kellner, Matthias ..... •MM 31.4
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Khan, Latif Ullah ..... BP 22.9
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Khoromskaia, Diana ..... SYED 1.2, •BP 16.2, •DY 17.2
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Koch, Elias .....•DY 8.2, DY 8.3
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Lichtl, Henrik ..... O 45.15, O 45.16, •O 90.5
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Liedke, Maciej Oskar ..... DS 2.5, KFM 15.6, MM 32.8
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Lim, Jaemin ..... O 92.13
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Limberg, Ulrich ..... •HL 8.3
Lin, Jiunn-Yuan ..... TT 5.13, TT 16.6
Lin, Kaiman ..... •HL 29.32
Lin, Minn-Tsong ... MA 32.2, O 101.2, TT 40.2, TT 57.2
Lin, Pu-Chou ..... •HL 45.11
Lin, Yayi ..... TT 5.6, •TT 11.5
Lin, Yuqing ..... MA 32.4, TT 40.4
Lindbergh, Göran ..... •CPP 16.1
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Lindner, Alexandra ..... MA 12.4
Lindner, Benjamin . BP 34.2, •DY 32.1, DY 32.3, DY 46.2
Lindner, Florian .. •KFM 5.5, MM 27.1
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Lindner, Jürgen ... MA 12.4, MA 12.6, MA 26.1, MA 41.13
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Ling, Ziyu ..... •MM 26.5
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Linz, Scott Daniel .•DY 20.3, •TT 28.3
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Lipavský, Pavel ..... TT 5.13
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Liu, D. ..... O 26.6
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Liu, Hanqing ..... HL 47.7
Liu, Hao ..... •CPP 25.14, •DY 23.14
Liu, Haoyang ..... MA 34.2
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Liu, Jung-Ching ..... O 45.13, •O 90.9
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Liu, Ming-Hao ..... DS 10.3, HL 17.9, HL 40.6, TT 39.6, TT 49.1, •TT 49.2, TT 49.8
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Liu, Yufei ..... TT 25.3
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Liu, Yuxin ..... •CPP 32.43
Liu, Zheng ..... •MA 23.4, MA 27.1
Liu, Zhengyuan ..... •O 11.2, O 19.2
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Lorenz, Florian .... •DY 29.7, DY 45.2, TT 59.2
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Lu, Haidong ..... KFM 1.2
Lu, Hanqian ..... MA 31.20, •O 99.7
Lu, Hao ..... •DS 6.3, •DS 6.4
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Lu, Zhiwei ..... MA 12.2
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Ludwig, Alfred ..... MM 6.7
Ludwig, Arne ..... HL 15.2, HL 15.5, HL 20.9, HL 20.11, HL 29.39, HL 29.51, HL 29.54, HL 29.58, HL 29.63, HL 29.66, HL 29.72, HL 29.75, HL 29.79, HL 42.2, HL 42.3, TT 47.5
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Lünemann, Daniel C. . . . . •CPP 30.6, HL 11.7, HL 40.12, HL 54.5
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Luo, Chen . . . . . MA 17.1, MA 41.38
Luo, Chengjie . . . . . BP 34.5, CPP 1.5, •CPP 45.4, DY 18.4, DY 46.5
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Luo, Lu . . . . . HL 29.55
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Lüpfert, Eckhard . . . . . DS 13.37
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Lüth, Hans . . . . . HL 51.1, TT 46.1
Luther, S. . . . . •TT 37.23
Luther, Stefan . . . . . BP 10.8, DY 14.8
Luther, Sven . . . . . TT 26.3
Lutz, Christopher P. . . . . MA 15.10
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Lv, Hua . . . . . •DS 3.8, DS 3.9, DS 4.3
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Lysogorskiy, Yury . . . . . MM 7.4
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Lytken, Ole . . . . . O 13.8
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M. Aladdin, Omar . . . . . •TT 38.6
M. Bonetti, Pietro . . . . . TT 16.11
M. Chakkingal, Aswathi . . . . . MA 40.3
M. Eich, Sebastian . . . . . MM 12.9
M. Fernandes, Rafael . . . . . TT 41.4
M. Juraschek, Dominik . . . . . KFM 8.5, MA 10.9, TT 13.9
M. Roy, Renjith . . . . . TT 37.41
M. Ugeda, Miguel . . . . . TT 5.2
M. Vasconcelos, Samuel . . . . . O 14.3
M. Vicente-Arche, L. . . . . DS 6.5
Ma, Chenxi . . . . . •HL 36.9, HL 42.5, HL 57.5
Ma, Chun Yu . . . . . HL 29.49
Ma, Hadiya . . . . . O 98.3
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Ma, Ji . . . . . O 9.7, O 12.8, O 97.7
Ma, Xuekai . . . . . HL 39.6
Ma, Yu-Han . . . . . DY 9.11
Maaß, Benjamin . . . . . HL 57.6
Maas, Christian . . . . . •MM 9.71
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Maasilta, Ilari . . . . . TT 55.1
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Maass, Robert . . . MM 16.6, MM 30.5
Mabrouk, Youssef . . . . . CPP 15.70
Maccari, F. . . . . MA 30.3
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Macheda, Francesco . HL 2.1, HL 31.4
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Mäck, Martin . . . . . •TT 47.12
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Maehrlein, Sebastian •MA 5.1, •TT 1.1
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Maes, Michael . . . . . BP 21.5, SOE 8.5
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Magerle, Robert . BP 17.72, •BP 17.74, •DY 4.1
Magrez, Arnaud . . . . . O 29.2, TT 20.2
Magrinya, Paula . . . . . BP 19.8
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Mahajan, Avinash . . . . . MA 21.3
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Mahendru, Bharti . . . O 45.9, •O 45.11, TT 42.10
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Maier, Simon . . . . . O 43.7
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Maier, Stefan A. . . . . DS 2.3
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Maile, Dominik . . . . . TT 47.2
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Maiti, Kalobaran . . . . . MA 15.32
Maitra, Ananyo . . . . BP 13.1, CPP 19.1, DY 15.1
Maity, S. . . . . MA 37.8
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Majcen, Fabian . . . MA 3.5, MA 20.10, •MA 31.38
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Majewski, Martin . . . . . •CPP 24.4
Major, András . . . . . BP 30.7
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Majstorovic, Filip . . . . . O 26.7, •O 72.1
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Mak, Ka Lai . . . . . DS 13.26
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Malik, Dominique . . . . . •O 33.12
Malik, Himani . . . . . O 98.7
Malindretos, Jörg . . . . . O 37.2
Maljuk, Andrey . . . . . TT 26.3
Mallada, Banjamin . . . . . O 75.1
Mallada, Benjamin . •BP 33.6, O 24.2, O 68.6, •O 100.6
Malmström, Eva . •BP 12.1, •CPP 18.1
Malok, Matjaž . . . . . HL 17.3, HL 29.2, TT 36.1, TT 36.2
Malter, Jannik . . . . . O 99.7
Malvestuto, Marco . . . . . HL 29.88
Mamiyev, Z. . . . . O 33.10
Mamiyev, Zamin . . . . . O 28.5, •O 28.7, O 33.6, O 33.13
Mammadli, Isa . . •CPP 25.8, •DY 23.8
mammadov, samir . . . . . •DS 1.9
Mañas-Valero, Samuel . . . . . HL 37.2, MA 7.4
Manchini, Andrea . . . . . O 96.4
Mancini, Andrea . . . . . O 96.5
Mandal, Haraprasad . . . . . •CPP 15.12
Mandal, Souraj . . . •BP 9.4, •CPP 12.4, CPP 15.21
Mandal, Suvendu CPP 14.3, CPP 25.5, DY 23.5
Mandalaparthy, Varun . . . . . CPP 32.2, •CPP 41.5
Mandloi, Salony . . . . . HL 2.5
Manfra, Michael . . . . . TT 25.1
Manfra, Michael J. . . . . HL 44.2
Manganelli, Constanza . . . . . HL 13.4
Mangeat, Matthieu . . BP 2.3, •BP 2.4, CPP 2.3, •CPP 2.4, DY 3.3, •DY 3.4
Mangeolle, Léo . . . . •MA 8.8, •TT 43.3
Mangeri, John . . . . . •MA 8.1
Mangin, Stephane . . . . . TT 5.10
Mangold, Florian . . . . . •O 96.5
Mania, Felix . . . . . DS 1.10
Manikowsky, Niklas . . . . . CPP 32.45, HL 45.2
Manjunath, Madhusudan . . . . TT 4.11
Mankovsky, Sergiy HL 39.8, MA 10.2, •MA 11.8, •MM 9.66, TT 13.2, •TT 14.8
Mankowsky, Roman . . . . . DY 31.7
Manmana, Salvatore R. . . . . O 57.4
Mann, Gerrit Johannes . . . . . •O 61.4, •TT 29.4
Mann, Julian . . . . . HL 29.68, HL 42.4
Mannathanath Chakkingal, Aswathi MA 15.27
Mannel, H. . . . . HL 57.4
Mannel, Hendrik . . . . HL 42.3, TT 47.5
Manning, Luca B. . . . . O 4.7
Manoharan, Sruthi . . . . . O 98.7
Manoj Kumar, Vishnu Narayan •DS 13.32
Manolescu, Andrei DY 33.13, HL 12.6, TT 12.6
Manolopoulos, David . . . . . CPP 27.2
Manser, Julia . . . . . HL 58.4
Manske, Dirk . . . . . TT 11.14
Mansy, Sheref . . . . . BP 26.2
Manthai, Tobias . . . . . HL 59.2
Manzoni, Anna Maria . . . . . MM 30.5
Manzoni, Cristian . . . . . CPP 30.6
Mao, Ning . . . . . MM 27.7
Maouene, Djamil Abdelkader Adel •CPP 15.64
Maradan, Dario . . . . HL 23.1, HL 31.10, TT 21.1
Maragkos, Fotios . . . . . TT 5.11
Maranzana, Luca . . . . . •MA 43.2
Marayatta, Nour . . . . . TT 58.5
Marbini, Arwin . . •BP 28.8, •CPP 35.8, •DY 36.8
Marcelli, Giorgia . . . . . •CPP 10.2
March, Anne-Marie . . . . . HL 11.6
Marchegiani, Giampiero . . . . . TT 55.7, TT 55.8
Marchetti, Cristina . . BP 6.2, CPP 7.2, DY 7.2
Marcks, Christian . . . . . O 12.4
Marcogliese, Lucas . . . . . •HL 6.10
Marcus, Charles M. . . . . HL 44.2
Marek, Štěpán . . . . . •O 85.3, O 92.4
Marganska, Magdalena . . . . . TT 11.1, •TT 44.3
Margraf, Johannes . HL 3.2, MM 17.2, MM 34.5
Margraf, Johannes T. . . . . CPP 15.3, MM 3.4, MM 3.9, •MM 9.44, MM 9.64, MM 31.6, O 32.8, O 41.4, O 81.5, O 96.8
Margraf, Jonas . . . . . •HL 29.24
Marie Freiberger, Eva . . . . . O 8.8
Marie, Xavier . . . . . HL 53.8
Marín, Francisca . . . . . •HL 13.4
Marini, Giovanni . . . HL 11.5, HL 39.25, TT 7.1
Marinova, Vera . . DS 13.38, DS 13.40, DS 13.41
Mariot, J.-M. . . . . O 101.1, TT 57.1
Markina, Daria . . . . . HL 29.7, HL 29.17
Markina, Daria I. . . . . HL 40.2
Märkle, Kerstin . . . . . CPP 15.44
Märklin, Timo . . . . . •TT 11.56
Markmann, Jürgen . . . . . MM 9.12, MM 21.2
Marković, Vladimir . . HL 13.6, HL 13.7
Marler, Bernd . . . . . KFM 18.5
Marlovits, Thomas . . . . . BP 30.8
Marmodoro, Alberto . . . . . •MA 32.4, •TT 40.4
Marocko, Marina . . . . . •HL 40.8
Marotta, Federico •BP 29.6, •DY 38.6
Marquardt, Florian . . . . . DY 34.3
Marques, Carolina A. . . . . O 16.2
Marques, Miguel . . •SYMD 1.5, HL 3.1
Marques, Miguel A. L. . . . . HL 3.3
Marques Salvador, Helder CPP 15.24
Marqués-Marchán, Jorge . . . . MA 6.6
Marquez, Jose . . . . . SYFD 1.2
Marsman, Martijn . . . . . O 27.9, O 92.6
Marsteller, Alexander . . . . . •DY 22.21, O 66.8
Martens, Thore . . . . . •TT 26.5
Marthaler, Michael . . DY 41.6, TT 56.6
Martín, Fernando . . . . . O 15.2, TT 6.2
Martín Jefremovas, Elizabeth MA 29.7, MA 41.35
Martin, Jens . . . . . TT 49.3
Martin, Marcel . . . . . •DS 3.1, DS 13.13
Martin, Nora S. . . . . •BP 26.9
Martin, Pierre . . . •BP 31.3, •CPP 42.3, •DY 43.3
Martin, Sylvain . . . . . MA 11.7, TT 14.7
Martín Valderrama, Carmen •MA 39.5
Martina, Riccardo . . CPP 21.4, O 58.9
Martinek, Jan . . . . . O 90.6
martinelli, lucio . . . . . O 39.2
Martinez, Franklin . . . . . O 72.6
Martinez, Jose . . . . . O 62.1
Martinez-Castro, J. . . . . O 38.5
Martinez-Castro, Jose O 83.2, O 88.6, TT 45.2
Martinez-Strasser, Carolina . . TT 53.5
Martini, Francesca . •HL 46.7, MA 4.1
Martins, Leandro . . . . . MA 20.6
Martuza, Muhammad Ali . . . . . O 37.1
Marty, Alain . . . . . MA 19.5
Marukara, Hashima . . . . . •O 23.15
Marwan, Norbert . . . . . DY 34.5
Marx, Achim . . . . . TT 11.52, TT 15.8, TT 15.9, TT 50.12
Marx, Bruno . . . . . HL 46.5
Marx, Dominik . . . . . TT 36.4
Marx, Dorian . . . . •BP 17.32, BP 17.63
Marx-Glowna, Berit . . . . . DS 13.56
Maryenko, Denis . . . . . •TT 24.7
Marzari, Nicola . . . . . MM 3.8, O 58.6
Mascher, Thorsten . . . . . BP 14.1
Masell, Jan . . . . . MA 6.10, MA 29.5, •MA 43.11
Masenda, Hilary . . . . . HL 29.15
Masilamani, Muthu . . . . . O 86.5
Masilamani, Muthu P.T. O 11.6, O 29.1, O 46.8, O 99.4, TT 20.1
Masilamani, Muthu Prasath Thirugnanasambandam Masilamani O 11.8
Masis, Sergei . . . . . TT 50.6
Maskanaki, Katerina . . . . . •DS 13.47
Maskill, Jan . . . . . MA 35.5
Masliuk, L. . . . . O 81.8
Maßmeyer, Oliver . . . . HL 8.5, HL 17.2, O 6.8, O 83.6, TT 45.6
Massabuau, Fabien C.-P. . . . . HL 52.6
Mast, Christof . . . . . BP 26.1, BP 26.2
Mast, Christof B. . . . . BP 14.25
Mastalerz, Michael . . . . . O 62.2
Matar, Toka . . . . . O 89.3
Matatagui, Daniel . . . . . CPP 32.32
Mateo, Luis M. . . . . O 68.4
Matera, Sebastian . . DY 22.1, DY 32.4, MM 3.5, MM 17.4, MM 32.5, O 21.1, O 21.2, O 84.4
Matetskii, Andrei . . . . . O 33.11
Matetskiy, Andrey . . . . . O 80.6
Mateus, Rita . . . . . BP 18.11
Mathes, Benedikt . . •HL 29.5, HL 46.2
Mathes, Lucian . . . . . •KFM 14.8,

