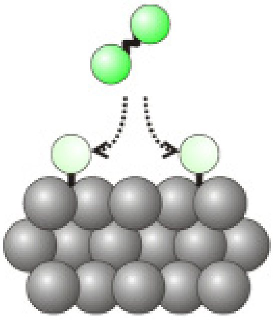
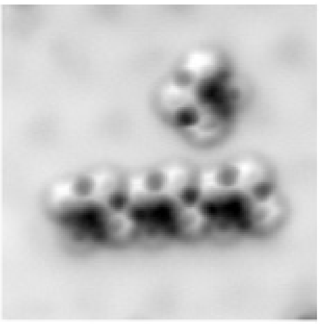
Deutsche Physikalische Gesellschaft DPG

Virtual DPG Spring Meeting 2021

of the Surface Science Division





1 – 4 March 2021

surfacescience21.dpg-tagungen.de/

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Content

Greeting

Dear Conference Guests,

On behalf of the DPG, I would personally like to welcome you to the virtual DPG-Frühjahrstagung (DPG Spring Meeting) of the Surface Science Division.

I am very pleased that despite the ongoing pandemic, we are able to hold this DPG Spring Meeting with an outstanding programme of keynote lectures, mini-symposia, interactive poster sessions to promote the exchange that is so important for science. This is invaluable, especially for the next generation of physicists for further scientific development and career planning, as at these DPG Spring Meetings, young researchers can present their theses to a larger scientific audience for the first time and able to network with potential employers.

However, our conference season this year also shows the great potential for innovation that lies dormant in the DPG. Thanks to the extraordinary commitment of our members, new and digital formats for events were developed and implemented in the Corona pandemic in a very short time. These are not only temporary alternatives, but can also help to increase the overall reach of the DPG events in the future - and thus the visibility of physics in politics and the public. This is of great importance for a society that relies heavily on the discoveries and innovations of the natural sciences and benefits from their findings, which are needed to address current and future societal challenges.

In short, we need physics as part of our culture today more urgently than ever!

For the success of this DPG Meeting, I would therefore like to express my great gratitude to all those involved. I would also like to especially thank the Wilhelm and Else Heraeus Foundation for their generous support of all DPG Meetings. My special appreciation goes to the responsible programme committee, Prof. Karsten Reuter (Head of the Surface Science Division, Director of the Theorie Department at the Fritz-Haber-Institute of the Max Planck Society in Berlin) and Prof. Dr. Ulrike Diebold (Deputy Head of the Surface Science Division, Institute of Applied Physics, Vienna University of Technology). I would like to thank the staff of the DPG Head Office for their support and supervision of all DPG Spring Meetings.

Dr. Lutz Schröter

President of the
Deutsche Physikalische Gesellschaft e. V.

Organisation

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Scientific Organisation

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Mini-Symposia

Coherent band structure engineering with light
Organisation:
Marcel Reutzel, Georg-August-Universität Göttingen
Stefan Mathias, Georg-August-Universität Göttingen

Ultrafast surface dynamics at the space-time limit
Organisation:
Melanie Müller, Fritz Haber Institute Berlin
Hannes Böckmann, Georg-August-Universität Göttingen

Infrared nano-optics
Organisation:
Alexander Paarmann, Fritz Haber Institute Berlin
Markus A. Huber, Universität Regensburg

Electrified solid-liquid interfaces
Organisation:
Nicolas Hörmann, Fritz Haber Institute Berlin
Mira Todorova, Max-Planck-Institut für Eisenforschung Düsseldorf

Machine learning applications in surface science
Organisation:
Oliver T. Hofmann, Technische Universität Graz, Austria
Karin Zojer, Technische Universität Graz, Austria
Stefan Kowarik, Karl-Franzens-Universität Graz, Austria

Dzyaloshinskii-Moriya Interaction in magnetic layered systems
Organisation:
Andres Arnau, Basque Country University San Sebastian, Spain
Mikhail M. Otrokov, Basque Country University San Sebastian, Spain
María Blanco-Rey, Basque Country University San Sebastian, Spain