KFM 14.13, MM 9.30, MM 32.8
Mathew Roy, Renjith ..... TT 37.21
Mathews, Prince .....•MM 11.5
Mathey, Ludwig ..... TT 42.5
Mathias, Stefan ... MA 12.8, MA 37.6, MA 43.1, MA 43.3, O 7.6, O 23.14, O 23.15, O 23.16, O 57.4, O 57.6, O 57.9, O 79.2
Mathieu, Mathieu ..... HL 6.6
Mathukhno, N. ..... HL 46.4
Mathwieser, Andreas ..... O 71.1
Matkovic, Aleksandar ..... O 80.4
Matreux, Thomas . BP 14.25, BP 26.1, BP 26.2
Matsarskaia, Olga ..... CPP 41.2
Matsidik, Rukiya ..... DS 15.5
Matsuda, Masaaki ..... MA 15.30, TT 37.18
Matsuda, Yuji ..... TT 3.3
Matsueda, Hiroaki ..... TT 25.2
Matsumoto, Haruka ..... TT 52.7
Matsumoto, Ryosuke ..... MM 28.3
Matsumoto, Yosuke ..... TT 33.5
Matsuzawa, Takumi . BP 8.4, CPP 9.4
Matta, B ..... O 33.4
Matta, Bharti .. O 28.3, O 33.1, O 33.2, O 33.8, O 33.16
Mattern, Max ..... O 23.7
Mattern, Maximilian ..... MA 26.10, •MA 26.12, MA 31.16
Mattern, Michael ..... MA 15.37
Mattersteig, Gunter ..... CPP 29.4
Matthäus, Franziska ..... BP 18.7
Matthes, Frank ..... O 80.1
Matthes, Tjorben ..... •HL 6.8
Matthias, Dana ..... BP 8.4, CPP 9.4
Mattoso, Samuel ..... •O 65.8
Matzdorf, René ..... O 69.2
Matzdorff, Tim ..... CPP 15.47
Maultzsch, Janina .... DS 3.4, DS 9.9, HL 62.4, TT 7.5
Maur, Moritz ..... TT 11.47
Maurer, Felix ..... BP 17.20
Maurer, Reinhard ... MM 18.4, O 28.4, O 42.4
Maurer, Reinhard J. . MM 18.5, O 31.6, O 42.1, O 42.6, O 47.1, O 47.2, O 67.10, O 73.5, O 84.1, O 96.6
Mauri, Francesco .... HL 2.1, HL 31.4
Mauser, Hans ..... CPP 32.38
Mauser, Norbert ..... MA 31.38
Maximov, Leo ..... TT 10.9
Mayer, Alexandre ..... AKPIK 5.2
Mayer, Benjamin . •HL 17.12, HL 29.14
Mayer Martins, Jonas ..... •DY 8.3, DY 24.4
Mayerhöfer, Thomas ..... •BP 33.7, •O 100.7
Mayo, Christopher ..... DY 21.6
Mayr, Sina ..... MA 15.16
Mayr, Stefan G. ..... CPP 15.18
Mayr, Thomas ..... •BP 14.10
Mayr-Schmölzer, Wernfried . MM 14.3
Mazare, Anca ..... CPP 10.1
Mazheika, Aliaksei ..... •AKPIK 3.3
Mazhnik, Efim ..... AKPIK 5.19
Mazibrada, David ... TT 8.3, TT 11.43, •TT 11.44, TT 11.46
Mazin, Igor ..... MA 9.11
Mazo, M. Alejandra ..... CPP 32.32
Mazza, Federico ..... TT 58.3
Mazzera, Margherita ..... HL 36.6
Mazzocchi, Francesco .... •KFM 15.3
Mazzola, Frederico ..... O 30.7
McAllister, Kaitlin H. ..... MA 3.5
McCallum, Terry ..... O 98.8
McClarty, Paul ..... MA 45.8
McCluskey, Conor ..... KFM 4.1
McCord, Jeffrey .... MA 6.2, MA 37.7, MA 41.18
McCormack, Oisin ..... KFM 15.5
McCulloch, Iain ..... CPP 3.4
McDonald, Steven ..... DY 22.2
McGinley, Max ..... •TT 27.1
McIver, James ..... O 57.5
McNeill, Christopher R. .... CPP 32.5
McQuaid, Raymond ..... KFM 9.1
McReynolds, Dylan ..... CPP 30.1, CPP 30.3
McRoberts, Adam DY 13.13, TT 19.13
Mead, Monica ... MM 32.1, •MM 32.4
Mearini, Simone ..... O 69.8
Mechler, Anna ..... O 12.4
Mecke, Joscha ..... •DY 24.8
Meckenstock, Ralf ..... MA 22.4
Medhekar, Nikhil ..... MM 19.1
Medina, Agustín ..... MA 15.46
Medrano, Cynthia P. C. ..... MA 28.6
Medrano Sandonas, Leonardo •BP 32.10, CPP 44.3, •MM 18.11
Medugorac, Marko ..... CPP 36.2
Meghwal, Vikash ..... O 98.7
Megias, Eugenio ..... SOE 4.2
Mehboodi, Sina ..... MA 41.38
Mehdipour, Hamid .....•HL 17.13
Mehdizadeh siahroudi, Faezeh •CPP 32.25
Mehdizadehlima, Mahnaz .. MM 36.4
Mehl, Sascha ..... O 65.11
Mehlhorn, Kurt ..... BP 21.1, SOE 8.1
Mehlhorn, Markus ..... •KFM 14.16
Mehlich, Kai ..... O 14.3, O 89.9
Mehner, Lisa ..... •O 23.6
Mehra, Yashasvi . •O 29.10, •TT 20.10
Mehring, Michael ... DS 13.1, DS 13.8
Mehrtens, Thorsten ..... DS 1.3
Mehta, A. ..... O 26.6
Mei, Yunhao ..... BP 17.21
Meibohm, Jan ..... •DY 9.3
Meier, Andreas ..... KFM 15.2
Meier, Dennis ..... DY 39.3, KFM 4.2, KFM 4.3, KFM 4.4, KFM 9.3, KFM 11.1, KFM 11.3, KFM 14.17, KFM 14.19, MA 2.10, MA 29.5, MA 41.35, MA 43.11, MA 43.14
Meier, Fabian ..... •MA 41.30
Meier, Jessica ..... O 69.3
Meier, Matthias ..... O 6.7, O 39.1
Meier, Quintin ..... KFM 8.3, O 99.1
Meier, Torsten ..... HL 39.10
Meierhofer, Manuel ..... O 10.6
Meiler, Tim ..... O 7.7
Meineke, Christian ... HL 63.5, O 24.9
Meinert, Christina ..... •O 49.4
Meinert, Helmut ..... HL 39.21
meinhardt, alexander ..... O 39.2
Meiring, Matthias ..... •TT 11.25
Meißner, Robert .... CPP 21.6, O 85.5
Meitzner, Rico ..... CPP 15.47
Meiwes-Broer, Karl-Heinz .... O 72.6, O 82.5
Meixner, Michael .. TT 17.12, •TT 43.4
Mejuto-Zaera, Carlos ..... •TT 3.9
Melchert, Henri ..... HL 2.10
Melchioni, Nicola ..... O 96.4
Melendez-Sans, Anna ..... TT 52.7
Melidonie, Jason ..... O 9.7
Melkov, Gennadii A. ..... MA 3.5
Melle-Franco, Manuel ..... O 68.5
Mellin, Maximilian ..... MM 8.3
Mello, Jehferson ... BP 29.7, DY 38.7
Mellor, Christopher J. ..... O 88.7
Melnikov, Alexey ..... MA 41.14
Meltschoch, Mona ..... •CPP 32.9
Melz, Marius ..... •TT 15.13
Memovich, Madeline ..... BP 30.8
Menai, Nabil .....•MA 11.11, •TT 14.11
Mena-Osteritz, Elena HL 11.8, HL 54.1
Menchón, Rodrigo ..... O 59.2
Menden, Peter ..... HL 18.8, O 24.9
Mendez, Bianchi ..... HL 46.9
Méndez-Córdoba, Fabio Pablo Miguel •MA 28.7
Mendozza, Raffaele ..... •BP 17.68
Meneghini, Carlo ..... HL 1.1
Meneghini, Giuseppe ... O 7.6, O 57.9
Menei, Tom ..... •TT 35.8
Meng Chong, Yan ..... DY 39.3
Meng, Kuan ..... •MM 29.1
Meng, Sheng . HL 11.4, O 15.7, O 43.1, O 57.3, O 67.8, O 99.2, TT 6.7
Meng, Tobias ..... TT 4.12, TT 10.10
Meng, Xiangzhi ..... •O 59.2
Meng, Yuhao ..... MA 15.3
Meng, Zi Yang ..... TT 18.2
Mengel, Lucia ..... •O 58.4, O 63.1
Mengis, Thibault ..... KFM 14.25
Menke, Henri TT 7.3, TT 7.5, TT 16.12, TT 17.4, TT 37.48
Menon, Krishnakumar S. R. .. O 89.11
Menon, Sarath .. MM 9.63, •MM 23.2
Mense, Cornelis ..... •BP 17.46
Mensing, Jonas .....•AKPIK 3.2
Menteş, Tevfik Onur ..... O 14.9
Mentink, Johan .... MA 3.1, MA 41.3, MA 41.34
Menzel, Andreas M. ..... BP 2.11, CPP 2.11, CPP 5.3, •CPP 43.5, DY 3.11, •DY 44.5
Menzel, Dirk ..... MA 29.6, MA 41.2, TT 9.2, TT 35.1
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Menzler, Heiko Georg ..... •TT 2.9
Merboldt, Marco .... O 23.16, •O 57.4, O 57.6, O 57.9, O 79.2
Mercurio, G. ..... O 67.5
Merdon, Christian .... HL 13.4, O 21.1
Merger, Claudia ..... SOE 7.9
Merino, Pablo ..... O 20.9
Merisescu, Patrick ... O 29.4, O 64.6, TT 20.4
Merkel, Konrad ..... •HL 16.2
Merkel, Milena ..... •CPP 40.1
Merkel, Rudolf ..... BP 17.82
Merker, Stefan ..... HL 52.7
Merle, Pascal ..... CPP 15.67
Merold, Veronika ..... BP 3.4
Merstorf, Marc ..... TT 37.40
Merten, Lena ..... CPP 8.3
Mertens, Fabian ..... MA 41.7
Mertens, Florian ..... KFM 14.16
Mertens, Julian ..... DS 13.58
Mertig, Ingrid ..... MA 9.6, MA 10.10, MA 11.1, MA 11.10, MA 16.1, MA 26.5, MA 29.12, MA 31.18, MA 32.6, TT 13.10, TT 14.1, TT 14.10, TT 40.6
Merz, Michael ..... TT 58.5
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Mesple, Florie ..... TT 39.3
Metelmann, Anja ..... TT 50.12
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Metternich, Daniel ..... MA 26.11, MA 43.10, MA 43.12
Mettus, Denis ..... MA 29.4
Metzler, Ralf DY 4.8, DY 24.5, DY 24.6, DY 37.1, O 69.5
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Mey, Oliver ..... •AKPIK 4.1
Meyer, Alida ..... BP 7.3, •BP 30.6
Meyer, Andreas .. MM 26.2, MM 29.3
Meyer, Bernd .MM 9.68, O 6.4, O 34.1, O 34.2, O 39.5, O 68.3
Meyer, Carola ..... BP 14.17
Meyer, Ernst ..... MM 21.10, O 45.13, O 86.1, O 90.9
Meyer, Jana ..... DS 13.35
Meyer, Lorenz ..... O 45.18, •TT 11.21
Meyer, Nina ..... MA 15.11
Meyer, Ruth ..... BP 11.6
Meyer, Sabrina ..... •HL 29.37
Meyer, Sebastian .... •MA 2.2, O 87.9
Meyer, Tami ..... O 67.9
Meyer, Tobias ..... DS 13.28, O 23.16
Meyer zu Heringdorf, Frank .... O 7.2, O 7.7, O 14.10, O 37.3, O 37.4
Meyer zu Heringdorf, Frank-J. O 61.1, TT 29.1
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Meyerheim, Holger ..... •MA 33.3
Meyer-Ortmanns, Hildegard . DY 34.6
Mezger, Markus ..... CPP 4.5
Miao, Guangyao ..... MA 15.9
Michael, Florian ..... •TT 33.6
Michael, Marios ..... •DY 31.2, O 87.6
Michaelides, Angelos ..... O 27.4
Michaelis de Vasconcellos, Steffen CPP 15.61, HL 20.24, HL 29.16, HL 29.25, HL 29.28, •HL 30.3, MA 15.22, MA 31.39, MA 41.11
Michalcová, Alena MA 30.4, MM 34.4
Michałek, Mateusz ..... SYQS 1.4
Michalicek, Gregor .... O 36.1, O 85.4, O 92.8
Michalsky, Ina ..... O 46.1
Michel, Daniel ..... HL 13.7
Michelini, Ana ..... HL 58.4
Michell, Rose Mary ..... CPP 15.55, •CPP 15.56
Michels, Andreas . MA 29.3, MA 33.4
Michely, Thomas ..... O 36.5, O 37.5, O 45.2, O 76.1, O 76.2
Michez, Lisa ..... MA 9.12
Michler, Peter ..... HL 7.1, HL 7.2, HL 29.59, HL 29.62, HL 29.73, HL 29.74, HL 39.23, HL 39.24, HL 42.1, •HL 47.1, HL 47.5, HL 57.10, HL 57.12
Midya, Jiarul ..... BP 19.10
Miedaner, Stefan ..... •O 23.10
Miedema, P. S. ..... O 67.5
Mier Gonzalez, Cristina ..... O 45.12, •O 90.7
Mieres-Perez, Joel ..... O 8.9
Miháliková, Ivana ..... •AKPIK 3.4, AKPIK 5.9
Mihlan, Levin ..... •DS 4.4
Mikadze, Luca ..... MA 15.1
Mikhailau, Uladzislau ..... •KFM 5.3
Mikolajick, Thomas ..... HL 23.4, KFM 11.4, TT 21.4
Mikulics, Martin ..... MA 48.6
Mikuni, Kouki ..... MA 12.5
Milanese, Chiara ..... MM 4.7
Milas, Maja .....•BP 17.81
Milewska, Anna CPP 15.62, CPP 16.3
Milivojević, Marko ... DS 4.10, DS 4.11
Miller, Kirill ..... DS 5.5
Miller, Nina •HL 13.2, HL 13.5, HL 32.3
Miller, R. J. Dwayne ..... O 40.6
Millis, Andrew ..... TT 39.5
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Milošević, Milorad V. ..... MM 36.7
Milovanovic, Dragomir ..... BP 30.7
Milting, Hendrik ..... BP 17.62
Min, Byungjoon ..... SOE 4.5
Minakova, Olga ... HL 45.5, •MA 10.7, TT 8.5, •TT 13.7
Minár, J. ..... O 101.1, TT 57.1
Minár, Ján ..... DS 13.33, HL 36.8, MA 13.6, MM 9.66, O 11.7, O 29.3, O 29.10, O 45.3, O 49.2, O 51.4, O 51.5, O 99.4, TT 20.3, TT 20.10, TT 41.10
Minarelli, Emma L. .....•TT 53.11
Minh Tran, Duc ..... MA 29.13
Minola, Matteo ..... MA 20.11
Mir, Mashood T. ..... MA 5.8, TT 1.8
Mir, Mashood Tariq ..... HL 29.93, •HL 29.94, HL 29.95
mir, showkat h. ..... DS 15.3
Miranda, Henrique ..... O 27.9
Miranda, Ivan ..... MA 12.5
Miranda, Rodolfo ..... O 9.7
Mirarchi, Giovanni ..... •MM 32.10
Mirau, Luca ..... BP 12.5, CPP 1.4, CPP 18.5, •CPP 38.2
Mirmohammadi, Sajad .... •TT 37.59
Mirny, Leonid A. ..... •SYED 1.5
Mironov, Alexey ..... TT 55.1
Miroshkina, Olga ..... •MA 22.3
mirza, waleed ahmad ..... •BP 11.3
Misawa, Ryo ..... TT 3.3
Misbah, Chaouqi ..... BP 31.10, CPP 42.10, DY 43.10
Mischke, Valentin ..... O 7.5, O 29.4, O 64.6, TT 20.4
Mishra, Akshat ..... •TT 17.10
Mishra, Aritra ..... •O 43.2
Mishra, Neeraj ..... O 67.11
Mishra, Seemant ..... •DY 37.4
Mishra, Shalini ..... MM 6.3, MM 6.4
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Perelshtein, Michael ..... TT 55.1
Perepadan Shaju, Roshal .. •CPP 21.5
Perera, Aurélien ..... MM 9.25
Perez, Dolores ..... O 17.1, O 68.4
Pérez Ríos, Jesús ..... DY 33.9
Perez Romero, Arturo ..... •TT 2.4
Pérez, Rubén ..... O 16.11
Pérez-Elvira, Elena .... O 59.4, O 97.7
Pérez-Román, Berta ..... CPP 32.32
Perfetti, Luca ..... HL 45.5
Perfetto, Enrico ..... •SYIS 1.2
Peria, Matteo ..... •CPP 33.4
Peris, Victor ..... BP 14.5
Perkins, Natalia ..... TT 33.3
Perl, Paul ..... •HL 29.1
Perna, Paolo ..... O 30.7
Pernice, Wolfram ..... MA 20.14
Pernice, Wolfram H. P. ..... HL 57.10, MA 31.39
Pernishova, Alexandra ..... O 24.5
Persichetti, Luca ..... •O 32.4
Persson, Mats ..... O 47.3, O 73.2
Peruani, Fernando .. BP 2.7, CPP 2.7, DY 3.7
Pervez, Waqas ..... •O 72.7
Pesch, P. ..... HL 29.29
Peshcherenko, Nikolai ..... •MM 27.7
Pesquera, David ..... O 96.10
Pestka, Benjamin ..... DS 4.8
Peter, Janis ..... TT 50.9
Peter, Oleg ..... HL 29.48
Peter, Petricia Sara ..... •HL 38.3, HL 40.10, •TT 30.3
Petermann, Eric ..... •MA 41.44
Peters, Jannick ..... •O 73.9, O 98.4
Peters, Julian I. U. BP 28.4, CPP 35.4, DY 36.4
Petersdorf, Lukas ..... AKPIK 6.4
Petersen, Christian ..... HL 8.2
Petersen, Clemens .. •HL 9.3, HL 9.4, HL 9.6, HL 39.14
Petracic, Oleg ..... •MA 39.3, O 12.7
Petreska, Irina ..... •DY 29.9
Petridou, Nicoletta ..... •SYED 1.2, CPP 43.2, DY 44.2
Petrinic, Irena ..... CPP 15.59
Petrocchi, Andrea ..... •MA 15.44
Petrova, Dimitrina DS 13.38, DS 13.40, DS 13.41
Petrović, Marin ..... •O 14.9, O 14.10, O 37.5
Petschke, Danny .. KFM 5.4, KFM 5.7
Pettinger, Nina ..... HL 11.1, HL 17.10
Petz, Dominik .. CPP 16.2, CPP 32.16
Petz, Sascha ..... MA 43.10
Petzold, Albrecht ..... CPP 15.55, CPP 15.56
Petzold, S. ..... HL 58.2, HL 58.3
Petzoldt, Philip ..... O 39.3, •O 63.1
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Pfaff, Corentin ..... TT 5.10
Pfaffinger, Lea ..... TT 5.7
Pfannstiel, Anton ..... KFM 14.11, KFM 14.12, KFM 14.21
Pfau, Bastian ..... MA 41.39
Pfeiffelmann, Timo ..... HL 52.7
Pfeiffer, Florian ..... •O 8.7
Pfeiffer, Frederik ..... TT 55.5
Pfeiffer, Mario ..... O 71.4
Pfeiffer, Martin ..... CPP 29.4
Pfeiffer, Ramon ... •DS 11.4, DS 13.62, DS 13.63
Pfeiler, Erwin ..... •AKPIK 6.3
Pfister, Clara ..... •O 48.4
Pfister, Ulrich ..... •HL 57.10
Pfitzner, Emanuel ..... BP 7.6
Pfitzner, Emmanuel . •BP 27.1, •O 91.1
Pflaum, Jens ..... CPP 32.3, O 10.5
Pfleiderer, Christian ..... MA 28.8, MA 29.4, TT 3.5, TT 7.9, TT 10.9
Pflug, Theo ..... DS 13.60, O 99.9
Pflügl, Laura .... •DS 13.23, DS 13.28, MM 9.15
Pforr, Jakob ..... HL 6.14
Pham, L.V. Duc ..... •MA 16.1
Pham, Tuan ..... •SOE 7.3
Phark, Soo-hyon ..... O 90.10
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Philip Alamcheril, Mephin •CPP 15.72
Philipp, Julian ..... BP 19.1
Phuc, Trung ..... O 45.3
Piatkowski, Nico ..... •AIW 1.2
Piazza, Francesco .. DY 31.4, TT 54.8
Pichler, Fabian ..... •TT 18.7
Picker, Julian ..... DS 13.12, HL 29.7, O 14.4, •O 14.7, O 14.12, O 49.6
Picó-Cortés, Jordi ..... •TT 32.6
Picozzi, Silvia ..... O 29.9, TT 20.9
Piehler, Jacob ..... KFM 14.25
Piel, Pierre-Maurice ..... HL 29.18, HL 29.19, •HL 40.1, HL 40.3, HL 60.5
Pielic, Borna ..... O 83.3, TT 45.3
Pieper, Max ..... •DY 16.2, •TT 22.2
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Pietronero, Luciano ..... SOE 10.1
Pietz, Anthony ..... •BP 4.2
Pietzonka, Patrick ..... DY 42.2
Pignedoli, A. ..... MA 6.11
Pignedoli, Alessandro .... •DY 22.20, MA 33.2, MA 41.31, MA 41.32
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Pijeat, Joffrey ..... O 68.2
Pilch, Patrick ..... MA 26.1, TT 9.11
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Pincelli, Tommaso .... O 10.5, O 18.3,