Free-standing functional molecular 2D materials
Organisation:
Armin Gölzhäuser, Universität Bielefeld
Andrey Turchanin, Friedrich-Schiller-Universität Jena

Manipulation and control of spins on functional surfaces
Organisation:
Fabian Paschke, Universität Konstanz
Katharina Kaiser, IBM Zürich, Switzerland
Rasa Rejali, Technische Universität Delft, The Netherlands
Georg A. Traeger, Georg-August-Universität Göttingen
Fabio Donati, Center for Quantum Nanoscience Seoul, South Korea
Yujeong Bae, Center for Quantum Nanoscience Seoul, South Korea
Andreas J. Heinrich, Center for Quantum Nanoscience Seoul, South Korea

Molecular scale investigations of liquid-vapor interfaces
Organisation:
Rémi Dupuy, Fritz Haber Institute Berlin
Clemens Richter, Fritz Haber Institute Berlin
Clara Saak, Universität Wien, Austria

Frontiers of Electronic-Structure Theory: Focus on Electron-Phonon Interactions
Organisation:
Claudia Draxl, Humboldt-Universität zu Berlin
Feliciano Giustino, Universität Texas Austin, USA
Matthias Scheffler, Fritz Haber Institute Berlin

Thematic Poster Sessions

Mini-Symposium: Coherent band structure engineering with light
Mini-Symposium: Ultrafast surface dynamics at the space-time limit
Mini-Symposium: Infrared nano-optics
Mini-Symposium: Electrified solid-liquid interfaces
Mini-Symposium: Machine learning applications in surface science
Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems
Mini-Symposium: Free-standing functional molecular 2D materials
Mini-Symposium: Manipulation and control of spins on functional surfaces
Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces
Mini-Symposium: Frontiers of electronic-structure theory
Metal substrates
Semiconductor substrates
Oxide and insulator surfaces: Structure, epitaxy and growth
Oxides and insulators: Adsorption and reaction of small molecules
Supported nanoclusters: Structure, reactions, catalysis
Organic molecules on inorganic substrates: Adsorption and growth
Organic molecules on inorganic substrates: Networks and overlayers
Organic molecules on inorganic substrates: Electronic, optical and other properties
Solid-liquid interfaces: Structure, spectroscopy
Solid-liquid interfaces: Reactions and electrochemistry
Graphene and beyond
2D Materials: Electronic structure, excitations, etc.

Topological insulators
Topology and symmetry-protected materials
Nanostructures at surfaces
Heterogeneous catalysis
Electronic structure of surfaces: Spectroscopy, surface states
Ultrafast electron dynamics at surface and interfaces
Electron-driven processes at surfaces and interfaces
Electronic structure theory: General
Surface reactions
Surface magnetism
Surface dynamics: Phase transitions and elementary processes
New methods
Scanning probe techniques: Method development
Tribology: Surfaces and nanostructures
Plasmonics and nanooptics

Programme
The scientific programme consists of **656** contributions:

8	Plenary talks
41	Invited talks
51	Talks
553	Posters
3	Paper discussions

Information for Participants

The virtuell conference will be held in the period 1–4 April, 2021

Conference Information

Conference Location
Web-based Conference – Login information will be provided a few days before the event starts.

Conference Time Zone
All times are in Central European Time (CET), UTC +1

Conference Website
https://surfacescience21.dpg-tagungen.de/

Conference Platform Functionalities
To use all features of the digital conference, you need an up-to-date browser. The latest versions of Chrome, Firefox, Safari, and Edge with Blink engine are fully supported. JavaScript must be active. For video calls, permission to access your microphone and camera is required. Please note that firewalls of company or institute networks can also limit the functionality.

Immediately after logging in (with your credentials), you will be directed to the conference platform, which is the central access point on the web during the entire event. Here, all functionalities of the platform are available to you clearly and intuitively.