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Pineda, Eloi ..... MM 16.2
Pineros, William D. ..... •DY 5.5
Pini, Michele ..... TT 54.8
Pinto, Adrian John ..... •BP 3.2
Pinto, Dinesh ..... MA 19.3
Pionteck, Mike ..... KFM 14.11
Pionteck, Mike Nico ..... •MM 34.2
Piovano, Andrea .... MA 13.1, TT 16.2
Piperidou, Athanasia ..... •DS 13.24
Piquero-Zulaica, Ignacio ..... O 51.1
Pirker, Luka ..... DS 4.7, O 14.8
Pirker-Díaz, Paula ..... •SOE 3.3
Piro, Oreste ..... BP 14.14
Piros, Eszter ..... TT 37.35
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Pistidda, Claudio ..... MM 4.7
Pistolesi, Fabio ..... O 43.6
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Pistor, Paul ..... HL 45.11
Pithan, Linus .... CPP 8.3, AKPIK 6.4
Pittalis, Stefano ..... HL 54.6
Pitthan, Eduardo ..... O 89.4
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Piva, Mario Moda ..... TT 10.1
Piva, Valentina ..... DS 5.3
Pizarro, J.M. ..... MM 18.10, MM 31.7
Pizarro, José M. .... BP 29.5, DY 38.5
Pizúrová, Naděžda ..... MA 38.7
Pizzi, Giovanni .... MM 3.8, MM 31.1, MM 31.9
Placke-Yan, Carsten ..... O 49.3
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Plainpan, Nukorn ..... MM 3.8
Plak, Katarzyna ..... BP 25.12
Planer, Jakub .... O 8.5, O 8.6, O 13.1
Plass, Christian T. .. HL 6.7, HL 29.42
Plass, Kathrin ..... •O 11.3
Plate, Franz ..... •O 17.8, O 17.9
Platero, Gloria ..... TT 32.6
Platonov, Alexey ..... •AKPIK 5.16
Plenio, Martin B. ..... O 92.13
Plentz, Jonathan ..... CPP 44.1
Plitt, David ..... •HL 29.27
Pliushchai, Anna . MM 9.33, MM 9.50
Plo, Juliette ..... O 88.7
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Ploier, Alexander .... DY 20.1, TT 28.1
Plokhikh, Igor ..... MA 41.43
Plucinski, Lukasz ..... DS 4.8, O 51.2, O 86.5, O 88.6
Pluhackova, Kristyna ..... •BP 3.7
Plumadore, Ryan ..... O 98.8
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Poccia, Nicola ..... DS 3.1, DS 13.13, TT 50.3, TT 50.4
Pochet, Pascal ..... HL 1.9
Podjaski, Filip ..... •CPP 27.4
Podlesnyak, A. ... MA 15.30, TT 37.18
Podlesnyak, Andrey ..... MA 15.28
Poelchen, Georg ..... TT 52.7
Pogna, Eva ..... •HL 18.3
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Pohl, D. ..... MA 6.11
Pohl, Darius ..... MA 39.6, •MA 39.7
Pohl, Greta ..... BP 17.62
Pohl, Linus ..... O 68.1
Pohl, Ulli ..... TT 41.1
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Pöhls, Jonas . O 7.6, O 23.14, O 23.16
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Polák, Marcel ..... TT 5.4, TT 5.5, •TT 42.12
Polat, Mine ..... BP 17.15, •BP 17.18
Polesya, Svitlana ..... •HL 39.8
Poletto, Luca ..... O 79.2
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Pollner, Zsigmond ..... HL 54.3
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Pomjakushin, Vladimir .... MA 15.27, MA 40.3, MA 41.43
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Pomyalov, Anna ..... MA 3.8
Poncé, Samuel ..... O 29.5, TT 20.5
Pongsangangan, Kitinan ... MM 27.9, •MM 27.10, •TT 47.7
Ponomaryov, Alexey ..... DS 10.1
Pontius, Niko .... MA 26.7, MA 31.15, MA 31.20, MA 31.25
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Popp, Andreas ..... O 86.8
Popp, Juergen ..... BP 27.2, O 91.2
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Poschmann, Michael ..... MM 12.6
Poshakinskiy, Alexander V. ... HL 6.4
Pospíšil, J. ..... MA 13.11
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Poths, Patricia ..... MM 3.5, •O 84.4
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Potthoff, Michael .. MA 16.4, TT 37.8
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Potzger, Kay ..... MA 28.1
Pou, Pablo ..... O 16.11
Poudel, Bhuwan ..... •CPP 17.3
Poul, Marvin ..... •MM 3.1, MM 6.6, MM 9.63, MM 23.2, MM 28.2
Pournaki, Armin ..... •SOE 10.10
Povarov, Kirill ..... •TT 9.3
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Powalla, Lukas ..... MA 41.5
Powell, Adam ..... O 98.8
Powell, Annie K. ..... MA 41.28
Požar, Martina ..... MM 9.25
Pozdnyakov, Sergey N. ..... MM 3.2
Pozsár, Dániel Tibor ..... •MA 8.6
Prabhu, Shriganesh ..... HL 46.11, MA 31.22, MA 31.31
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Pradhan, Soumen ..... •DS 5.5
Prado-Navarrete, Enrique .... HL 15.6
Prager, Lukas .... •DS 13.51, TT 49.13
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Prange, Christian ..... TT 37.41
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Prass, Sebastian ..... CPP 32.25
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Predin, Sonja ..... •TT 31.6
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Prehl, Janett ..... •DY 6.4
Preibsch, Alina ..... O 13.2
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Preis, Kevin ..... DS 13.7
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Presselt, Martin ... CPP 15.47, DS 1.8
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Prodan, Lilian ..... MA 2.5, MA 2.8, MA 4.5, MA 15.39, MA 28.2, •MA 28.3, MA 28.6, MA 31.47
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Protik, Nakib ..... HL 24.3, HL 51.6, TT 46.6
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Pucci, Fabrizio ..... BP 3.3
Puddu, Alessandro •HL 51.5, •TT 46.5
Pudell, Jan-Etienne ..... •O 23.7
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Puig, Joaquin ..... TT 24.8
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Pulkkinen, Aki ..... •HL 36.8, O 29.3, O 45.3, TT 20.3
Pulkkinen, Aki Ismo Olavi ..... O 51.5
Püllmann, Maximilian ..... DS 7.7
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Purwar, Shubham ..... MA 31.22
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Qaiumzadeh, Alireza ..... MA 45.2
Qamar, Minaam ..... •MM 4.1
Qazi, Saib Jahan ..... •CPP 15.48
Qdemat, Asmaa ..... O 12.7
Qi, Ruoxuan .. CPP 32.18, •CPP 32.19
Qi, Yang ..... O 101.6, TT 57.6
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Qian, Chen ..... MM 18.4, •MM 18.5
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Qiao, Junfeng ..... MM 31.9
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Qiao, Yulong ..... •DY 31.3
Qin, Jin ..... O 60.6
Qiu, Haixin ..... •TT 2.7
Qiu, Jiajia ..... KFM 14.4
Qiu, Jianxiang ..... TT 25.3
Qiu, Jonny ..... MA 17.4
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Radulescu, Aurel ..... BP 19.4
Radulov, Iliya ..... MA 30.2
Rafeek, Rafna ..... •DY 42.3
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Raftrey, David ..... MA 33.5
Raghav, Abhishek ..... •MM 7.5
Raghuvansy, Sushma ..... •DS 5.2
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Rahimi-Iman, Arash . TUT 1.1, TUT 1.2, TUT 1.3, BP 1.1, BP 1.2, BP 1.3, AKPIK 1.1, AKPIK 1.2, AKPIK 1.3, •AKPIK 3.5, AKPIK 5.2
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Rahn, Marein .... MA 15.28, MA 28.8, MA 40.8, TT 54.3, TT 58.6
Rahn, Marein C. ..... MA 28.3
Rai, Banik ..... •MM 9.46
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Rajabzadeh, Armin ..... MM 11.1
Rajak, Piu ..... HL 29.88
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Ramirez, Francisco ..... MM 3.8
Ramkumar, Shivani G. ..... BP 18.11
Ramming, Philipp ..... CPP 15.34
Ramos, Rafael ..... MA 9.8
Rampp, Michael A. •DY 13.8, •TT 19.8
Ramsauer, Bernhard ..... •O 31.1
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Ran, Yan ..... •CPP 40.3
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Ranalli, Luigi ..... HL 1.13, TT 5.8
Rand, David ..... •SYED 1.3
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Rayan, Diaa EL-Rahman ... MA 38.10, •MM 12.5
Raz, Oren ..... DY 9.10
Razavi, Atieh .... CPP 14.3, •CPP 31.5
Razpopov, Aleksandar ..... MA 40.4
Razumovskiy, Vsevolod I. ... MM 11.3
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Rebanal, Clara ..... O 15.2, TT 6.2
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Rebarz, Mateusz ..... DS 8.2
Reber, Simone ..... BP 17.43
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Reck, Johanna ..... DS 9.4
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Reecht, Gaël .. O 15.1, O 23.1, O 24.11, O 46.3, •O 47.4, TT 6.1
Reed, Joshua ..... BP 5.1
Reents, Timo ..... •MM 31.1
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Reich, Johanna ..... O 44.1
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Reticcioli, Michele ..... HL 20.20, •MA 41.47, •MM 9.20, O 63.8, O 85.6, TT 5.8
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Rettig, Laurenz .... MA 31.20, O 10.5, O 18.1, O 18.2, O 18.3, O 29.7, O 99.3, O 99.6, TT 20.7
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Reva, Verena ..... DS 5.1
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Richter, Johannes ..... MA 40.10
Richter, Julia ..... •MM 36.4
Richter, Klaus ..... DS 10.3, DY 13.1, DY 13.11, DY 20.9, DY 45.6, HL 11.10, TT 19.1, TT 19.11, TT 28.9, TT 42.3, TT 59.6
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Rickhaus, Peter ..... MA 18.3
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Riedel, Felix ..... DY 37.9
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Rieger, Heiko ..... BP 2.3, BP 2.4, •BP 20.6, CPP 2.3, CPP 2.4, DY 3.3, DY 3.4, •DY 25.6, DY 42.1
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Riek, Claudius ..... •AIW 1.3
Riemelmoser, Stefan ..... •HL 46.3
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Rimek, F. ..... •HL 57.4
Rimek, Fabio ..... HL 42.3, TT 47.5
Rinaldi, Christian ..... DS 15.2
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Rizzoli, Silvio O. ..... BP 7.2
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Roberts, Ann ..... O 60.9, O 87.3
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Rudorf, Sophia .... •BP 29.3, BP 29.6, •DY 38.3, DY 38.6
Rudzinski, J.F. .. •MM 18.10, MM 31.7
Rudzinski, Joseph F. ..... •TUT 2.1, BP 29.5, DY 38.5, •O 1.1
Ruf, Leon ..... TT 42.6, •TT 42.7
Ruffieux, Pascal .... MA 34.3, O 12.8, O 45.14, O 59.5, O 84.5
Rugeramigabo, Eddy ..... HL 29.73, HL 29.74, HL 36.9, HL 42.5
Rugeramigabo, Eddy P. .... HL 20.13, HL 29.78
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Ruggenthaler, Michael O 87.6, O 87.8
Ruggeri, Mariangela ..... MM 9.20
Rühle, Rebecca ..... HL 7.1, •HL 7.2
Ruhmlieb, Charlotte ..... O 87.7
Ruhtinas, Aki ..... TT 55.1
Ruiz Alvarado, Isaac Azahel . •O 51.3, O 74.4
Ruiz Gómez, S. ..... MA 12.1
Ruiz- Gómez, Sandra ..... MA 15.13
Ruiz Perez, Atzin ..... HL 6.11
Ruland, Holger ..... MM 12.6
Rulands, Steffen ..... •SYAI 1.3
Rule, Kirrily C. ..... TT 9.2
Rumiantsev, Egor ..... MM 9.62
Runeson, Johan ..... •CPP 27.2
Runeson, Johan E. ..... CPP 13.3
Runge, Christian ..... MA 3.10
Runge, Daniel ..... O 21.1
Runge, Erich ..... DY 22.4, •HL 39.12, MM 27.3, MM 31.10, O 86.7, O 88.8
Runge, Henning ..... O 41.2
Rungger, Ivan ..... MM 34.6
Runnger, Ivan ..... HL 23.3, TT 21.3
Rupp, Anna ..... HL 37.1
Rupp, Jennifer L.M. ..... MM 12.8
Ruppel, Michael ..... O 68.3
Ruppert, Michael G. .. BP 27.5, O 91.5
Rupprecht, Lea ..... •BP 17.30
Ruschel, Lucas M. ..... MM 9.53, •MM 20.3, MM 26.2
Ruschel, Lucas Mathias .... MM 26.1
Rüsing, Michael ..... •KFM 18.7
Rüßmann, P. ..... O 38.5
Rüßmann, Philipp .... O 101.2, TT 5.3, TT 11.22, TT 57.2
Russell, Danny ..... MM 9.30
Russell, Danny R. ..... KFM 14.13, •MM 9.67
Rüssman, Philipp .... •O 15.6, •TT 6.6
Rüssmann, Philipp ..... TT 32.1
Russo, Matteo ..... HL 29.92
Russo, Valeria ..... O 69.10
Rusz, Ján ..... MA 39.6, MA 39.7
Rüth, Julian ..... O 58.3
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Rütten, Lisa M. ..... O 45.8, O 45.9
Ruvalcaba Briones, Ricardo . BP 33.3, O 100.3
Ruz, Benjamín ..... O 50.4
Ryabov, Artem ..... DY 37.4
Rybicki, Marcin ..... CPP 15.30
Rybski, Diego ..... •SOE 4.1
Ryburn, Finlay .... MA 3.12, MA 31.41
Ryder, Christopher ..... DY 4.4
Ryee, S. ..... O 33.10
Ryee, Siheon ..... •TT 39.5, TT 49.9
Ryndyk, Dmitry ..... O 17.8
Ryndyk, Dmitry A. ..... CPP 36.1
Rysov, Rustam ..... CPP 8.3
Ryzhak, Diana ..... •HL 15.6
S. Bar, Michael ..... HL 20.15
S. C. Mazzoni, Mario ..... O 14.3
S. Ghiasi, Talieh ..... HL 37.2
S. Hofmann, Johannes ..... DY 29.6
S. J. van der Zant, Herre ..... HL 37.2
S. Nair, Akhil ..... •MM 3.10
S. Pillai, Hemanth ..... •O 58.8
S. Ramírez, Irián ..... TT 5.2
Saalwächter, Kay ..... CPP 32.28
Saavedra, D.A. ..... BP 5.3
Saavedra, Daniel .... BP 14.22, O 21.5
Saavedra, Daniel A. ..... •O 50.4
Sabapathy, Ouviyan ..... HL 6.10
Sabass, Benedikt ..... BP 25.2
Sabath, Franziska .. •CPP 10.4, O 6.9, O 16.4, O 63.3
Sabir, Miwan ..... O 87.5
Sachdeva, Parrydeep Kaur . •HL 52.5
Sack, Ingolf ..... BP 18.5
Sadeghi, Mohsen ..... •BP 3.8
Sadeghi, Zeynab . MA 23.6, •MA 27.3
Sadeqi-Moqadam, Mohsen . KFM 9.3
Sadowski, J. ..... O 101.1, TT 57.1
Sadrollahi, Elaheh . •MA 28.6, TT 33.4
Safari, Mohammad Reza ..... O 80.1
Safarifard, Vahid ..... O 73.10
Safeer, Affan . O 36.5, O 45.2, •O 76.1, O 76.2
Safi, Inès ..... TT 47.3
Sagwal, Amandeep . O 20.9, •O 46.10, O 46.12, O 97.3
Saha, Pratim ..... HL 44.1
Saha, Rafikul Ali ..... HL 1.1
Saha, Rupayan ..... •DY 22.6
Saha, Saptarshi ..... •DY 29.1
Saha, Surajit ..... TT 9.12
Saha, Suropriya ... CPP 25.1, DY 23.1
Sahay, Prakhar ..... HL 16.6
Sahebmohammadi, Leila ... •CPP 4.5
Sahinovic, Armin ..... •O 28.6
Sahle, Christoph ..... MM 9.9
Sahle, Christoph J. ..... MM 9.3
Sahoo, Bhabani Sankar ..... HL 59.2, •HL 59.4, HL 62.2
Sahoo, Bibhut ... •CPP 25.2, •DY 23.2
Sahoo, Chakradhar .... O 88.1, O 88.2
Sahoo, Krishna Rani ..... •MA 41.11
Sahoo, Manaswini ..... TT 26.3
Sahoo, Prasana ..... O 88.1
Sahoo, Priyatosh ..... •MA 30.5
Saigal, Nihit ..... HL 53.2
Saika, Bruno ..... TT 52.6
Sailler, Sebastian ..... •MA 11.12, MA 15.18, MA 15.38, MA 17.4, •TT 14.12
Saito, Hiroto ..... •MA 15.43
Saitoh, Eiji .. MA 9.8, MA 11.3, TT 14.3
Saitta, Antonino Marco .... CPP 33.4
Saive, Rebecca ..... HL 29.20
Sajan, Sandra ..... •TT 5.2, TT 16.1
Sajjad, Arooj ..... CPP 25.6, DY 23.6
Sakamoto, Kazuyuki .. O 86.6, O 89.5
Sakar, Baha ..... •DS 7.7
Sakong, Sung ..... •O 4.3
Sakrowski, Robin ... MM 9.3, MM 9.9
Sakuma, Noritsugu ..... MA 35.3
Sakurai, Hidehiro ..... O 98.6
Sakurai, Hiroshi ..... HL 36.8
Sala, Arnau ..... HL 36.3
Sala, Giacomo ... MA 11.12, MA 11.13, MA 15.25, TT 14.12, TT 14.13
Salak, Andre ..... KFM 18.5
Salamat, Ashkan ..... MM 9.9
Salamon, Soma ..... MA 38.3
Salaverria, Sergio ..... O 17.1, O 68.4
Salazar, Catalina ..... KFM 14.19
Salazar Mejia, C. ..... MA 22.6
Salazar, Raphaël ..... O 29.3, O 51.5, TT 20.3
Salazar-Mejía, C. .. MA 22.5, MA 31.6
Salditt, Tim ..... BP 30.7
Saleh, Muhammad ..... •O 58.9
Salgado-Linares, Ignacio .... •TT 3.6
Salikhov, Ruslan .. MA 12.6, MA 26.1, MA 31.9, MA 41.13
Salinas, Andrea Capa ..... O 99.3
Salinas, Pablo E. ..... O 21.5
Salinga, Martin ... HL 39.13, MM 9.26
Salje, Ekhard K. H. ..... KFM 14.17
Sallermann, Moritz ..... TUT 4.3, •MA 33.13, O 2.3
Salusti, Francesco ..... HL 29.67, •HL 57.11
Salvalaglio, Marco ..... KFM 15.10, •MM 10.1
Salvan, Georgeta ..... DS 7.4, DS 7.6, DS 13.1, DS 13.4, DS 13.8, MA 31.46
Samad, Abdus ..... O 89.9
Samad, F. ..... MA 37.8
Samad, Fabian .. •MA 15.26, MA 31.9
Samal, Pankaj Kumar . O 65.11, O 81.7
Samanta, Amit K. ..... BP 30.8
Samanta, Tapas . MA 22.7, MA 41.30
Sammartino, Francesco ..... •O 40.3
Sammüller, Florian ..... DY 5.6
Samtsevich, Artem ..... MM 17.9
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samuely, p ..... TT 11.17
Samuely, T. ..... O 38.5
Sanchez, Ana M. .... HL 51.1, TT 46.1
Sánchez, Cristián G. ..... O 85.9
Sánchez, Miguel ..... •TT 7.8
Sanchez, Pedro ..... BP 14.12
Sanchez, Pedro A. ... DY 21.1, DY 21.2
Sánchez, Rafael ..... TT 53.10
Sánchez Sánchez, Miguel ... TT 39.2
Sánchez-Barquilla, Raquel ... O 14.11, O 21.6, O 32.2, O 41.1, •O 81.6
Sanchez-Garcia, Elsa ..... O 8.9
Sánchez-Grande, Ana ..... O 9.7
Sánchez-Portal, Daniel ..... O 59.2
Sanchez-Valle, Carmen .... HL 20.24
Sandberg, Johannes ..... MM 20.5
Sander, Mathias ..... DY 31.7
Sander, Wolfram ..... O 8.9, O 9.5
Sanders, Charlotte .... DS 1.1, O 67.9, O 79.6, O 89.8
Sanders, Charlotte E. ..... O 23.12
Sandev, Trifce ..... DY 29.9, •DY 37.8
Sandfeld, Stefan ..... MM 28.4
Sandholzer, Kilian ..... •TT 8.9
Sandner, Daniel ..... HL 54.8, •O 79.7