In the header, you will find the main menu, which allows you to access the different areas of the conference – and to switch back and forth between them:

⇨ **Your Profile**
In the upper right corner of the screen, you will find access to your profile. All your data is stored here. Additionally, introduce yourself with a short description or a statement and mark your interests. Should you wish to network more closely with other participants, authors, or exhibitors during the congress, you can send them your virtual business card. Your e-mail address will also appear on this card.

⇨ **Programme**
Here you will find an overview of the individual conference days and the respective contributions including short descriptions.

⇨ **Discussion Forum**
Use the opportunity to exchange ideas with participants or start a thematic exchange via the „Create Thread“ button. Fill out the form and publish your contribution, which can now be commented on and discussed. A video chat room is linked to each contribution, where you can exchange ideas in small groups during the breaks, for example.

⇨ **Networking**
Get an overview of the conference participants, make contact requests, and thus expand your network. An important aspect of every conference is the opportunity to maintain old contacts and make new ones. The menu item „Networking“ gives you an overview of the people registered for the conference in an area that is only accessible to participants. There you will also find, among other things, your profile, which you can individualize.
To view the profile of another conference participant, click on a corresponding virtual business card. A separate button allows you to send a contact request to exchange your e-mail addresses. If a conference participant also appears as a speaker or poster author, the respective contributions are stored in the profile – so you always have an overview of which of your contacts is speaking.

⇨ **Poster Room**
View the submitted poster contributions and the corresponding abstracts and exchange ideas with the authors. During the poster sessions you will also have the opportunity to join a group video chat at each poster to exchange and discuss.

⇨ **Search**
If you want to find specific content and/or programme items, use the search function to find them very quickly. On the right side of the header, you will find your profile as well as a list of your contacts, and access to the chat function. The latter includes conversations already held with conference participants, but you can also start new conversations including the possibility for individual video chats.

To make access to the lecture programme as convenient as possible, the individual conference days can be individually controlled. Thus, you can access the current live stream or on-demand offers of the conference in an ordered Electronic Programme Guide. If you want to mark contributions in the run-up to or during the conference, you can highlight them with a „star“. You will find the programme items marked in this way under „My Favorites“.

⇨ **Electronic Programme Guide**
Join the live stream or live zoom session to follow the current presentation.
Browse the programme for each day. By clicking on the individual contributions you will get additional information, such as the abstract. In addition to the basic information, you can ask the author a question about his or her contribution. This is publicly accessible. If you send a contact request to the participating authors, they can also exchange information bilaterally or arrange for an individual video chat.

⇨ **Time Shift & On-Demand Content**

If you have missed a presentation or want to listen to it again, you can still access the contributions up to 14 days after the event using your access data.
The poster contributions and the networking opportunities with other conference participants will also be available to you until two weeks after the conference.

In case of any technical issue please contact us at: +49 (0)69 75306 777

Notice Board

All changes regarding the schedule of the conference will be updated currently. The information is identical to the programme updates of the scientific programme and are available at the scientific programme in other formats as well (ordered by publication date, filterable by conference part and as an rss-feed). Please use the form at *https://surfacescience21.dpg-tagungen.de/programm/notice-board-form* to submit amendments, cancellations, etc.

Wilhelm and Else Heraeus Communication Programme

Within this programme the active participation by young DPG members – from Germany and abroad – at the virtual DPG-Frühjahrstagungen (DPG Spring Meetings) is financially supported.
For the virtual DPG-Frühjahrstagungen (DPG Spring Meetings), the conference fee (and exclusively the "early bird rate") is subsidised at 100 % (*submission of an application was open until 7 February 2021. Subsequent applications are unfortunately not possible*). After the conference, your participation in the conference will be checked on the basis of the login data and the funding will be finally confirmed or rejected if no participation took place.

Payment will be made – after prior notification by e-mail – by the end of April 2021 at the latest by bank transfer to the account you specified in your application.