Sandner, Fabian ..... HL 18.8
Sandonas, Leonardo M. .... MM 36.3
Sandor, Bulcsu ..... SOE 7.10
Sandoval-Guzmán, Tatiana . BP 18.12
Sangeetha, N. S. .... TT 3.10, TT 3.11, TT 3.12, TT 37.32
Sangiovanni, Giorgio ..... DS 9.8, MA 15.31, O 61.7, O 101.3, TT 7.5, TT 17.2, TT 29.7, TT 34.2, TT 37.48, TT 39.1, TT 43.1, TT 49.9, TT 57.3
Sankar, Raman ..... MA 7.2, O 101.2, TT 57.2
Sankeshwar, Vijayalaxmi ... MA 46.1, •MA 46.2
Sann, Joachim ..... HL 45.12
Sanna, S. ..... KFM 14.18
Sanna, Simone CPP 15.11, CPP 15.13, HL 46.10, KFM 14.3, KFM 14.6, KFM 14.11, KFM 18.4, MM 34.2, O 8.7, O 17.12, O 47.5
Sano, Masaki ..... SYED 1.4
Sant, Roberto ..... O 29.9, TT 20.9
Santa, Botond ..... HL 54.3
Santana Andreo, Julia ..... •MM 22.3
Santander, Ricardo ..... •BP 14.1
Santen, Ludger ..... BP 11.2
Santer, Svetlana .•BP 28.1, •CPP 35.1, •DY 36.1
Santiso, Jose ..... O 96.10
Santo, Elton ..... MA 8.5
Santos Franca, Aldilene ..... O 71.5
Santos, Lea F. ..... DY 29.5
Santos, Marcos Cuervo .... MA 45.10
Santos, Paulo V. ..... HL 6.4
Santra, Saswati ..... HL 33.3, O 21.8
Sanyal, Biplab ... MA 6.12, •MA 11.14, MA 33.6, •TT 14.14
Sappler, Benjamin ..... •TT 17.9
Sara, Anam ..... •CPP 15.67
Saraceno, Clara ..... O 7.5
Sarafimov, Blagoj ..... MA 15.19
Saraiva, Breno ..... O 89.3
Sarau, George ..... CPP 10.1
Saravanan, M. P. ..... MM 6.3
Sardinero, Ignacio ..... •TT 51.3
Saric, Andela ..... BP 19.7
Saritas, Ozan ..... •TT 11.4
Sarkar, Kanchan ..... •AKPIK 2.4
Sarkar, R. ..... TT 16.3
Sarkar, Sagar ..... MA 43.8
Sarkar, Suchetana ..... O 17.8, O 17.9
Sarker, Partha ..... •TT 33.10
Sartori, Fabio .... •BP 21.5, •SOE 8.5, SOE 10.11
Sarvaharman, Seeralan ..... •DY 32.5
Sasaki, Yuta ..... MA 48.3
Sasi, Sarath •O 29.3, O 99.4, •TT 20.3
Sasioglu, Ersoy ..... MA 9.6
Saßnick, Holger-Dietrich ... MM 22.3
Sassenfeld, Hannah ..... •HL 9.1
Sassetti, Maura .... HL 12.2, TT 12.2, TT 48.4
Sastre, Judit ..... BP 26.8
Sata, Sai Preetham ..... •DY 33.8
Sathe, V. G. ..... MM 6.4
Satheesh, Sayooj ..... MA 41.5
Sato, Shunsuke ..... DY 20.7, TT 28.7
Sato, Toshihiro ..... •MA 13.5
Sato, Yudai ..... •TT 16.10
Sato, Yukio ..... KFM 1.3
Satoh, Takuya ..... MA 12.5
Sattler, Alexander ..... •TT 35.7
Sau, Jyotirmoy ..... MM 9.46
Sauer, Frank ..... DS 7.7
Sauerwein, Felix ..... KFM 14.21, KFM 14.25
Saunders, Benedict ..... •O 28.4
Saunderson, Tom G. ..... O 88.6
Saunot, Aymeric ..... •O 88.3
Sauter, Eduard ..... HL 29.80
Sauter, Eric ..... O 63.5
Sauter, Gabriel ..... •CPP 27.6
Sauther, Schorsch ..... TT 7.9
Savaldor, Helder ..... CPP 38.5
Savan, Alan ..... MM 6.7
Saveh, Hooman .... BP 21.4, SOE 8.4
Savelkouls, Jaqueline ..... MM 9.25, MM 9.55
Savey-Bennett, Heidi ..... TT 33.4
Savoie, Marc ..... O 98.3, O 98.8
Savoini, Matteo ..... DY 31.7
Savvidi, Kamila ..... •O 85.5
Sawatzki, Jakob ..... DS 15.4
Sayar, Mohsin ..... •HL 11.9
Sayenko, Dmitry ..... •HL 39.14
Sbierski, Björn .... MA 21.5, •MA 21.6
Scagnoli, V. ..... MA 30.3
Schaal, Maximilian ... O 50.2, •O 97.2
Schaarman, William . HL 51.1, TT 46.1
Schaberg, Lars Leander ... KFM 18.5
Schabesberger, Jan ..... DS 3.10
Schädlich, P ..... O 33.4
Schädlich, Philip .... O 28.3, O 33.14, O 33.16, O 33.18, O 101.4, TT 57.4
Schaedel, Laura ..... BP 11.2
Schaefer, Clara ..... •BP 17.14
Schaefer, Luca ..... •DY 5.1
Schaefer, Thomas ..... TT 16.12
Schaeffer, Malte ..... •MA 15.4
Schaeper, Anja ..... BP 17.22
Schäfer, Christian .... O 87.4, TT 42.8
Schäfer, Felix ..... HL 40.11
Schäfer, Jörg . O 61.7, O 74.7, TT 29.7
Schäfer, Julia M. ..... CPP 29.4
Schäfer, Julien ..... •MA 31.40
Schäfer, Kilian ..... •MA 30.7
Schäfer, L. ..... MA 30.3
Schäfer, Marie-Christine ..... •O 22.1, O 73.1
Schäfer, Marlon ..... HL 47.5
Schäfer, Moritz R. .. MM 9.73, O 34.3, •O 85.2
Schäfer, Nils Andre ..... HL 58.1, •KFM 18.4
Schäfer, Peter ..... •MM 9.9
Schäfer, Rudolf .. •MA 23.3, MA 33.5
Schäfer, Sascha . HL 29.56, MA 41.12, O 10.2, O 10.9
Schäfer, Thomas ... TT 7.3, TT 17.12, TT 34.6, TT 43.4
Schäffer, Moritz Richard .. CPP 15.64
Schäffer, Tilman ..... BP 22.5
Schäffer, Tilman E. ..... BP 15.4
Schaffrath, Nico •CPP 25.4, •DY 23.4
Schaible, Eric ..... CPP 30.3
Schaible, Sophie ..... •O 10.7
Schamriß, Lukas ..... •TT 36.5
Schäning, Anton ..... HL 46.9
Schaper, Sebastian . HL 40.1, TT 38.7
Schäpers, Thomas ... HL 51.1, TT 4.1, TT 42.8, TT 46.1
Scharff, Konrad ..... •MA 3.6
Scharfstädt, Moritz ..... •HL 29.11
Schatt, Leonhard ..... •CPP 15.1
Schatz, George C. ..... CPP 15.12
Schauerte, Alexander ..... •CPP 15.4, CPP 15.8
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Schaumann, Gregor ..... •PSV III
Schaumburg, F. ..... HL 29.29
Schaumburg, Felix ..... HL 29.8, •HL 29.27, O 49.4
Schawe, Jürgen ..... •MM 26.6
Schebek, Maximilian ..... •DY 33.5
Schedler, Benno ... •BP 7.3, BP 14.19
Scheele, Marcus ..... DS 13.21
Scheer, David ..... •TT 25.4
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Scheer, R. ..... HL 45.9
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Scheffel, Benjamin ..... O 98.8
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Scheffler, Matthias . DY 33.12, HL 3.7, HL 17.4, HL 29.84, HL 52.5, •MA 35.1, MM 3.6, MM 3.10, O 85.8, O 89.10, O 92.10, TT 34.13
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Scheibel, Thomas ..... BP 17.30
Scheiber, Daniel ..... MM 11.3
Scheidt, Joshua ..... O 17.2
Schelchshorn, Michael ..... •O 12.6
Scheler, Ulrich ..... •CPP 45.1
Schellenberger, Andreas .... TT 41.9, •TT 43.13
Schellhammer, Sebastian .. •BP 12.3, •CPP 18.3, CPP 22.3, CPP 22.4, CPP 29.3, CPP 30.4, CPP 36.3, HL 16.5
Schemmelmann, Sven ..... •O 86.6, O 89.5
Schenk, Richard J. ..... HL 52.7
Schenk, Sebastian ..... O 6.1
Schepers, Anna ..... •BP 22.4
Scherb, Sebastian .... O 11.2, •O 36.2
Scherer, Theo ... KFM 15.2, KFM 15.3
Schertel, Andreas ..... O 26.4
Scherz, A. ..... O 67.5
Scheu, Christina ..... •MM 15.1
Scheuchenpflug, Ludwig .. •MA 29.1, TT 41.3
Scheuerer, Philipp ..... O 24.10
Scheurer, C. ..... O 81.8
Scheurer, Christoph ..... DY 28.6, DY 33.10, HL 3.2, KFM 12.5, KFM 13.7, MM 8.2, MM 8.4, MM 9.22, MM 17.4, MM 17.8, MM 17.9, MM 18.2, MM 22.2, MM 32.2, MM 32.5, O 9.3, O 21.1, O 32.3, O 52.3, O 81.2, O 84.4
Scheurer, Mathias ..... TT 43.2
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Schewe, Lukas ..... •O 86.8
Schick, Daniel .... MA 10.4, •MA 10.8, MA 26.10, MA 26.12, O 23.7, TT 13.4, •TT 13.8
Schied, Monika ..... •O 5.3
Schiegl, Felix ..... HL 18.8
Schiek, Manuela ..... DS 9.2
Schienbein, Philipp ..... •CPP 17.4
Schier, Richard ..... •O 92.1, O 92.11
Schierning, Gabi ..... MM 9.4, O 6.6
Schilberth, Felix ... MA 2.5, •MA 28.8
Schilcher, Maximilian J. ..... HL 45.6
Schildbach, Michael ..... O 23.9
Schiller, Frederik M. ..... MA 46.4
Schiller, Karl ..... •O 7.5
Schilling, Julian-Steven ... •CPP 32.3
Schilling, Marcel ... HL 33.2, HL 33.4, HL 33.7, HL 39.3, HL 39.4
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Schimmel, Sebastian ..... TT 24.8, TT 35.3
Schimpf, Lennart .. •MA 11.1, •TT 14.1
Schindler, Florian ..... HL 1.6
Schindlmayr, Arno HL 20.16, MA 41.21
Schink, Severin ..... BP 4.6
Schio, Luca ..... O 68.7
Schirk, Johannes .. TT 11.42, TT 55.5
Schirmeisen, André ... BP 27.5, O 8.7, O 16.11, O 31.9, O 35.4, O 91.5, TT 8.6, TT 8.7, TT 36.8, TT 36.9
Schirmer, Yokozuna ..... •CPP 24.7
Schiroli, Riccardo ..... •BP 14.25
Schlabach, Sabine ..... MM 4.2
Schlagel, D. L. ..... MA 22.6
Schlaich, Alexander PSV I, CPP 15.32, •CPP 17.1, CPP 32.24, CPP 32.34, CPP 33.1
Schlappa, J. ..... O 67.5
Schlatmann, Rutger ..... CPP 24.7
Schlawin, Frank ..... MA 28.7
Schleberger, Marika . O 23.11, O 33.15
Schleicher, Lukas . HL 38.3, HL 40.10, TT 30.3
Schleife, Andre ..... O 92.9
Schlesag, Marcel ..... O 69.2
Schlettwein, Derck ..... CPP 15.42, HL 20.23, HL 45.8
Schlichting, Hartmut ..... O 13.7
Schlickum, Uta .... KFM 13.3, O 16.6, O 20.10
Schliemann, John ... TT 11.1, TT 44.3
Schlipf, Martin ..... O 27.9, •O 92.6
Schlitz, Richard ... MA 3.10, MA 9.12, •MA 10.12, MA 11.12, MA 15.18, MA 15.38, MA 32.5, O 59.9, •TT 13.12, TT 14.12, TT 40.5
Schlömer, Henning ..... •TT 16.9
Schlosser, Jakob ..... •HL 63.5
Schlueter, C. ..... MM 6.5
Schlueter, Christoph ..... DS 13.48, KFM 5.2, KFM 11.4, MA 31.43
Schlünzen, Frank ..... CPP 30.3
Schlupp, Peter ..... HL 29.40
Schlüter, Henrik ... DY 13.10, TT 19.10
Schmalhorst, Jan ..... MA 13.10, MA 15.36, MA 15.37, MA 41.45, O 6.6
Schmalian, Jörg ..... MA 9.1, O 12.1, TT 34.5
Schmalzl, Karin .... MA 13.1, MA 13.8
Schmauder, Siegfried ..... CPP 15.54
Schmelz, Bruno . •BP 17.11, BP 17.75, BP 18.4
Schmerwitz, Yorick ..... TT 37.52
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Schmid, Alexander ..... •O 23.21
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Schmid, Christoph .. TT 11.8, TT 11.9, TT 11.56, TT 25.7
Schmid, Clemens ..... •TT 5.10
Schmid, Friederike ... BP 3.6, BP 9.2, BP 19.6, CPP 12.2, CPP 15.72, •DY 24.11, DY 27.11
Schmid, Luca ..... •O 82.3
Schmid, Michael .... MM 9.70, O 6.7, O 6.9, O 39.1, O 39.5, O 44.3, O 63.4, O 63.8, O 89.2, •O 89.4
Schmid, Sebastian ..... •HL 54.3
Schmidt, Annette ..... MA 38.3
Schmidt, Bernd ..... •TT 8.6, TT 8.7, TT 36.8, TT 36.9
Schmidt, Burkhard ..... HL 36.3
Schmidt, Davina ..... MA 15.38
Schmidt, Frederik ..... •HL 20.16
Schmidt, G. ..... HL 58.2, HL 58.3
Schmidt, Gordon ..... HL 32.2
Schmidt Hansen, Jesper ... MM 16.3
Schmidt, Heidemarie ..... TT 5.6
Schmidt, Heiko ..... DY 4.5
Schmidt, Henri Jörn ..... •BP 17.5
Schmidt, Jack ..... •TT 8.7
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Schmidt, Jan Robert ..... •DY 45.2, •TT 59.2
Schmidt, Jan-Niclas ..... •O 37.2
Schmidt, Jay ..... •TT 11.35
Schmidt, Jonathan ..... •HL 3.1
Schmidt, Kai P. .... TT 26.7, TT 37.28
Schmidt, Kai Phillip . TT 2.3, TT 37.11, TT 37.38, TT 37.51, TT 41.9, •TT 43.7, TT 43.10, TT 43.13
Schmidt, Leon ..... KFM 12.1
Schmidt, Marcel ..... HL 29.75
Schmidt, Marcus .. MA 15.28, TT 9.7, TT 37.24, TT 37.25
Schmidt, Markus ..... TT 9.8
Schmidt, Matthias ..... DY 5.6
Schmidt, Oliver G. ..... MA 38.5
Schmidt, Paul Philip ..... •O 69.5
Schmidt, Philipp ..... HL 17.5
Schmidt, Richard .. DY 13.12, TT 19.12
Schmidt, Robert CPP 15.61, CPP 40.1, HL 20.24, HL 29.16, HL 29.25, HL 29.28, MA 15.22, MA 31.39, MA 41.11
Schmidt, Thomas .. DS 9.5, DS 13.57, •DS 13.58, MA 16.3, MA 33.4, TT 4.12, TT 51.4
Schmidt, Thomas L. MA 29.3, TT 35.8
Schmidt, Timo .... MA 43.1, MA 43.3, MA 43.12
Schmidt, Volker .. CPP 33.2, MM 21.8
Schmidt, Winfried ..... •BP 31.10, •CPP 42.10, •DY 43.10
Schmidt, Wolf Gero .. HL 6.1, HL 31.9, KFM 18.2, O 47.5, O 51.3, O 55.1, O 73.7, •O 74.4, O 86.7, O 90.1
Schmidt-Grund, Rüdiger ..... DS 8.2, DS 13.60, HL 6.9
Schmiedeberg, Michael ... CPP 25.9, •CPP 43.9, DY 23.9, DY 27.13, •DY 44.9
Schmiedinghoff, Gary ..... •TT 9.11
Schmitt, Cedric ..... •DS 9.8, O 55.3, O 61.7, TT 29.7
Schmitt, Christin .. MA 9.8, •MA 11.3, •TT 14.3
Schmitt, David . O 7.6, O 57.4, O 57.6, O 57.9, O 79.2
Schmitt, M. ..... MM 6.5
Schmitt, Markus ... DY 13.4, DY 20.9, DY 20.13, TT 17.3, TT 19.4, TT 28.9, TT 28.13
Schmitt, Matthias ..... O 86.10
Schmitt, Michael ... •BP 27.2, •O 91.2
Schmitt, Peter ..... MA 34.7
Schmitt, Robert ..... O 71.1
Schmitt, Simeon ..... •DY 27.8
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Schmitz, Guido ... MM 9.18, MM 12.9, MM 14.2, MM 29.1, MM 29.2, MM 30.4, MM 32.1, MM 32.4, •MM 34.1
Schmitz, Gunnar .... MM 9.73, O 54.1
Schmitz, Jelena ..... •O 23.8
Schmitz, Peter C. ... O 101.2, TT 57.2
Schmitz, Valentina ..... BP 14.4
Schmitz-Antoniak, Carolin .. MA 28.9
Schmolka, Niklas ..... •MA 41.45
Schmoll, David ..... •MA 20.1
Schmoranzerová, Eva ..... MA 23.6, MA 27.3
Schmuck, Johannes HL 11.1, HL 17.10
Schmutzler, Stephan ..... •MA 15.9, O 40.2
Schnabel, Allard ..... MA 2.10
Schnabel, Michael ..... •DY 29.8
Schnack, Jürgen ... DS 4.4, DY 13.10, DY 16.2, •MA 34.4, MA 41.24, TT 19.10, TT 22.2
Schnapp, Marius ..... CPP 15.14
Schneck, Emanuel ..... BP 5.1

Schneemann, Andreas ..... O 17.9
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Schneider, Andrea ..... •BP 3.9
Schneider, Andreas SOE 3.4, SOE 10.8
Schneider, Andreas C. ..... DY 33.3
Schneider, Benedikt MA 21.5, MA 21.6
Schneider, C. ..... HL 46.4
Schneider, Carina ..... •CPP 6.3
Schneider, Carlo ..... •O 52.4, O 52.5
Schneider, Christian ..... HL 2.10, HL 40.12, HL 57.9, HL 62.1, TT 11.32, TT 11.40, TT 11.42, TT 55.6
Schneider, Christian MF .... TT 11.33
Schneider, Claus ..... MA 48.6
Schneider, Claus M. ... O 51.2, O 80.1, O 86.5, O 101.2, TT 57.2
Schneider, Claus Michael ... MA 15.6, MA 32.2, O 69.8, TT 40.2
Schneider, Eileen ..... HL 62.4
Schneider, Eric . •BP 17.36, •MM 9.55
Schneider, Florian ..... O 63.3
Schneider, Hans Christian ... MA 9.7, MA 9.8, MA 26.13, MA 31.24, MA 34.6
Schneider, Imke .. MA 20.4, TT 43.11, •TT 43.12
Schneider, Jochen ..... MA 38.2
Schneider, Konstantin D. .... •TT 36.2
Schneider, Linus ..... •HL 29.20
Schneider, Lucas ..... O 59.8
Schneider, M. Alexander ..... O 14.5, O 50.8, O 74.5
Schneider, Michael ..... MA 41.39
Schneider, Reiner ..... DS 13.36
Schneider, Robin ..... BP 17.17
Schneider, S. ..... MA 6.11
Schneider, Tim ..... HL 20.23
Schneider, Tim P. ..... •HL 45.8
Schneider, Tobias ..... •HL 39.6
Schneider4, Jochen ..... DS 13.61
Schneidt, Veronika ..... DS 3.7
Schneidwind, Astrid ..... •SYFD 1.1
Schnell, Adrian F. ..... •BP 3.4
Schnelle, Walter ..... O 23.1
Schnieber, Timo ..... HL 47.5
Schnitzerlein, Miriam ..... •BP 20.8, •DY 25.8
Schnitzspan, Leo .. MA 41.1, MA 41.4
Schnohr, Claudia S. . DS 11.1, HL 52.7, HL 52.8
Schnorr, Laurin ..... HL 15.2, HL 15.5, HL 29.63
Schnyder, Andreas ..... TT 10.5
Schnyder, Andreas P ..... TT 10.4
Schober, Jan-Christian ..... O 81.1
Schobert, Arne ..... O 36.5
Schock, Robin T. K. •HL 17.3, HL 29.2, TT 36.1, TT 36.2
Schoepe, Wilfried ..... •TT 47.13
Schöhs, Yannick ..... •DY 27.5
Schoinas, Nikolaos . HL 23.3, TT 21.3
Scholle, Robin ..... •TT 3.1
Schöllhorn, Michael ..... TT 11.56
Schollwöck, Ulrich ..... TT 54.10
Scholz, Gordon .... •MM 9.3, MM 9.9
Scholz, Josef ..... BP 22.8
Scholz, Katharina ..... •BP 25.11
Scholz, M. ..... MM 6.5, O 26.6
Scholz, Markus ..... MA 8.3
Scholz, Reinhard ... CPP 1.1, •CPP 6.1
Scholz, Sven ..... HL 29.63
Schölzel, F ..... O 33.4
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Schömig, Richard ..... •CPP 15.32
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Schön, Carl-Friedrich ..... KFM 14.20
Schondelmaier, Daniel ..... DS 7.4
Schönecker, Stephan ..... MM 3.7
Schönfeldt, Mario ..... MA 30.2
Schöngrundner, Paul ..... •O 44.2
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Schönhense, Gerd . KFM 5.2, MA 8.3, O 11.7, O 86.10
Schöning, Sonja ..... MM 9.57
Schönleber, Marco ..... •TT 37.10
Schoop, Leslie ..... O 79.6, TT 54.2
Schöpf, Jörg ..... •DS 5.3, O 76.1
Schöppl, Florian ..... •DS 10.3
Schörmann, Jörg ... HL 51.4, TT 46.4
Schorn, Dennis .... •BP 2.1, •CPP 2.1, •DY 3.1
Schorre, Florian ..... BP 17.77
Schott, Christina ..... O 23.21
Schöttke, Fabian ..... O 11.1, •O 14.8
Schowalter, Marco .... DS 1.3, DS 5.2, HL 9.5, HL 46.9, HL 52.6
Schraad, Simon ..... •CPP 15.24
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Schrader, Carolin ..... •MA 19.5
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Schrefl, Thomas MA 31.38, •MA 35.3
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Schreiber, Jan Vincent .... •DS 13.44
Schreiber, Lars ..... HL 12.4, TT 12.4
Schreiber, Lars R. ... HL 6.10, HL 36.3
Schreiber, Lucas ..... •HL 29.45
Schreiber, Susanne •BP 10.7, •DY 14.7
Schreiner, Rupert ..... O 66.7
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Schrijer, Joëlle J. A. ..... O 20.11
Schröder, Alexander HL 29.56, O 10.2, O 10.9
Schröder, Benjamin .... O 7.1, O 23.17
Schröder, Christian ..... KFM 14.23, KFM 15.9
Schröder, Frederik ..... •HL 2.13
Schröder, Konrad ..... TT 26.12
Schröder, Pascal ..... DS 11.4
Schröder, Philip ..... •TT 35.1
Schröder, Rasmus R. ..... CPP 26.2
Schröder, Stefan ..... •CPP 20.1, CPP 32.11
Schroeder, Uwe ..... KFM 11.4
Schroedter, Erik ..... •DY 29.2
Schröer, Julian .. DS 13.45, •HL 29.22
Schroeter, Niels B M ..... TT 54.5
Schröter, Lutz ..... •PSV VI
Schröter, Matthias ..... DY 21.5
Schröter, Niels ..... O 38.3
Schubert, Alina ..... •HL 2.3
Schubert, Andreas ..... DS 6.2
Schubert, Jürgen ..... MA 39.3
Schubert, Juri Franz ..... •BP 13.8, •CPP 19.8, •DY 15.8
Schubert, Leon G. ..... •DS 13.15
Schubert, Leonie ..... HL 20.3
Schubert, Marco ..... TT 38.6
Schubert, Markus Andreas .. HL 15.6
Schubert, Martin C. ..... HL 1.6
Schubert, Roland ..... DS 13.20
Schubert, Ulrich ..... BP 17.25
Schubert, Ulrich S ..... CPP 15.47, CPP 15.48, CPP 29.2, CPP 32.45, CPP 44.1, HL 45.2
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Schuck, Alfons Georg ..... •MA 20.5
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Schug, Felix .... •CPP 40.6, MM 9.45
Schuh, Dieter ..... TT 38.1
Schuhmann, Cedric ..... SOE 1.3
Schüle, Carolin Sabrina .... •DS 13.11
Schuler, Ben ..... BP 8.4, CPP 9.4
Schuler, Bruno ..... O 5.6, O 5.7
Schüler, Julian ..... MA 3.12
Schüler, Leonard ..... TT 41.3
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Schüler, Michael ... MA 31.32, O 11.5, O 43.3, O 57.3, O 57.4
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Schüller, C. ..... HL 29.13
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Schuller, Marlis ..... •MA 21.3
Schulte, Stefan ..... O 45.6
Schultheiss, Helmut ..... MA 3.1, MA 20.13
Schultheiss, Jan KFM 11.3, KFM 14.19
Schultheiss, Katirn ..... MA 3.1
Schultheiss, Katrin ..... MA 20.13
Schultz, Christof ..... CPP 24.7
Schultz, Johannes MA 26.8, MA 37.5, O 82.7
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Schulz, Florian ..... O 87.7
Schulz, Julian ..... BP 17.39
Schulz, Justin ..... •KFM 15.5
Schulz, Katrin ..... O 79.7
Schulz, Niklas L. ... TT 25.5, •TT 25.6
Schulz, Steven ..... BP 21.8, SOE 8.8
Schulz, T. ..... HL 45.9
Schulz, Tommy ..... •HL 2.12
Schulze, Aaron ..... TT 9.2
Schulze, Dirk ..... HL 6.9
Schulze, Patricia S. C. ..... HL 1.6
Schulze, T. ..... MA 15.8
Schulz-Harder, Helmuth-André •MM 21.8
Schumacher, Hans W. ..... HL 17.8, HL 23.1, HL 31.6, HL 31.10, TT 21.1
Schumacher, Hans Werner .. HL 30.1, MA 37.10, O 33.5, O 33.18
Schumacher, Stefan HL 39.6, HL 57.1
Schumacher, Thorsten ..... O 87.1
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Schuster, Jörg ..... HL 51.8, TT 36.3, TT 46.8, AKPIK 5.3
Schütt, Kristof T. ..... O 17.2
Schütt, Michael ..... TT 41.4
Schütte, Friedrich ..... •CPP 15.18
Schütte, Marc ..... HL 40.9
Schütz, Florian ..... HL 29.89
Schutzeichel, Lars ..... •SOE 7.8
Schvartzman, Mark ..... CPP 15.23
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Schwade, Martin ..... •HL 3.8
Schwager, Benjamin ..... HL 29.57, HL 29.64, HL 29.71, •HL 38.2, MA 41.8, •TT 30.2
Schwäke, Lynn ..... •CPP 32.11
Schwan, Lennart ..... •MM 9.57
Schwanewedel, Ben ..... •MA 11.9, •TT 14.9
Schwanitz, Paul ..... •CPP 15.41
Schwark, Arthur von U.-S. .. MA 20.11
Schwarm, Mica ..... TT 2.4
Schwartz, Rico ..... DS 3.7, HL 2.3, HL 29.4, HL 29.12
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Schwartzkopff, Sebastian .. CPP 8.3, •CPP 32.38
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Schwarz, Nico ..... •HL 42.3, TT 47.5
Schwarz, Ulrich .. BP 17.46, BP 25.11, CPP 6.4
Schwarz, Ulrich S .. BP 11.5, BP 17.42, BP 17.45, BP 25.4, BP 28.5, BP 34.3, •BP 35.1, CPP 35.5, •CPP 46.1, DY 36.5, DY 46.3, •DY 47.1
Schwarz, Ulrich T. ..... DS 7.4
Schwarze, B. V. ..... TT 24.2
Schwarzkopf, Jutta ..... KFM 14.7
Schwarzkopf, Matthias .... CPP 24.3
Schwarz-Selinger, Thomas MM 9.30, MM 32.8
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Schweikhard, Lutz ..... O 72.6
Schweins, Ralf ..... CPP 41.2
Schweiss, Sophia ... •BP 27.7, O 31.7, •O 91.7
Schweitzer, Christine ..... BP 25.12
Schweitzer, Pascal ..... •CPP 15.42
Schweizer, Matthias ..... MA 31.33
Schweizer, Matthias R. ..... MA 3.4, •MA 3.8, MA 3.11, MA 31.27
Schwendele, Martin ..... •TT 11.67
Schwendke, Philipp ..... •O 88.4
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Schwenke, Alexander ..... •TT 37.17
Schwenke, Philipp ..... •MA 29.2, MA 41.19
Schwermer, Isabel ..... MA 46.8
Schwierz, Nadine .... BP 3.4, BP 19.1
Schwille, Petra ..... •PSV IV
Schwingenschlögl, Udo .. •CPP 24.5, HL 6.13, O 89.9, •TT 53.6
Schwinghammer, Philip ..... •HL 52.1
Schwirblat, Margarete ..... BP 14.17
Schwöbel, Gabriel ..... •MA 31.28
Schwoerer, Heinrich ..... HL 29.87
Sciortino, Alfredo ..... BP 31.11, CPP 42.11, DY 43.11
Scita, Giorgio ..... BP 17.7
Scoles, Amanda ..... •TT 11.32
Scontrino, Emilio ..... •O 45.6
Sebastiani, Daniel ..... •CPP 5.1, CPP 15.66
Šebesta, Jakub ..... •MA 41.29
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Sedghi, Mohammad ..... MA 15.12
Seeja Sivakumar, Nikhil ..... O 20.11
Seeley, Laurence .. BP 30.9, BP 30.10
Seema, Seema .. DS 13.48, MA 31.44
Seemann, Lukas ..... •DY 8.4
Seewald, F. ..... MA 15.8
Segadlo, Kai ..... •CPP 24.6
Segets, Doris ..... HL 29.8, O 12.4
Sehrt, Jan T. ..... MM 9.55
Seibel, Christopher MA 26.9, O 23.20, O 42.5, O 67.10
Seibold, Götz .... MM 32.10, TT 11.10, TT 11.11
Seibold, Kilian ..... SYQS 1.4
Seibt, Michael ..... O 4.3
Seidel, Jürgen ..... KFM 14.16
Seidel, Konrad ..... TT 47.1
Seidel, Leon ..... •MA 26.11
Seidel, Stephan ..... •AIW 2.2
Seidler, Dennis ..... MA 41.18
Seifert, Jakob ..... HL 39.14
Seifert, Paul ..... •O 11.12
Seifert, Tom ..... O 5.5, O 20.2
Seifert, Tom S. ..... MA 48.5
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Seiler, Adrian ..... •O 24.8
Seiler, Anna ..... •PRV I, O 57.9
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Seiler, Magdalena ..... •MM 9.17
Seipel, Simone ..... •TT 37.30
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Seitz, Christoph ..... O 41.2
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Sek, Grzegorz ..... HL 47.7
Sekania, Michael ..... MA 40.10
Selbach, Sverre M. ..... KFM 9.3
Seleš, Patrick ..... •O 14.10
Selhuber-Unkel, Christine .... •BP 8.6, •CPP 9.6
Selig, Malte ..... O 10.5
Sell, Marlene ..... •O 34.2
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Sellies, Lisanne ..... •PRV II, O 24.10
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Selve, Sören ..... O 89.6
Selyshchev, Oleksandr ..... DS 13.30, DS 13.31
Semeniuk, Konstantin ..... TT 9.5, •TT 58.1
Semisalova, Anna ..... MA 22.4
Şen, Onur Can ..... •MM 4.10
Senarath, Aditha ..... HL 18.4
Sénéchal, David ..... TT 34.7
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Seniutinas, Gediminas ..... HL 6.6, MA 18.3
Seno, Hiroshi ..... BP 18.3
Sentef, Michael ..... O 43.3, O 57.4, O 57.5, O 85.9, •O 87.6
Senthiappan Vellaiappan Uthayasurian, Vedhanth ..... •HL 29.16
Senyk, Yurii ..... TT 37.14
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Serafin, Francesco ..... BP 13.10, CPP 19.10, DY 15.10
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Serbyn, Maksym .... DY 13.3, TT 19.3
Serebrennikova, Alexandra CPP 33.2, CPP 37.2
Sereda, Beniamin ..... •SOE 3.5
Seres, Imre ..... O 7.3
Serga, Alexander A. . MA 3.4, MA 3.5, MA 3.8, MA 3.11, MA 31.27, MA 31.28
Serha, Rostyslav O. •MA 3.5, MA 3.11, MA 20.1, MA 31.28
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Setescak, Alexander ..... •MA 15.45
Setescak, Christoph ..... O 49.5
Setescak, Christoph S. ..... •O 101.5, •TT 57.5
Setina, Janez ..... O 66.2
Setoudeh, Maryam ..... •BP 18.8
Settanni, Giovanni ... BP 3.6, BP 19.6
Setti, Thirupathaiah ..... MA 31.22
Setvin, Martin ... •HL 20.20, MM 9.2, O 6.3, O 42.2, O 49.10, O 65.10, O 81.7
Sevik, Cem ..... MM 36.7
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Sevlikar, Shraddha ..... MM 11.3
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Shabala, Natalia .. •MA 10.5, •TT 13.5
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Shadman Awsaf, Chowdhury •MA 31.15
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Shaevitz, Joshua W. ..... BP 4.4
Shafer, Padraic ..... DS 5.3
Shahi, Nisha ..... TT 51.1
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Shaikh, Monirul ..... MA 6.12
Shaji, Athira ..... •HL 1.6
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Shakhayeva, Billura ..... •CPP 20.5
Shakirov, Timur ..... CPP 15.68
Shamim, Saquib ..... HL 12.1, TT 12.1
Shamrovska, Polina ..... •DS 13.30
Shamsulbahrin, Sofia ..... KFM 1.5
Shan, H. ..... HL 46.4
Shanbhag, Shridhar Sanjay ... HL 2.9, HL 29.24, •HL 29.26
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Shao, Yaping ..... DY 21.8
Shapiro, D. ..... MA 30.3
Sharangi, Purbasha ..... •MA 31.5, MM 9.53, MM 20.2
Sharikow, Eugen ..... O 68.1
Sharma, Abhinav ..... BP 6.5, BP 6.7, CPP 7.5, CPP 7.7, DY 4.8, DY 7.5, DY 7.7, •DY 24.2, DY 24.5, DY 24.6
Sharma, Abhishek ..... •DS 13.53, MM 9.15
Sharma, Anirudh ..... CPP 3.4
Sharma, Auditya ..... DY 29.5
Sharma, Avdhesh Kumar .... •MA 4.3
Sharma, Chithra ..... MA 41.39
Sharma, Chithra H. ..... •TT 49.3
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Sharma, Nand Lal ..... HL 47.5
Sharma, Niyorjyoti ..... KFM 9.3
Sharma, Pragati ..... MM 6.4
Sharma, Rohit ..... •TT 4.3
Sharma, Sandeep ..... CPP 3.4
Sharma, Sangeeta ..... MA 26.7
Sharp, Ian ..... DS 4.5
Sharp, Ian D. . DS 2.3, DS 10.4, HL 9.1, HL 20.18, HL 32.3, HL 33.3, O 21.8, O 65.5, O 65.6
Shaw, Syl ..... •HL 12.3, •TT 12.3
Shayduk, Roman ... MA 26.12, O 23.7
Shea, Jeanine ..... •BP 2.5, •CPP 2.5, •DY 3.5
Shee, Payel ..... •TT 41.2
SHEHADA, SUFYAN ..... •MA 46.10
Sheina, Valeria ..... O 90.10
Sheka, Denis D. ..... MA 18.3
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Shen, Chen ..... MM 3.7, AKPIK 6.4
Shen, Shangbin ..... MA 37.4
Shen, Yi-Hsin ..... MA 32.2, O 101.2, TT 40.2, TT 57.2
Shen, Z.X. ..... O 26.6
Sheng, B. ..... HL 58.2
Sheng, Shaoxiang ..... O 5.9
Shepelin, Nikita ..... MM 3.8
Shepherd, Sam ..... CPP 33.3
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Shevtsova, Olga ..•MA 19.4, MA 37.9
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Shih, Ching-Wen ..... HL 24.2
Shiloh, Roy ..... O 26.5
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Shinaoka, Hiroshi ..... TT 2.1
Shinwari, Tauqir ..... DS 3.8, DS 3.9, •DS 4.3, MA 26.7
Shiotani, Taiki ..... •MA 30.6
Shiotari, Akitoshi ..... BP 33.4, O 5.2, O 20.4, •O 72.13, O 100.4
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Shkodich, Natalia ..... MA 17.3
Shoji, Tetsuya ..... MA 35.3
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Shradha, Sai ..... •HL 29.7, HL 40.2
Shrestha, Binamra ..... HL 42.2
Shrestha, Sulabh . HL 20.13, HL 29.78
Shu, Guo-Jiun ..... MA 32.2, TT 9.11, TT 40.2
Shu, Sinan ..... •MA 41.1
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Shubbak, Yahya .. MA 15.15, MA 38.1, •MA 38.9, MA 41.22
Shugai, Anna ..... •O 73.8
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Shyta, Vira ..... TT 42.13
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Siboni, Henrik ..... •BP 17.13
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Siday, Tom ..... •HL 18.8
Siddiqui, Aamir ..... •MM 9.58
Sideri, Ioanna K. ..... O 68.7
Sidis, Yvan ..... MA 31.2
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Siebenkotten, Dario ..... •O 96.3
Siebert, Moritz ..... HL 12.1, HL 13.6, •HL 13.7, TT 12.1
Siebrecht, Janis ..... O 16.12
Siegl, Julian ..... TT 11.1, TT 44.3
Siegle, Leander ..... O 82.1
Siemann, Gesa ..... O 67.9, •O 79.6
Siemens, Jan ..... BP 34.3, DY 46.3
Siemon, Leon ..... •KFM 14.25
Sierda, Emil .. O 49.8, O 59.3, O 59.10
Sievers, Sibylle ..... MA 37.10
Sifft, Markus ..... HL 23.6, •HL 23.7, TT 21.6, •TT 21.7
Sigel, Reinhard ..... •CPP 15.33
Silber, Robin ..... MA 15.4, MA 15.11, •MA 23.2
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Silies, Martin ..... HL 11.7
Sill, Annekatrin .. CPP 20.2, CPP 41.4
Silva-Dias, Leonardo ..... •BP 17.69
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Sim, GiBaik ..... TT 27.5
Sim, Junyoung . O 5.5, O 20.2, O 20.3, •O 36.7
Simanenko, Alexander ..... O 65.11
Simeth, Wolfgang ..... TT 3.5
Simhofer, Marcel ..... •MM 23.4
Simmchen, Juliane ..... •BP 13.6, •CPP 19.6, •DY 15.6
Simmel, Friedrich C ..... BP 17.10
Simmonds, Maxim ..... CPP 32.43, •HL 45.10
Simões, Frederico ..... HL 1.10
Simon, Maik ..... TT 47.1
Simon, Paul ..... TT 5.12
Simon, Quentin ..... KFM 1.6
Simoncelli, Michele ..... MM 27.4
Simoncig, Alberto ..... HL 29.88
Simonov, Arkadiy ..... KFM 15.11
Simons, Clara ..... MA 48.5
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Simpson, Grant ..... O 46.4, O 73.2
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Šindler, Michal .... •MA 48.4, TT 5.13, TT 16.6
Sing, M. ..... MM 6.5
Sing, Michael DS 5.5, O 86.2, O 86.10
Singer, L. ..... MA 15.8
Singer, Mirko ..... BP 28.5, CPP 35.5, DY 36.5
Singh, Akriti ..... TT 9.12
Singh, Anupam ..... MA 33.3
Singh, Arpana ..... HL 29.86
Singh Bhakuni, Devendra .... DY 29.5
Singh, Devinder ..... •MM 20.4
Singh, Japsreet ..... O 55.2
Singh, Jaskaran ..... •BP 17.53
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Singh, Maanwinder ..... TT 10.10
Singh, Mahima ..... MM 9.46
Singh Negi, Devendra ..... MA 39.6
Singh, Nirpendra ..... TT 53.6
Singh, Palwinder ..... HL 29.30
Singh, Roja ..... HL 1.3
Singh, Shivani ..... O 8.3
Singh, Sunil ..... BP 31.6, CPP 42.6, DY 43.6
Singh, Sunil P ..... BP 3.10, CPP 45.5
Singh, Suyash ..... •O 45.14
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Sinz, Björn ..... •HL 11.1
Siri, Olivier ..... O 80.4
Sivakumar, Nikhil S. ..... O 36.2
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Siviero, Matilde ..... HL 39.2
Sivis, Murat . HL 18.7, HL 63.4, O 48.2
Siwick, Bradley J. ..... O 89.1
Skála, Tomáš ..... O 65.3, O 65.11
Skalli, Anas ..... AKPIK 3.1
Skibitzki, Oliver ..... HL 15.6
Skobjin, Gregor .. •MA 9.12, MA 15.18
Skokov, K. ..... MA 30.3, MA 31.7
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Skolaut, Julian ... MA 33.7, •MA 33.8
Skourski, Y. ..... MA 33.1
Skourski, Yurii ..... DS 10.1, MA 15.7
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Skrzynska, Katarzyna ..... HL 20.24
Škvára, Jan ..... O 65.11, O 81.7
Skwarek, Volker ..... CPP 15.7
Skylaris, Chris-Kriton ..... MM 17.1
Slager, Robert-Jan ..... MA 16.2
Slautin, Boris .. KFM 18.6, •AKPIK 2.3
Slepukhin, Valentin ..... BP 14.5
Sleziona, Vivien ..... O 20.5
Slimi, Younes ..... DS 13.60
Slipchenko, Mykola ..... HL 29.44
Slobodianiuk, Denys ..... MA 20.1
Smaliarova, Tatiana ..... MA 38.4
Smart, Thomas J. ..... TT 11.5
Šmejkal, Libor ..... •PRV V, MA 9.4, MA 9.8, MA 9.11, MA 9.13, MA 13.3, MA 16.5, MA 26.13, MA 47.5, TT 53.2
Smekhova, Alevtina ..... MA 31.23
Smeyers, Robin ..... HL 29.69
Smirnov, Dmitry ..... MA 34.9
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Smirnova, Olga ..... •MA 5.3, •TT 1.3
Smith, Adam ..... DY 41.1, TT 56.1
Smith, Ana Sunčana ..... CPP 15.73, CPP 25.13, DY 23.13
Smith, Ana-Sunčana ..... BP 17.81, BP 17.82, CPP 15.74, CPP 25.8, DY 22.5, DY 23.8
Smith, Elspeth ..... •O 4.1
Smith, Trevor ..... HL 39.16
Smoliarova, Tatiana ..... MA 17.3, •MA 37.4
Smolinski, David ..... PSV I
Smolla, Andree ..... DY 27.12
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Smržová, Darina ..... MA 2.9
Snoeijer, Jacco ..... CPP 14.4
Snoeken, Michiel ..... •HL 53.4
Snow, Tim ..... CPP 30.1
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Snyder, Gerald Jeffrey ..... MM 15.1
Soavi, Giancarlo ..... HL 2.2, HL 2.4, HL 2.7, HL 2.9, HL 29.5, HL 29.23, HL 29.24, HL 29.26, HL 29.33, HL 46.2, HL 53.7
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Sodemann, Inti ..... MA 4.8
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Sofer, Z. ..... HL 60.6
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Sohn, Seoyun ..... •MM 21.2
Sokaras, Dimosthenis ..... KFM 15.7
Sokeng, Aurelien D. ..... CPP 3.6
Sokolov, Dmitry ..... TT 52.5
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Solano, Eduardo ..... HL 1.1
Solar-Polo, Diego ..... O 15.8, TT 6.8
Soldatov, Ivan ..... MA 23.3, MA 33.5
Soldemo, Markus ..... O 81.4
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Soler, Diego ..... O 64.2, O 68.6
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Soll, Aljoscha ... HL 17.11, •HL 29.35, HL 60.7
Sollich, Peter .... BP 17.68, CPP 25.2, DY 22.3, DY 22.11, DY 23.2
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Solomon, Gemma C. ..... CPP 27.5
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Sommer, Michael .. CPP 4.6, DS 13.4, DS 15.5
Sondermann, Elke ..... MM 29.3
Song, Fei ..... O 22.4
Song, Jin-Dong ..... HL 57.6
Song, K. W. ..... HL 46.4
Song, Xiaohong ..... HL 39.10
Song, Y. ..... O 81.8
Song, Yihua ..... MM 17.8, •MM 17.9
Sonner, Michael ... •DY 13.5, •TT 19.5
Sonnweber-Ribic, Petra .... MM 4.11, •MM 33.1