The Deutsche Physikalische Gesellschaft thanks the Wilhelm and Else Heraeus Foundation for the generous financial support of young academic talents. We hope that young physicists will continue to seize the offered opportunity for active scientific communication at scientific conferences. A total of about 35,000 young academics were supported by this programme so far.

Information for Speakers

All speakers are invited to use our offer for a testsession one week before the conference starts. The nessesary information for the testsession about day, time and login information will be send out by e-mail to the speakers. We would like to ask you to consider the following points for your presentation:

- Please use the same equipment with which you successfully completed your technical check to avoid technical problems during your presentation.
- Please be in the Zoom session of the virtual room where you will give your presentation at least 5 minutes before the session starts.
- Please sign in at Zoom with your full name so that we and the technicians can identify you as a speaker and give you the rights to share your screen, microphone and camera in Zoom.
- Please make sure that you respect your presentation time!

Information for poster presentations

The interactive poster sessions combine the classic contributed talks and posters in an attractive digital form. In addition to the posters, which are accessible throughout the whole conference, it is also possible to present the core messages of the poster in a short 3 minute video abstract, which can also be accessed on-demand.

We would like to ask you to consider the following points when creating your posters and videos:

- Please create your poster as a JPG file in portrait format (DIN A0; 84.10 cm wide and 118.90 cm high). The file must not exceed a maximum size of 25 MB.
- Please create your 3 minute video abstract in MP4 format. The file must not exceed a maximum size of 150 MB.

- The above criteria are based on the technical requirements of the conference platform used. Therefore, different formats are unfortunately not possible.

The posters will be accessible to all registered participants throughout the conference and for up to two weeks after the end of the conference. Please be available for discussion (group video chat via Jitsi) at your poster throughout the poster session.

Social Events

Opening
by the Chair of the Surface Science Division
Prof. Dr. Karsten Reuter, Fritz Haber Institute, Berlin
Monday, 1 March, 09:45, R1. All participants are kindly invited.

Annual Meeting of the Surface Science Division
Thursday, 4 March, 13:00, R1

Announcement of Gerhard Ertl Young Investigator Prize
Thursday, 4 March, 16:00, R1

The DPG on Instagram
In the anniversary year the DPG will present an inspiring personality or an everyday physical phenomenon on Instagram (@dpgphysik) every day. Who inspires you? What fascinates you? Submit online suggestions for the 175 Inspirers and the 175 Impulses.
You can find the entries at http://175inspirierende.dpg-physik.de and http://175impulse.dpg-physik.de. Contact: 175inspirierende@dpg-physik.de or impulse@dpg-mail.de.

Acknowledgement
The Deutsche Physikalische Gesellschaft (DPG) wants to thank the following institutions for supporting the conference:

- Wilhelm and Else Heraeus-Foundation, Hanau
- Deutsche Gesellschaft für Materialkunde e.V. (DGM),
- and all staff who make the success of the conference possible.

Deutsche Physikalische Gesellschaft DPG

Jetzt bewerben!

DPG-Mentoring-Programm und Leading for Tomorrow

An der Schwelle zum Berufseinstieg bietet die DPG zwei besondere Programme an, gerade wenn der Berufseinstieg eventuell in Industrie und Wirtschaft erfolgen soll.

Bewerbungszeitraum 1. bis 31. März

Weitere Infos unter: www.mentoring_L4T.dpg-physik.de

Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

Key Notes

O 2.1	Mon	10:00–10:30	R1	**Chasing excited electrons in energy, momentum space, and time** — •Martin Aeschlimann
O 28.1	Mon	15:30–16:00	R1	**Physical chemistry and chemical physics of environmental interfaces** — •Vicki Grassian
O 29.1	Tue	10:00–10:30	R1	**Electrochemistry of platinum: new views on an old problem** — •Marc Koper
O 56.1	Tue	15:30–16:00	R1	**Meta-stable intermediates of OER catalysis: connecting their time-resolved spectra to thermodynamic descriptors** — •Tanja Cuk, Ilya Vinogradov, Aritra Mandal, Suryansh Singh, Hanna Lyle
O 57.1	Wed	10:00–10:30	R1	**Tunneling spectroscopy of magnetic adatoms on superconductors** — •Katharina J. Franke
O 84.1	Wed	15:30–16:00	R1	**Surface structure by way of machine learning** — •Bjørk Hammer
O 85.1	Thu	10:00–10:30	R1	**On-surface reactions and molecular charge-state transitions by atom manipulation** — Katharina Kaiser, Shadi Fatayer, Florian Albrecht, •Leo Gross
O 111.1	Thu	15:30–16:00	R1	**Light-matter interaction at the atomic scale** — •Klaus Kern