Soomro, Maaz . . . . . O 52.2
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Sorbello, Riccardo . . . . . HL 6.13
Sorgenfrei, Felix . . MM 9.69, •TT 7.10
Soroco, Cecilia . . . BP 31.9, CPP 42.9, DY 43.9
Sorrentino, Andrea . . MA 33.5, O 59.7
Sosa Barth, Fiona •MA 32.5, •TT 40.5
Sosniok, Tom . . . . . •BP 17.1
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Soteriou, Despina . . . . . BP 17.51
Sotgiu, Simone . . . . . DS 9.8, •HL 2.1, •HL 31.4
Sothmann, Björn . . . HL 29.72, O 18.7, O 67.1, O 99.6, TT 37.37
Soto, Nicolás A. . . . . O 21.5
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Soubatch, Serguei . . . O 33.16, O 62.1, O 80.6, O 101.4, TT 57.4
Soubelet, Pedro . . . •HL 31.3, •HL 53.1
Soultati, Anastasia . DS 4.9, DS 13.47, DS 15.6
Sourais, Alexandros G. . . . . DY 27.12
Sourd, Jeremy . . . . . MA 15.7
Souri, Somayeh . . . . •HL 11.8, HL 11.9, HL 54.1, HL 54.5
Sovic, Karlo . . . . . •O 32.8
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Spachtholz, Raffael . •O 24.10, O 43.7
Spaldin, Nicola . . . . . MA 2.3
Spaldin, Nicola A. . . . . MA 18.4
Spallek, Domenik . . . . . •KFM 15.8
Spallelk, Domenik . . . . . O 26.2
Spanheimer, Kai Luca . . . . . CPP 25.5, •CPP 43.7, DY 23.5, •DY 44.7
Spanier, Lukas . . . . . CPP 15.39
Spanier, Lukas V. . . . . •CPP 3.1, CPP 15.35, CPP 31.2
Spånslätt, Christian . . . . . TT 47.3
Spantzel, Lukas . . . . . BP 17.21
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Spasova, Marina . . . . . MA 38.4
Späth, Christoph . . . . . DS 13.21
Spears, Alexander . . . . . •O 42.6
Speliotis, T. . . . . MA 13.11
Speller, Sylvia . . . . . BP 17.22, HL 16.4, O 52.1, O 72.7
Spencer, Michael S. HL 45.5, MA 10.7, •TT 8.5, TT 13.7
Sperl, Matthias . . . . . DY 21.6
Sperlich, Andreas . . . . . CPP 15.14, CPP 15.15, HL 6.3, HL 6.12, HL 16.7, HL 29.45, HL 29.46, HL 29.47
Spetzler, Benjamin . . . . . O 88.8
Spickmann, Florian . . . . . •O 48.2
Spiecker, Martin . . . . TT 55.3, TT 55.4
Spielvogel, Henrik . . . . . HL 45.13
Spies, Maximilian . . . . . CPP 32.37, •HL 45.7
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Spillane, Katelyn . . . . . BP 17.76
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Spirito, Davide . . . . . HL 15.6
Spitzer, Nikolai . . HL 29.54, HL 29.58, HL 29.75
Splettstoesser, Janine . . . . . TT 47.3
Splith, Daniel . . . . . HL 20.2, HL 20.15
Spoddeck, Matthias . . . O 13.3, O 50.3
Spolenak, Ralph . . . . . O 60.3
Sprafke, Alexander . HL 45.1, HL 45.3, O 60.5
Sprau, Christian . . . . . CPP 15.44
Spree, Lukas . . . . . •O 12.10
Sprengel, Carla . . . BP 17.15, BP 17.18, •BP 22.7
Sprengel, Wolfgang . . . . . MM 23.4
Spreter, Vincent Leon . . . . . •HL 20.7
Spring, Merit . . . . . DS 5.5
Springate, Emma . . . . O 23.12, O 67.9, O 79.6
Springborn, Johann Richard . . •O 54.1
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Springl, Christoph . . . . . MM 32.8
Spruijt, Evan . . . . . BP 19.11
Sprung, Michael . . CPP 8.3, DS 13.34
Sreekala, Lekshmi . . . . . MM 7.1
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Sriramoju, Raja Vyshnavi . . CPP 30.3
Srivastava, Anubhav . . . . . TT 27.5
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Środa, Maksymilian . . . . . TT 2.1
Staab, Torsten . . . •KFM 5.4, KFM 5.7
Staabs, Maximilian . . . . . •MA 12.8
Staacke, Carsten . . . . . MM 9.21
Stadler, Fabian . . . . TT 11.58, TT 47.11
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Stähler, Julia . . . . O 9.1, O 67.1, O 67.2, O 67.3, O 88.4
Stallberg, Klaus . . . . . O 50.9
Stampfer, Christoph . . DS 4.8, HL 2.1, HL 17.5, HL 17.6, HL 29.11, HL 31.4, HL 40.9, HL 53.5
Ständer, Christian . . TT 8.3, TT 11.46, TT 11.48, TT 11.49, •TT 55.11
Stange, Daniel . . . . . BP 18.5
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Stankard, Stephanie . . . . . •O 49.11
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Stanković, Igor . CPP 15.30, CPP 23.5
Stannarius, Ralf . . . . DY 21.3, DY 21.7, DY 33.8
Stanojević, Katarina . . . . . •HL 17.5
Stapf, Siegfried . . . . . CPP 15.67
Stará, Veronika . . . . . O 13.10
Starick, Tommy . . . . . DY 4.5
Starikov, Sergei . . •MM 11.2, MM 11.3
Stark, Alexandra . •MM 4.11, MM 33.1
Stark, Holger . . . . . BP 2.5, BP 13.7, BP 28.4, BP 28.6, BP 31.3, BP 31.8, CPP 2.5, CPP 19.7, CPP 35.4, CPP 35.6, CPP 42.3, CPP 42.8, CPP 43.8, DY 3.5, DY 15.7, DY 36.4, DY 36.6, DY 43.3, DY 43.8, DY 44.8
Stark, Máté . •O 16.10, O 24.6, O 24.7, O 24.8, O 68.10, O 90.2
Stärk, Philip . . . . . CPP 33.1
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Starke, Adrian Henrik . . . . . •HL 29.71
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Starkov, Grigorii . . . •HL 51.7, TT 15.11, •TT 46.7, TT 53.8
Starostin, Vladimir . . . . . AKPIK 5.4, AKPIK 6.3, AKPIK 6.4
Stasi, Michele . . . . . BP 26.8
Staško, Daniel . . . . . MA 40.1
Staub, Urs . . . . . DY 31.7, MA 31.20
Stauber, Tobias . . . . . TT 7.8, •TT 39.2
Stausberg, Niklas . . . . . •SOE 10.6
Stavrič, Srdjan . . . . . O 29.9, TT 20.9
Stavropoulos, P. Peter . . . . . MA 9.4, •MA 40.4
Stechel, Tim . . . . . •CPP 30.5
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Steeger, Paul . . . •HL 20.24, HL 29.16, HL 29.25, O 83.7, TT 45.7
Steele, Julian A. . . . . HL 1.1
Steenbock, Torben HL 39.11, •HL 57.8
Stefancu, Andrei . . . . . O 79.7
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Steil, Daniel . . . . . MA 12.8, MA 43.1, •MA 43.3, O 7.6, O 23.14, O 57.4, O 57.6, O 57.9, O 79.2
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Stein, David . . . . . MA 41.11
Stein, Markus . . . . . HL 17.2, HL 40.11
Steinbach, Florian . . . . . •BP 14.17
Steinbach, Simon . . . . . O 13.8
Steinbauer, Michael Karl . . MA 15.47, •MA 45.7
Steinbrecher, René . . . . . CPP 31.2, CPP 31.4
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Steinfeld, Judith . . . . . AKPIK 5.10
Steingelb, Genrietta . . . . . •HL 20.6
Steinhäußer, Aaron . . . . . MA 38.5
Steinhoff, Alexander . . . . . •SYIS 1.4, HL 2.12
Steinhuber, Mathias . . . . . DY 13.1, •DY 20.9, TT 19.1, •TT 28.9
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Steinigeweg, Robin . DY 20.3, TT 28.3
Steinke, Florian . . . . . DY 34.4
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Steinmann, Andy . . . . . O 71.5
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Stelzer, Ernst H.K. . . . . BP 18.7
Stenger, Nicolas . . . . HL 2.13, HL 62.3
Stenz, Christian . DS 13.54, •DS 13.55, DS 13.57
Stepanov, Evgeny . TT 43.6, •TT 54.7, TT 54.12
Stepanova, Mariia . . . . . MA 43.11
Stepanow, Sebastian . . . . . O 59.9
Stephan, Sven . . . . . HL 11.7, HL 62.1, O 72.8
Sterin, Pavel . . . . . HL 29.80
Sternemann, Christian . . . . . MM 9.9, MM 9.25, MM 9.55
Sternemann, Lasse . . . . O 7.5, O 29.4, O 64.6, TT 20.4
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Stevens, Laurie . . . . . •CPP 21.4
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Stiehm, Noah . . . . . •DS 8.2, DS 13.60, HL 6.9
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Stienen, Sven . . . . . MA 12.6
Stienkemeier, Frank . . . . . DY 37.9
Stier, Andreas . . . . . •HL 31.7, •HL 59.7
Stier, Andreas V. . . . . HL 31.3, HL 53.1
Stierl, Dario . . . . . DS 13.20
Stierle, Andreas . . . . CPP 38.1, O 39.2, O 41.2, O 81.1, O 89.3
Stierle, Felix . . . . . •MM 9.59
Stiewe, Finn-F. . . . . MA 15.11
Stilp, Fabian . . . O 12.5, O 12.6, •O 98.1
Stimpel-Lindner, Tanja . . . . . O 38.2
Stimper, Vincent . . . . . O 18.1
Stöberl, Stefan . . . . . BP 17.77
Stock, Henry . . . . . •HL 29.53
Stock, Sebastian . . BP 12.5, CPP 18.5
Stockert, Oliver . . . . . TT 41.1
Stockert, Ulrike . . MA 40.3, •MM 9.42
Stockmann, Gregor . . . . . •O 72.3
Stoehr, Rainer . . . . . MA 8.5
Stoffel, Wieland G. . . . . TT 5.1
Stogiannidis, Georgios . . . . . •BP 5.5
Stöhr, Meike . . . O 8.3, •O 17.7, O 69.1, O 69.6
Stöhr, Rainer . . . . . MA 37.9
Stoica, Mihai . . . . . MM 26.6
Stojanovic, Nikola . . DS 13.42, O 24.3
Stoll, A. . . . . •TT 11.28
Stoll, Alexander . . . TT 11.27, TT 11.43
Stoll, Enrico . . . . . AKPIK 5.1
Stoll, Florian . . . . . TT 37.3
Stolte, Evert . O 45.12, O 90.7, •O 90.8
Stolwijk, Judith . . . . . •PSV IX
Stolz, Wolfgang . . . . . HL 15.4
Stoodley, Matthew . . . . . O 73.5
Stooß, Henrik CPP 32.24, CPP 32.34, •CPP 33.1
Stork, Björn . . . . . BP 22.7
Storm, Philipp . . . . . HL 52.8
Stosch, Rainer . . . . . O 33.2, O 33.5
Stosiek, Matthias . . •MM 18.6, TT 5.7
Stötzner, P. . . . . •HL 45.9
Strahl, Janina . . . . . •TT 37.2
Strampe, Laura . . . . . •BP 25.12
Stranak, Patrik . . . . . HL 36.10
Strand, Hugo . . . . . TT 37.61
Strand, Hugo U. R. . . . . TT 17.10
Strangmüller, Stefan . . . . . MM 8.1
Straßburger, Julian . . . . . MA 31.26, MA 41.30
Strasdas, Jeff . . . . . •DS 4.8, MA 15.2
Straßheim, M. . . . •MA 22.5, MA 31.6, MA 31.7
Strasser, Nina . . . . . KFM 5.5
Stratakis, Emmanouel . . . . . HL 53.8
Strathkötter, Pascal . . . . . DS 13.20
Straub, Michael . . . . . HL 2.5
Straube, Arthur V. . . . . DY 4.9
Straubinger, Thomas . . . . . HL 33.2
Strauch, Hannah C. . . . . •MA 37.6
Strauß, Dirk . . . . . KFM 15.3
Strauß, Johanna . . . . . •TT 37.21
Strauss, Dirk . . . . . KFM 15.2
Strebel, Oliver . . . . . •DY 27.4
Streibel, Verena . . . . HL 9.1, HL 20.18, HL 33.3
Streller, Fabian . . . . CPP 22.5, •DS 6.7
Striebel, A. . . . . •TT 11.61
Striebel, Adrian . . . . . TT 8.1, TT 11.64
Střihavková, Julie MA 10.12, TT 13.12
Strik, Julian H. . . . . MA 46.7, •O 59.3, O 59.10
Strinic, Ana . . . . . •TT 8.4
Strittmatter, A. . . . . HL 58.3
Strittmatter, André . HL 32.2, HL 52.2
Strobel, Tim . . . . . HL 47.5
Strobel, Urs . . . . . •TT 11.29, TT 50.6
Strobl, Frederic . . . . . BP 18.7
Stroh, Karen . . . . . MA 12.8
Strohmair, Simone . . . . . HL 39.9
Strohmeier, Marcel . TT 11.2, •TT 24.6
Stroj, Sandra . . . . . HL 57.11
Stroppa, Alessandro . . . . . •MA 13.9, MA 41.47, MM 9.20, MM 12.4
Strothmann, Robert . . . . . •CPP 15.3
Strüber, Christian . . . . . MA 31.21
Strunk, Christoph . . . TT 5.7, TT 11.18, TT 11.35, TT 11.36, TT 25.1, TT 38.1, TT 42.3
Strunskus, Thomas . . . . . CPP 8.2, CPP 32.11, DS 13.32
Struve, M. . . . . •HL 46.4
Struve, Marti . . . . . HL 2.10
Stubenrauch, Jakob . . . . . •BP 34.2, •DY 32.3, •DY 46.2
Stummvoll, Mike . . . . . O 16.6
Stumpf, Steffi . . CPP 32.33, CPP 44.1
Stunault, Anne . . . . . MA 13.8
Stupar, Matija . . . . . O 7.5
Šturala, Jiří . . . . . HL 29.35, HL 60.7
Sturm, Chris . . . . . HL 39.14, HL 39.15, HL 46.8
Sturm, Jonathan . . . . . •TT 53.9
Stutzer, Lars . . . . . •DY 42.5
Su, Haoqing . . . . . HL 20.4
Su, Linfeng . . . . . •MM 9.1
Su, Yixi . . . . . O 51.2
Subach, Sergey . . . . . O 98.2
Subotnik, Joseph . . . . . MA 34.10
Subramanian, Palaniappan . DS 13.33
Suchanek, Thomas . . . . . •DY 32.2
Suchecki, Krzysztof BP 21.2, SOE 8.2
Sudarsan, Akhil . . . . . •BP 19.1
Sudbø, Asle . . . . . MA 29.7, MA 47.2
Suen, Cissy . . . . . MM 6.10
Suess, D. . . . . MA 12.1
Suess, Dieter . . . . . MA 15.13, MA 20.1, MA 20.10, MA 33.12, MA 43.1, MA 43.3, MA 43.5, MA 45.10, TT 5.12
suetani, hiromichi . . . . . •DY 8.11
Sufyan, Osamah . . . . . •DY 39.1
Sügers, Christoph . . . . . O 24.7
Sugimoto, Yoshiaki . . . . . O 98.6
Suhr, Maximilian . . . . . •KFM 14.13, MM 9.30
Sukanya, Sukanya . . . . . KFM 13.3
Sukenik, Nir . . . . . •BP 4.5
Sukhanov, Aleksandr . . . . . MA 15.28, •TT 54.3
Sukhanov, Aleksandr S. . . . . MA 28.3
Sukharev, Maxim . . . . . O 96.1
Sukuhanov, A.S. . . . . MA 6.11
Sulaiman, Cathy . . . . •O 14.11, O 33.21
Sulaiman, Vanessa . . . . . TT 26.7, •TT 37.28
Sulejman, Shaban B. . . O 60.9, O 87.3
Sulkowska, Joanna I . . . . . •BP 30.5
Süllow, Stefan . . . . . MA 29.6, TT 9.2, TT 35.1
Sulpizi, Marialore . . . . . CPP 21.4, CPP 25.20, DY 23.20, O 4.1, O 4.10, O 58.9
Sulpiziz, Marialore . . . . . •O 4.6
Sultan, Salik . . . . •CPP 43.8, •DY 44.8
Sumayya, Sumayya . . . . . •HL 20.17
Sun, Benyao . . . . . KFM 14.15
Sun, Fei . . . . . TT 5.9, TT 52.5
Sun, Haonan . . . . . •MM 36.8
Sun, Jiale . . . . . DS 1.10
Sun, Junsong . . . . . TT 53.7
Sun, Kun CPP 3.7, CPP 8.2, CPP 24.3, CPP 32.35, CPP 32.36
Sun, Luye . . . . . O 62.3, O 62.6

Sun, Ningwei ..... O 17.8
Sun, Qiang ..... O 17.6, O 22.4
Sun, Shoutian ..... O 58.7
Sun, Yuhan ..... •MA 41.5
Sun, Zhiyuan ..... O 57.3, TT 2.10
Suncana smith, Ana ..... CPP 15.23
Sundaramurthy, Vignesh ..... TT 52.1
Sundaresan, Athinarayanan . MA 21.3
Sündermann, Eric BP 17.36, •BP 17.37
Sundermann, Martin ..... MA 40.8
Sundermeyer, Jörg .... O 62.1, O 68.1
Sundiyal, Tigmanshu ..... HL 8.5
Sunko, Veronika ..... TT 52.5
Sünner, Moritz ..... O 49.4
Suo, Zhigang ..... CPP 15.53
Surendralal, Sudarsan ..... MM 4.3
Suresh Kumar, Subhalakshmi •CPP 32.5
Sürgers, Christoph ... O 16.10, O 24.6, O 24.8, O 45.1, O 68.10, O 90.2
Susilo, Norman ..... HL 39.4
Süss, Dieter ..... MA 31.38
Suter, Tim ..... DY 31.7
Šutta, P. ..... O 101.1, TT 57.1
Sutter, Florian ..... DS 13.37
Sütterlin, Jana ..... •BP 17.25
Suvorov, Oleksandr ..... O 67.9
Suwanna, Sujin ..... HL 6.5
Suyolcu, Y. Eren ..... TT 52.1
Suzuki, Kosuke ..... HL 36.8
Suzuki, Ryo ..... BP 18.3
Svaluto-Ferro, Enea ..... MM 3.8
Švec, Martin . O 20.7, O 20.9, O 46.10, O 46.12, •O 97.3
Svendsen, Mark ..... O 96.1
Swart, Ingmar ..... O 101.7, TT 16.10, TT 57.7
Swatosch, Philipp ..... •HL 39.22
Sweetman, Adam ..... O 74.6
Swerev, David ..... MA 17.1
Swiderski, Richard BP 14.23, •BP 26.5
Switalla, Isidor ..... MM 9.29
Swoboda, Philipp ..... •TT 37.36
Sychev, Dmitrii ..... CPP 31.3
Syga, Simon ..... •BP 2.7, •CPP 2.7, •DY 3.7
Syrowatka, Frank ..... HL 45.3
Syskaki, Maria Andromachi MA 41.36
Syskaki, Maria-Andromachi MA 29.7, MA 29.13
Szabó, Dorothée Vinga ..... MM 4.6, MM 9.13
Szabó, P. ..... O 38.5, TT 11.17
Szajna, Konrad ..... MM 9.2, O 6.3, O 49.10
Szalai, Alan ..... BP 7.1
Szameit, Alexander .. HL 2.3, HL 6.13
Széchenyi, Gábor ..... MA 8.7
Szigeti, Bertalan ..... MA 43.7
Szombathy, Dominik ..... •DY 41.4, •TT 56.4
Szostak, Bogumiła ..... •CPP 23.4
Szpak, Nikodem .... HL 23.2, TT 21.2, •TT 49.7
Szulc, Krzysztof ..... •MA 29.14
Szunyogh, László •SYES 1.2, MA 9.10, TT 51.6
T. B. Goennenwein, Sebastian MA 17.4
T. Costa, Antomio ..... HL 40.7
T. Elm, Matthias ..... HL 20.23
T. Koch, Christoph ..... KFM 15.12
T. Press, Adrian ..... BP 17.21
T. Zhou, Benjamin ..... TT 34.10
Taake, Chris ..... MA 22.7
Tabanera-Bravo, Jorge ..... •BP 20.5, •DY 25.5
Tabaru, Timuçin Emre DS 6.1, DS 6.8, •MM 21.7
Tabataba-Vakili, Farsane .... •HL 37.1
Taboada Antelo, Luis ..... BP 32.12
Tacon, M. Le ..... MM 6.5
Tada, Hirokazu .. HL 20.23, HL 45.13, MM 27.8
Tada, Mizuki ..... MM 27.8
Tadge, Finja ..... HL 36.4
Taghizade, Narges ..... •CPP 13.2
Tagliavini, Michelangelo .... TT 37.7, TT 37.40, TT 37.45, TT 37.46, TT 37.47, •TT 58.3
Tagmatarchis, Nikos ..... O 68.7
Taguchi, Yasujiro .. MA 6.10, TT 31.3, TT 37.31
Taha, Eman ..... •CPP 5.5
Taheri, Fereydoon ..... •DY 24.10
Taheriniya, Shabnam ..... MM 9.49, •MM 36.10
Tahn, A. ..... MA 6.11
Tailleur, Julien ..... DY 24.7
Tajik, Mohammad ..... O 99.6
Takagi, Hidenori .... TT 33.5, TT 52.1, TT 54.2
Takagi, Yasumasa ..... MA 31.13
Takahashi, Yukiko ... O 83.4, TT 45.4
Takayasu, Hideki ..... SOE 4.3
Takayasu, Misako ..... SOE 4.3
Takegami, Daisuke ..... •TT 52.7
Takeuchi, Ichiro ..... AKPIK 2.3
Taleb, Masoud .... •MM 9.6, MM 21.4
Talebi, Nahid ..... MM 9.6, MM 21.4, O 26.7, •O 61.3, O 72.1, •TT 29.3
Talei Jeid, Roham ..... •MM 30.3
Talei, Roham ..... MM 14.2
Tamai, Anna . HL 2.5, O 29.5, TT 20.5
Tan Qai Shen, Ryan ..... HL 29.17
Tan, Xin Liang ..... MA 32.2, O 101.2, TT 40.2, TT 57.2
Tan, Zihan ..... •BP 28.4, •CPP 35.4, •DY 36.4
Tanabe, Kenji ..... •MA 35.4
Tanaka, Elly ..... BP 18.12
Tanaka, Motomu .. BP 17.14, BP 18.3, BP 25.11
Tanaka, Yukio ..... TT 48.1
Tang, Evelyn ..... •SYQS 1.2
Tang, Peizhe ..... O 57.3
Tang, Xiankang . MM 31.2, •AKPIK 6.1
Tangi, Malleshwararao ..... MA 33.3
Taniguchi, Hiroki .. •KFM 1.3, KFM 1.4
Taniguchi, T. ..... HL 29.13, HL 40.9
Taniguchi, Takashi . DS 3.7, DS 13.15, HL 17.5, HL 17.6, HL 17.9, HL 23.4, HL 29.4, HL 29.12, HL 29.96, HL 37.2, HL 40.8, HL 40.11, HL 53.5, HL 59.5, HL 62.1, O 88.1, O 88.2, TT 18.4, TT 21.4
Tantos, Christos ..... •O 66.1
Tanuku, Venkata M.S.G. ..... BP 13.5, CPP 19.5, DY 15.5
Tanuma, Yuri ..... O 30.3, O 68.7
Tarabunga, Poetri Sonya ... •DY 41.5, •TT 56.5
Tarama, Mitsusuke •BP 16.4, •DY 17.4
Tarasenko, Róbert ..... TT 58.2
Tarasevitch, Alexander ..... O 23.11
Tarasov, Alexander ..... CPP 32.43
Tarasov, Ivan ..... MA 17.3, MA 38.4
Tardivo, Pietro ..... BP 18.12
Tas, Bengü ..... MM 11.3
Taskin, Alexey ..... DS 13.16
Taskin, Alexey A. ..... HL 29.82
Taskina, Alena ..... BP 3.11
Tasnadi, Ferenc . MM 9.32, •MM 37.1
Tasto, Janosch ..... •KFM 15.7
Taubenberger, Anna ..... •BP 15.2
Taubenberger, Anna V. ..... BP 18.5
Täuber, Daniela ... BP 17.17, BP 17.21
Täuber, Isabel ..... •MA 2.8
Taubner, Thomas .. •HL 18.5, HL 63.1, O 33.12, O 60.1, O 60.4, O 71.1, O 71.2, O 72.11, O 87.9
Taucer, Marco ..... O 98.3, O 98.8
Tausendpfund, Niklas ..... •DY 13.4, •TT 19.4
Tautz, F. S. ..... O 38.5
Tautz, F. Stefan ..... HL 40.4, O 10.6, O 17.2, O 62.1, O 79.5, O 80.6, O 83.2, O 88.6, O 101.4, TT 11.5, TT 11.6, TT 45.2, TT 57.4
Tautz, Frank Stefan .. O 16.7, O 33.11, O 79.3
Tautz, Stefan . O 45.5, O 45.6, O 45.7, O 59.1
Tavacoli, Joe ..... BP 17.10
Tavakoli, Ariyan ..... •MA 34.6
Tavernelli, Ivano ..... O 62.4, TT 17.11
Taylor, James M. ... MA 3.3, MA 18.1
Taylor, Victoria C. A. ..... MA 31.20, •O 61.8, O 99.7, •TT 29.8
Tazlerů, Stáňa ..... MA 48.4
te Vrugt, Michael ..... •DY 24.4
Tea, Lingsam ..... CPP 41.2
Tebbe, David ..... HL 53.5
Techert, Simone . CPP 34.2, DS 13.19
Tegeder, Petra . CPP 15.10, CPP 26.2, CPP 27.6, DS 15.4, O 46.1
Tegenkamp, C. ..... •O 33.3, O 33.4, O 33.10
Tegenkamp, Christoph ..... •DS 4.1, DS 7.3, DS 7.6, DS 13.3, DS 13.6, DS 13.7, DS 13.8, O 28.1, O 28.5, O 28.7, O 33.1, O 33.2, O 33.5, O 33.6, O 33.7, O 33.9, O 33.13
Tehranchi, Ali ..... •MM 7.1
Teichert, Christian ..... O 80.4
Teichert, Fabian . TT 36.3, •AKPIK 5.3
Teichert, Johannes F. ..... BP 17.72
Tekgül, Esra Kendir ..... DS 6.1
Telang, Prachi ..... MA 22.1
Teller, Justus ..... •TT 42.8
Temirov, Ruslan ..... O 45.5, O 45.6, O 45.7, O 59.1
Tempere, Jacques ..... HL 1.13
Tena-Solsona, Marta ..... BP 26.8
Teng, Esther ..... O 90.8
Tepper, Lucas .... •BP 34.4, •DY 46.4
ter Burg, Cathelijne ..... •DY 18.4
Terbeck, Manuel ..... •HL 29.19
Tereshchenko, Oleg ..... HL 61.4
Terfort, Andreas ..... CPP 15.9
Terletska, Hanna .. TT 37.39, TT 47.8
Ternes, M. ..... O 38.5
Ternes, Markus O 16.7, O 45.6, O 45.7, O 83.2, O 88.6, TT 45.2
Terres, Sophia ..... HL 63.5
Terzi, Aybike ..... O 32.3
Tesař, Roman ..... MA 48.4, •TT 5.13
Tesch, Davy ..... •O 60.5
Tesler, Alexander ..... •CPP 10.1
Tessarek, Christian ..... •HL 8.2
Tesser, Ludovico ..... TT 47.3
Tessmer, Ingrid ..... BP 7.1
Teubler, Raimund ..... CPP 37.2
Tewari, Akshay ..... •TT 16.2
Tewatia, Preeti .. MA 34.1, •MA 41.27
Tewonoue Djota, Anne Nadine •HL 31.5, •HL 57.7
Teza, Gianluca ..... •DY 9.10
Thaemer, Martin ..... O 84.3
Thake, Henry ..... •O 73.5
Thakur, Sangeeta . MA 17.1, MA 26.7, MA 31.15
Thakur, Shagun . DS 13.19, •DS 13.22, MM 9.15
Thaler, Marco ..... •BP 33.3, O 13.5, O 83.3, •O 100.3, TT 45.3
Thallmair, Sebastian ..... •BP 30.1
Thalmann, Karin S. ..... •CPP 13.3, MM 12.7
Thämer, Martin ... BP 27.4, DS 13.29, O 4.8, O 91.4
Thamizhavel, Arumugam . MA 15.32, TT 41.2, TT 58.2
Thamm, Matthias ..... TT 31.5
Thampi, Ashish .... BP 21.8, SOE 8.8
Thampi, Sumesh .. •BP 6.1, •CPP 7.1, •DY 7.1
Thase, Anastasiia ..... •MM 4.7
Thatte, Advait ..... •BP 26.8
Theile, Jannik ..... •CPP 15.50
Theilen, Marcel ..... O 57.8, O 79.3, •O 79.5
Thein, Marinus ... BP 31.4, CPP 42.4, DY 43.4
Theiss, Tobias ..... DS 7.3
Themann, Julian ... HL 24.1, HL 24.3
Then, Patrick ..... BP 17.17, BP 17.21
Theofylaktopoulos, Vasilis •HL 40.13
Therien, Alexander ..... O 98.3
Thery, Manuel ..... BP 11.2
Thewes, Filipe ..... •DY 27.7
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Thewes, Roland ..... BP 8.1, CPP 9.1
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Thiele, Jan Christoph BP 7.2, •BP 7.6
Thiele, Uwe ..... BP 4.2, CPP 14.2, CPP 14.4, DY 4.11, DY 18.1
Thielemann-Kühn, Nele .... MA 31.25
Thiemann, Fabian ..... •O 40.1
Thieme, Josua ..... •TT 51.1
Thieme, Marc ..... •MM 31.10
Thiering, Nicola ..... MM 9.25
Thies, Andreas ..... HL 2.3
Thingstad, Even ..... PLV IX
Thirion, Louis ..... TT 7.11, •TT 17.4, TT 37.52
Thirunavukkuarasu, Komalavalli •MA 34.9, TT 37.21
Thole, Lars ..... HL 17.1, HL 29.1
Thomale, Ronny ..... HL 6.13, O 60.6, O 86.2
Thomas, Andy .... MA 9.12, MA 15.11
Thomas, Felix ..... CPP 15.4
Thomas, Gwyn R. ..... O 74.5
Thomas, Hannappel ..... HL 20.8
Thomas, Heidi .... BP 12.3, CPP 18.3
Thomas Phillips, Ewan ..... DY 27.2
Thomas, Rico ..... DS 13.8
Thomas, Teslin R. . TT 3.10, TT 37.32, TT 54.6
Thomas, Teslin Rose ..... •TT 3.12
Thomé, Nicolas .... DY 27.5, •DY 34.1
Thompson, James O. F. ..... O 23.12
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Thonig, Danny ..... •MA 12.2
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Thoss, Michael . CPP 13.3, MA 34.10, O 42.4, TT 15.10, TT 47.12
Thulasiram, Parasar R. ..... •TT 41.7
Thunström, Patrik . MM 9.69, TT 7.10
Thurn-Albrecht, Thomas .... CPP 4.1, CPP 4.4, CPP 15.55, CPP 15.56, CPP 32.28
Thurner, Stefan .... SOE 4.7, SOE 4.8
Tian, Haoyang .... •TT 18.6, •TT 35.6
Tian, Sida ..... •TT 11.14
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Tiberto, Paola ... MA 31.5, •MM 20.1, MM 20.2
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Till, Muenker ..... BP 17.26
Timm, Adina . O 29.6, •O 36.3, O 36.4, TT 20.6
Timm, Carsten ... •TT 24.9, TT 24.10, TT 34.9, TT 35.5
Timm, Matthew ..... O 42.3
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Timmer, Daniel ... CPP 30.6, •HL 11.7, HL 11.9, HL 54.5
Timo, Betz ..... BP 17.26
Timoshin, Nikita ..... •AKPIK 5.14
Tindall, Joseph ..... MA 28.7
Tinnefeld, Philip ..... •BP 7.1
Tipp, Fabian ..... CPP 20.3
Tipp, Leonie ..... MM 9.3, MM 9.9
Tippner, Felix ..... •DY 9.8
Tirrito, Emanuele ... DY 41.5, TT 56.5
Tirunilai, Aditya Srinivasan . MM 35.1
Titkov, Ilya E. ..... HL 39.21
Titova, Anastasiai ..... MM 11.7
Tittl, Andreas ..... O 96.5
Titze, Tim ..... MA 12.8, •MA 43.1, MA 43.3
Tiwari, Achyut ..... •TT 37.41
Tiwari, Chandranshu ..... •BP 31.6, •CPP 42.6, •DY 43.6
Tiwari, Dhruv ..... •DY 29.6
Tiwari, Kajal ..... DS 13.17
TIWARI, VATSANA •DY 20.5, •TT 28.5
Tiwary, Tiark ..... •TT 11.2
Tjeng, L.H. ..... MA 40.5
Tjeng, Liu Hao ..... TT 52.7
Tjhung, Elsen ..... DY 5.7, DY 22.2
Tkáč, Vladimír ..... TT 58.2
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Tkach, Olena KFM 5.2, MA 8.3, O 11.7, •O 86.10
Tkatchenko, Alexandre .... •SYAI 1.2, BP 32.10, MM 18.11
Tober, Steffen ..... •O 89.3
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Tobisch, Sarah ..... O 39.5, O 42.2, •O 44.3
Todorova, Mira ..... MM 4.3, MM 7.3, MM 7.4, MM 11.6, MM 32.9, O 27.3, O 65.8
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Tödter, Sophia ..... •O 9.4, O 98.5
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Tohyama, Takami ..... MA 40.9
Toichi, Yuichiro ..... O 86.6, O 89.5
Tokita, Alea Miako ..... MM 9.73
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Trauzettel, Björn .. HL 51.7, MA 41.44, TT 10.7, TT 15.11, TT 46.7, •TT 53.7, TT 53.8
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Tritthart, Martin .•DY 28.4, •KFM 14.1
Trivedi, Nandini ..... MA 4.6
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Urban, Joanna M. .•HL 45.5, MA 10.7, TT 8.5, TT 13.7
Urbánek, Michal ... MA 3.2, MA 20.10
Urbaszek, Bernhard .....HL 29.7, HL 29.17, HL 40.2
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Vahedi, Javad .....•TT 43.9
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Universitätsstraße 31
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ADDITIVE Soft- und Hardware für Technik und Wissenschaft GmbH Max-Planck-Straße 22 b, 61381 Friedrichsdorf *ADDITIVE steht für Berechnen, Visualisieren, Automatisieren für Statistik und Wissensmanagement im Qualitäts-/Ingenieurwesen mit den Produkten Minitab, Origin, Mathematica und ADDITIVE-Cloud-Services.*	**H6**	**A54**
ADL Analoge & Digitale Leistungselektronik GmbH Bunsenstraße 30, 64293 Darmstadt *ADL is developer and manufacturer of various power supplies for thin film coatings and plasma etching as DC Plasma Power supplies, Uni- and Bipolar pulse generators and Power supplies for Ion Sources.*	**Economy Bldg.**	**E04**
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AHF analysentechnik AG Kohlplattenweg 18, 72074 Tübingen *Optical filters (also custom-specific), LED microscopy light sources, image splitters, fluorescence quality monitoring tools, patterned illumination systems for science and research.*	**H6**	**A53**
AIP Publishing 1305 Walt Whitman Road, Suite 300, Melville NY 11747-4300, *APL Quantum, AVS Quantum Science, Journal of Applied Physics, Applied Physics Letters, and more.*	**Foyer Audimax**	**A41**
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53170 Bonn

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Forschungszentrum Jülich Ernst-Ruska-Centrum (ER-C) — **Economy Bldg.** — **E14**

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Staib Instrumente GmbH — **Tent** — **T11**

Hagenaustraße 22, 85416 Langenbach

In situ growth monitoring for MBE, RHEED, TorrRHEEDTM, AUGERProbeTM, AES, XPS, UPS, REELS, electron and ion sources, complete surface analysis systems, STAIB MultitecTM.

Sumitomo (SHI) Cryogenics of Europe GmbH — **Foyer Audimax** — **A28**

Daimlerweg 5 a, 64293 Darmstadt

Cryocoolers: @4K: GMJT (9watt); RDK-101D(L); RDE-412D4; RDK-415D2; RDE-418D4; RP-062B2(S); RP-082B2(S); RP-182B2S @10K: CH-204; CH-210 @20K: RDK-500B2 @77K: CH-110; CH-160D2; New compressor: E77A.

Surface Concept GmbH — **Economy Bldg.** — **E18**

Am Sägewerk 23 a, 55124 Mainz

MCP based detectors, ToF momentum microscopes, Fast analoge readout electronics.

SweepMe! GmbH — **Tent** — **T12**

Bienertstraße 18, 01187 Dresden

Messtechniksoftware

Technische Informationsbibliothek Hannover (TIB) — **Tent** — **T16**

Welfengarten 1B, 30167 Hannover

Wissenschaftliche Fachliteratur.

Technische Universität München Forschungs-Neutronenquelle — **Economy Bldg.** — **E15**

Lichtenbergstraße 1, 85747 Garching

As a cooperation between TU München, Forschungszentrum Jülich, and Helmholtz-Zentrum hereon, the Heinz Maier-Leibnitz Zentrum is a user facility for cutting-edge research with neutrons and positrons.

tectra GmbH — **Foyer Audimax** — **A36**

Reuterweg 51-53, 60323 Frankfurt/M.

UHV Komponenten, Dünnschichttechnik, Plasmaquellen.

THORLABS GmbH — **Foyer Audimax** — **A02+A05**

Münchner Weg 1, 85232 Bergkirchen

Optische & optomechanische Komponenten, Test & Measurement Systeme, optische Tische und Vibrationskontrolle, Nanopositionierungen, Lichtquellen sowie Imaging, Mikroskopie und Life Science Komponenten.

TOPAG Lasertechnik GmbH — **H6** — **A56**

Nieder-Ramstädter Straße 247, 64285 Darmstadt

Laser und optische Messtechnik.

TOPTICA Photonics AG — Tent — T06

Lochhamer Schlag 19, 82166 Gräfelfing / München

New Tunable Diode Lasers, New Laser Frequency Stabilization, Femto Fiber Lasers, Wavelength Meters.

VACOM Vakuum Komponenten und Messtechnik GmbH — **Foyer Audimax** — **A23**

In den Brückenäckern 3, 07751 Großlöbichau

Vakuumkammer

vakuumfinder.de c/o CompoNext GbR — **Tent** — **T10**

Freiligrathstraße 35, 07743 Jena

Vakuumkomponenten, Vakuummesstechnik, Vakuumkammern, Kryotechnik, Critical Design Review, Vakuumpumpenservice, Auftragsfertigung.

Vaqtec-scientific Mario Melzer — **Economy Bldg.** — **E07**

Thulestraße 18B, 13189 Berlin

Komponenten der UHV- und HV-Technik: u.a. Stromdurchführungen, Schaugläser, Schichtdicken-Messgeräte

VASTA PTE. LTD. — **Tent** — **T08**

Blk 81 Ayer, Singapore 139967, Singapore

VASTA offers advanced solutions for cryogenic RF connectivity, single-photon detection, portable spectroscopy and Raman analysis, and low-temperature electrical transport measurement.

Wiley-VCH GmbH — **Foyer Audimax** — **A15**

Boschstraße 12, 69469 Weinheim

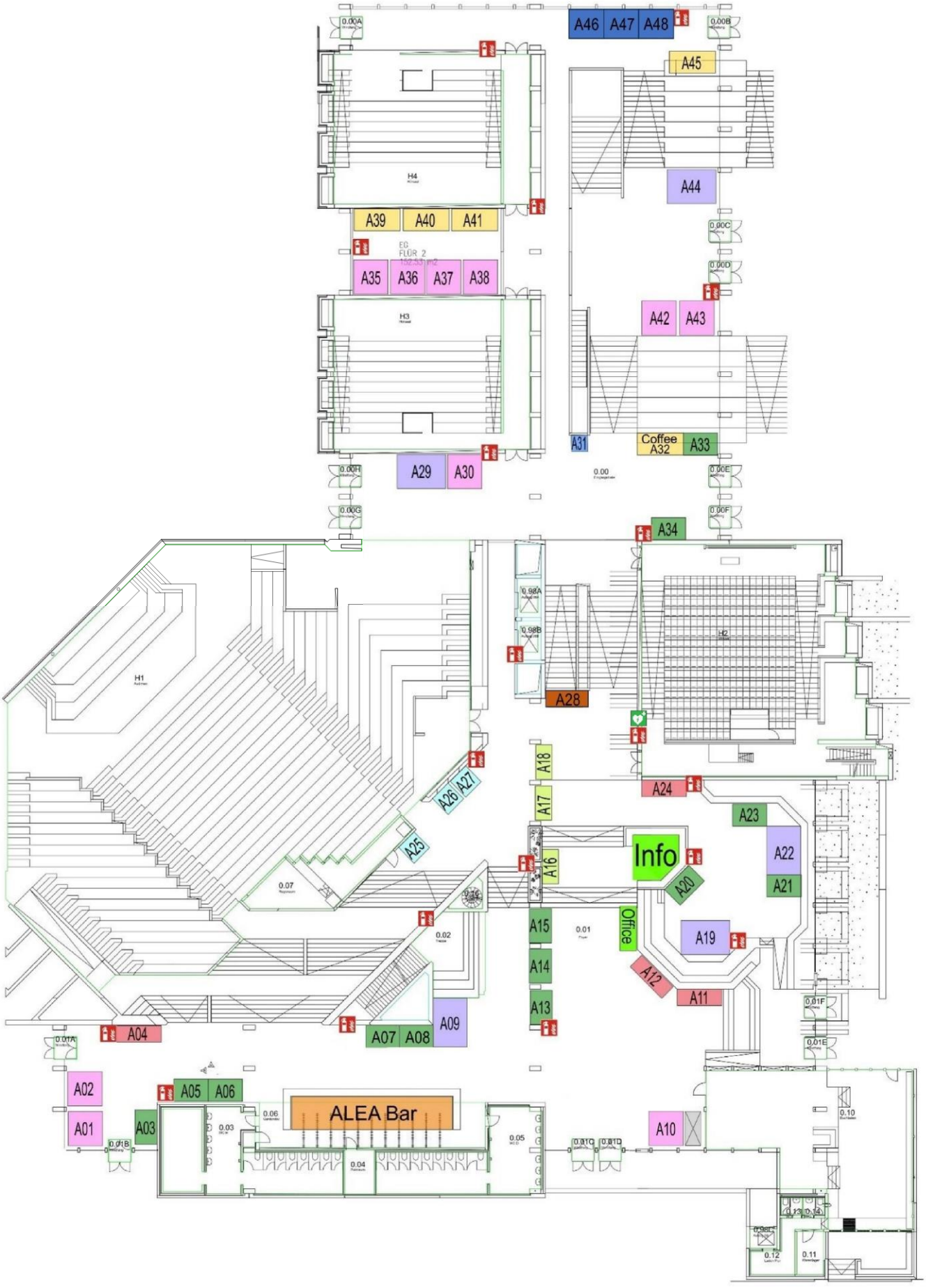
Verlag - Fachzeitschriften und Fachbücher.

Zurich Instruments Germany GmbH — **Foyer Audimax** — **A22**

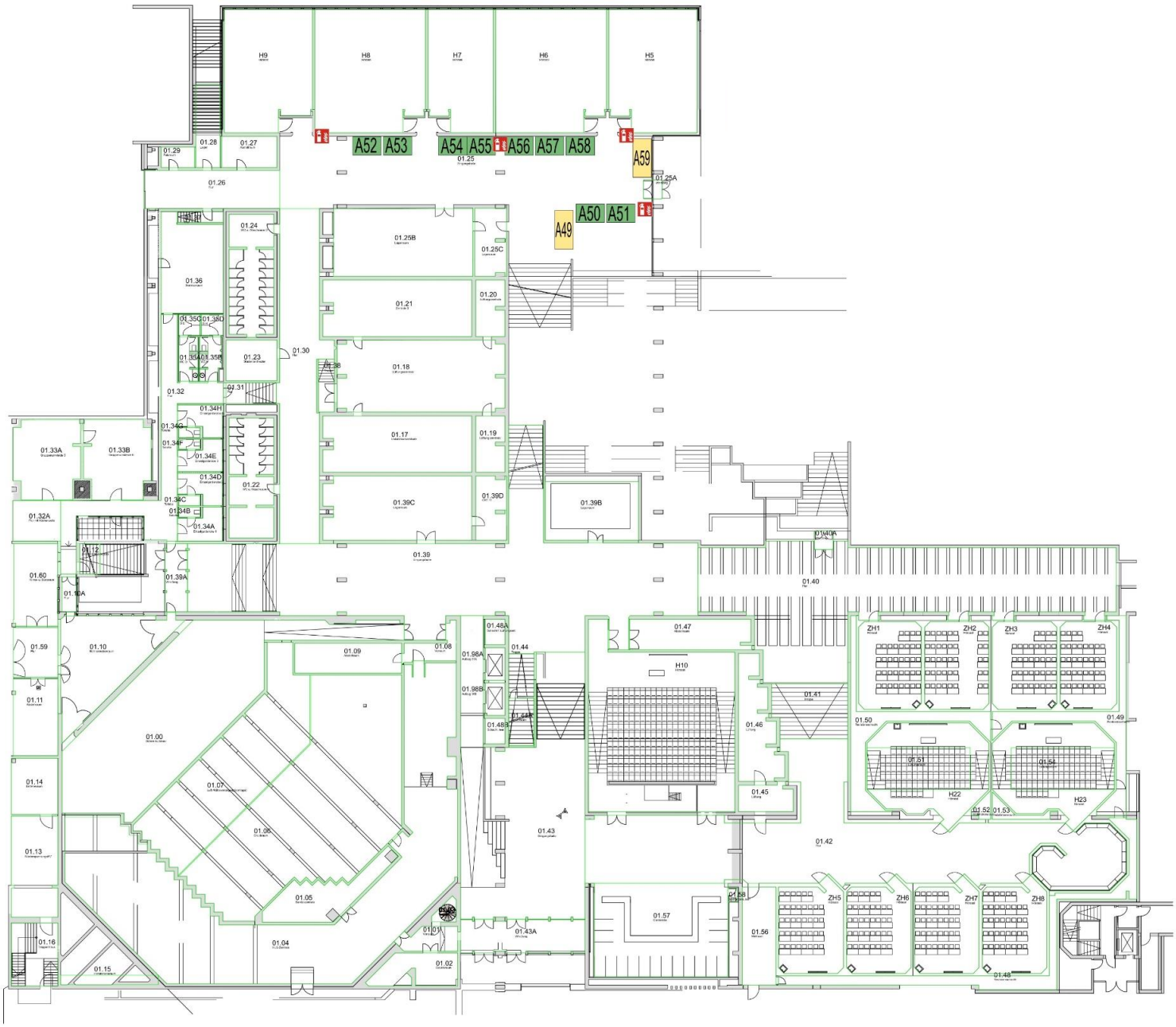
Mühldorfstraße 15, 81671 München

Lock-in Amplifier, Impedance Analyzer, Arbitrary Waveform Generator, Quantum Control System, Oscilloscope.

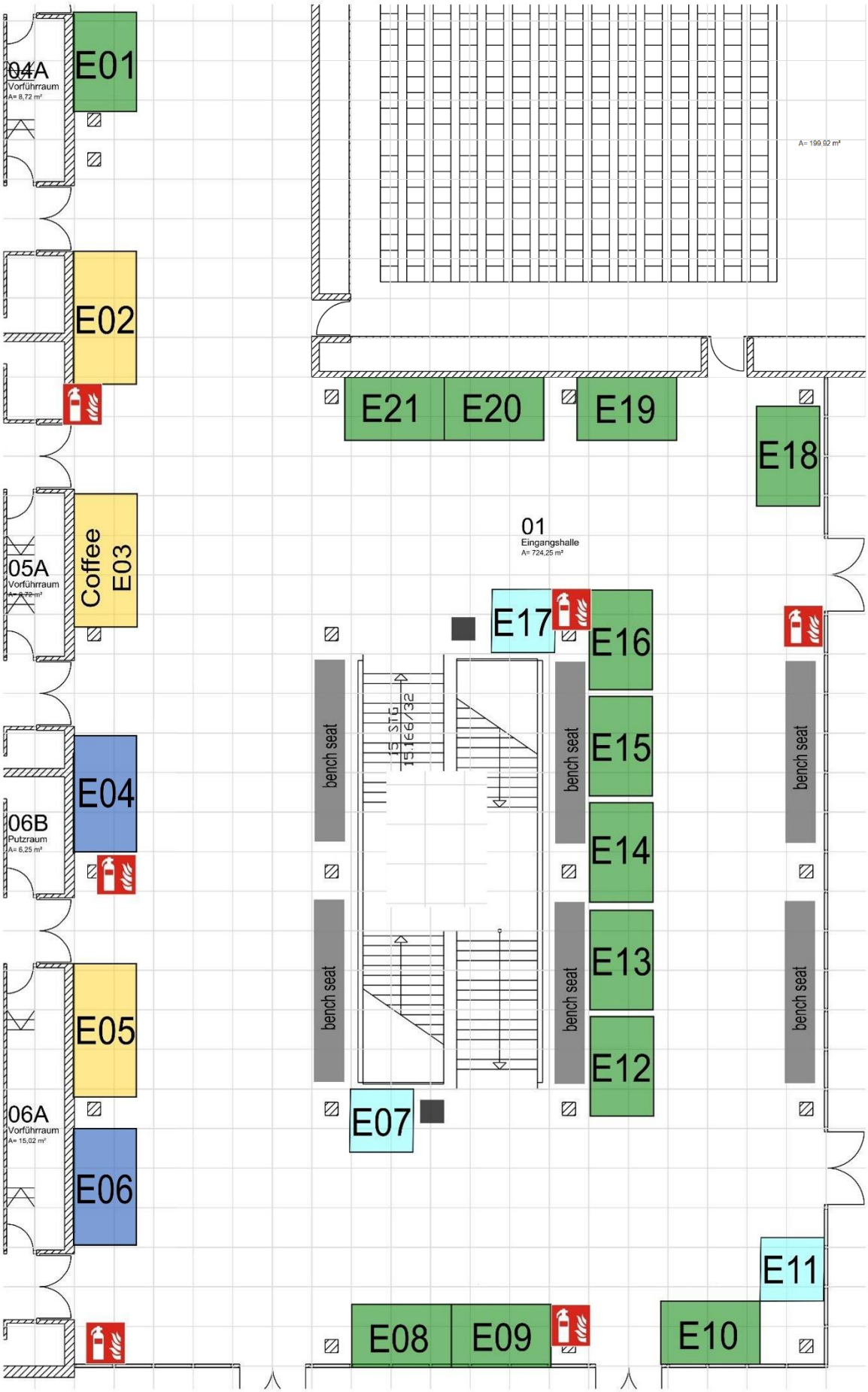
Exhibition ZHG A - Foyer Audimax



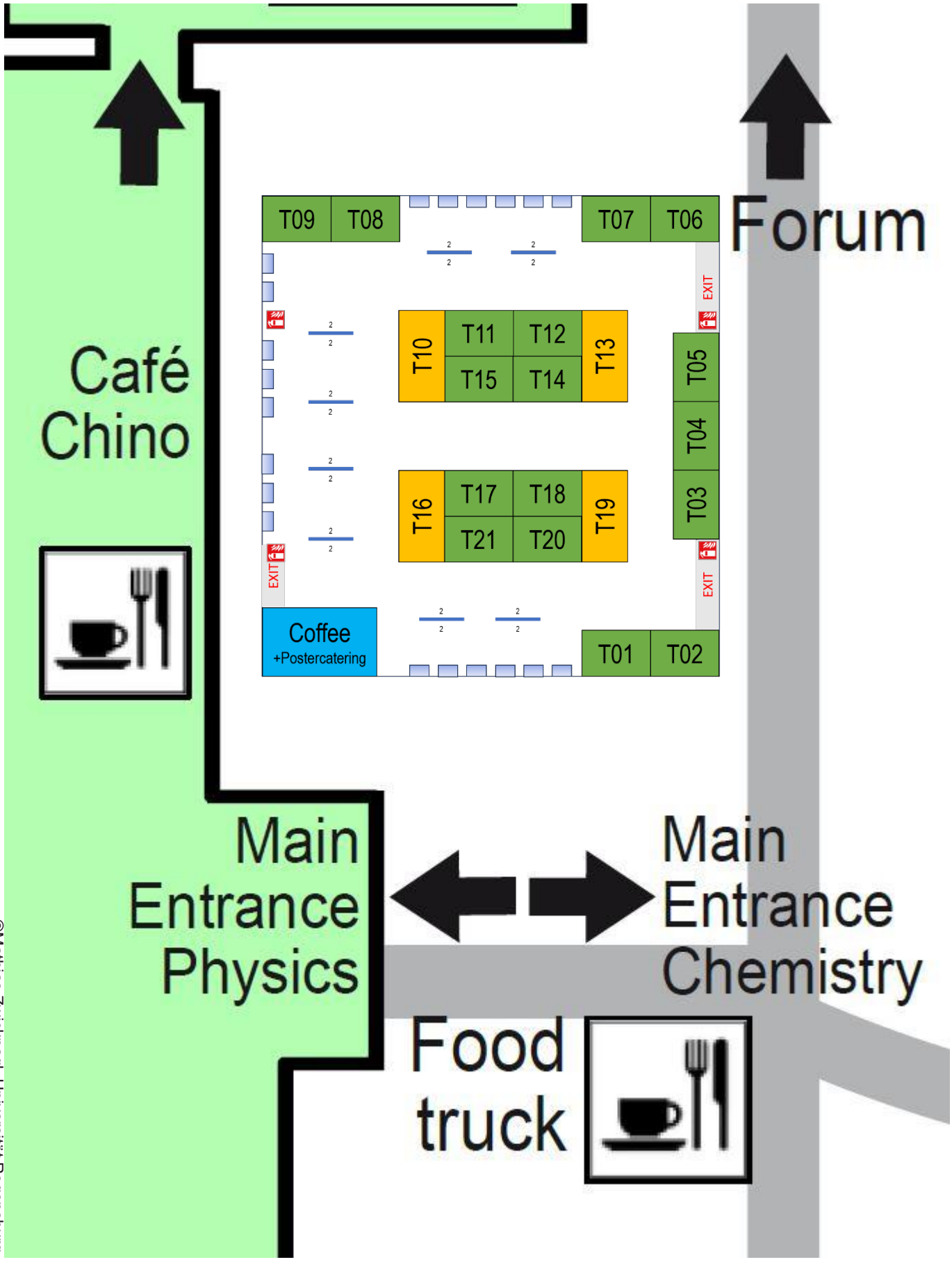
Exhibition ZHG A - Basement



Exhibition - Economy Bldg. (R&W)

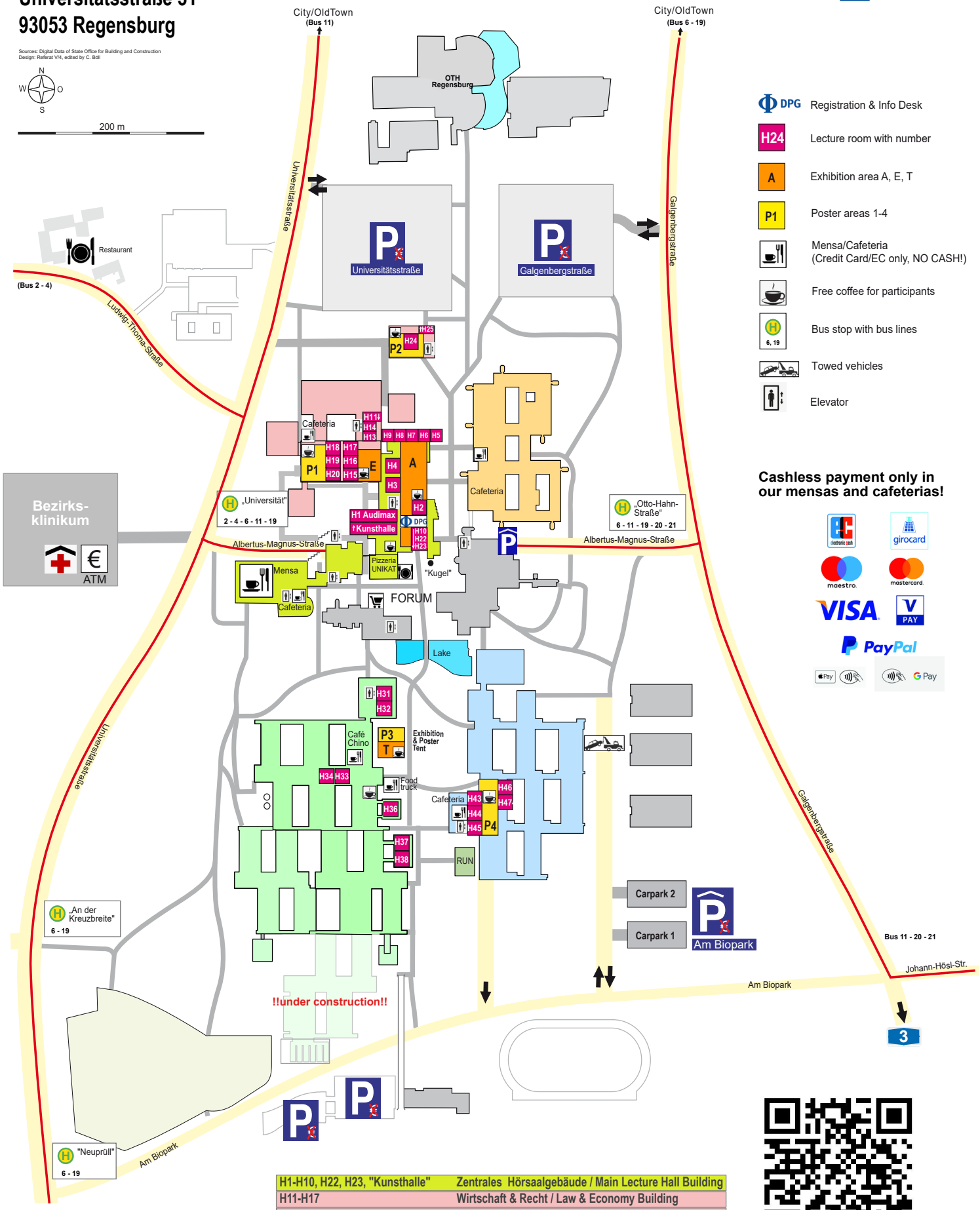


Exhibition - Tent



Universität Regensburg - Campus Map DPG Spring meeting 2025

Universitätsstraße 31
93053 Regensburg



DPG Registration & Info Desk

H24 Lecture room with number

A Exhibition area A, E, T

P1 Poster areas 1-4

Mensa/Cafeteria
(Credit Card/EC only, NO CASH!)

Free coffee for participants

6, 19 Bus stop with bus lines

Towed vehicles

Elevator

Cashless payment only in our mensas and cafeterias!

girocard
maestro
mastercard
VISA
V PAY
PayPal
Pay
G Pay

H1-H10, H22, H23, "Kunsthalle"	Zentrales Hörsaalgebäude / Main Lecture Hall Building
H11-H17	Wirtschaft & Recht / Law & Economy Building
H18-H21	Sammelgebäude / Multi-purpose Building
H24-H26	Vielberthgebäude / Vielberth Building
H31, H32	Mathematik / Mathematics
H33-H36	Physik / Physics
H37-H38	Biologie & Vorklinik / Biology & Pre-Clinical Medicine
H43-H47	Chemie / Chemistry

Exhibition Areas (Tue - Thur 10am - 6pm)
A Main Lecture Hall Building
E Law & Economy Building
T Tent at Physics Building

Please refer to the "UR Walking App" to find your way across the campus


Start
Sunday, March 16
Monday, March 17
Tuesday, March 18
Wednesday, March 19
Thursday, March 20
Friday, March 21
08:15
08:30
08:45
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08:25 Opening remarks (Audimax)
Plenary Talk (H1 Audimax)
Plenary Talk (H1 Audimax)
Plenary Talk (H1 Audimax)
Plenary Talk (H1 Audimax)
Plenary Talk (H1 Audimax)
SYED (H1 Audimax)
SKM Dissertation Prize Symposium (H2)
Sessions of divisions
SYIS (H1 Audimax)
Sessions of divisions
SYFD (H1 Audimax)
Sessions of divisions
SYAI (H1 Audimax)
Sessions of divisions
SYES (H1 Audimax)
Women in Quantum Physics
AKC (H2)
Sessions of divisions
Prize Talk (H2)
Lunch Talk (H1 Audimax)
Prize Talk (H2)
Lunch Talks (H1, H4)
Prize Talk (H2, H4)
Lunch Talks (H1, H3)
Prize Talk (H2, H4)
Lunch Talks (H1, H3)
Closing Talks (H1 Audimax & H2)
Plenary Talks (Audimax + H2)
AG Klima Lounge (H7)
Sessions of divisions
Plenary Talks (Audimax + H2)
Plenary Talks (Audimax + H2)
Registration
16:00-18:30 Tutorials (H2, H3, H4)
SYMD (H1 Audimax)
Sessions of divisions
Ceremonial Session with Award Ceremony and Ceremonial Talk (Audimax)
SYMS (H1 Audimax)
Sessions of divisions
SYQS (H1 Audimax)
Sessions of divisions
18:30-21:30 Welcome Evening (Mensa)
19:00-20:00 Public Evening Talk (in German) (H1 Audimax)
Post-Deadline-Session (O) (H1)
Einstein Slam (Audimax)
jDPG Kneipentour (Meeting Point: "Kugel", Forum)
SKM Evening (Mensa)
908
10.02.2025