Invited Talks

O 3.1	Mon	10:30–11:00	R1	**Actuating and probing a single-molecule switch at femtosecond timescales** — Dominik Peller, Carmen Roelcke, Lukas Z. Kastner, Thomas Buchner, Alexander Neef, Johannes Hayes, Florian Albrecht, Rupert Huber, •Jascha Repp
O 3.2	Mon	11:00–11:15	R1	**Real space-time imaging of valence electron motion in molecules** — •Manish Garg
O 3.3	Mon	11:15–11:45	R1	**Ultrafast structural phase transitions probed by low-energy electron diffraction** — •Claus Ropers
O 3.4	Mon	11:45–12:00	R1	**Probing the ultrafast electron dynamics in the quantum spin Hall system Bismuthene with time-resolved ARPES** — •Julian Maklar, Raul Stühler, Maciej Dendzik, Tommaso Pincelli, Shuo Dong, Samuel Beaulieu, Martin Wolf, Ralph Ernstorfer, Ralph Claessen, Laurenz Rettig
O 3.5	Mon	12:00–12:30	R1	**Atomic-resolution imaging of THz-driven dynamics on charge-ordered surfaces** — •Sebastian Loth
O 4.1	Mon	10:30–11:00	R2	**Ion permeation across atomically thin materials** — •Marcelo Lozada-Hidalgo
O 4.4	Mon	11:30–12:00	R2	**Macroscopic Two-Dimensional Polymers: Synthesis and Structure Control** — •Zhikun Zheng
O 15.1	Mon	13:30–14:00	R1	**The ultrafast Einstein-de Haas effect triggered by ultrafast demagnetization** — •Steven L. Johnson, Christian Dornes, Yves Acremann, Matteo Savoini, Martin Kubli, Martin J. Neugebauer, Elsa Abreu, Lucas Huber, Gabriel Lantz, Carlos A. F. Vaz, Henrik Lemke, Elizabeth M. Bothschafter, Michael Porer, Vincent Esposito, Laurenz Rettig, Michael Buzzi, Aurora Alberca, Yoav W. Windsor, Paul Beaud, Urs Staub, Diling Zhu, Sanghoon Song, James M. Glownia
O 16.1	Mon	13:30–14:00	R2	**Combining 2D materials and optical metasurfaces** — •Isabelle Staude
O 16.4	Mon	14:30–15:00	R2	**Electronic properties of freestanding ultra-thin small-molecular and multilayer graphene films** — •Thomas Weitz
O 17.1	Mon	13:30–14:00	R3	**Predominance of non-adiabatic effects in zero-point renormalization of electronic energies** — •Xavier Gonze, Anna Miglio, Véronique Brousseau-Couture, Gabriel Antonius, Yang-Hao Chan, Steven Louie, Bogdan Guster, Matteo Giantomassi, Michel Côté

O 17.2	Mon	14:00–14:30	R3	**Huge quantum effects on the 250 K superconducting lan- thanum hydride** — •Ion Errea
O 17.3	Mon	14:30–15:00	R3	**Out-of-equilibrium lattice dynamics in two-dimensional materials** — •Fabio Caruso
O 17.4	Mon	15:00–15:30	R3	**Ultrafast optical control of complex oxide functional properties: New insights from theory and first-principles calculations** — •Nicole Benedek
O 30.1	Tue	10:35–11:10	R1	**A Theoretical Framework for Investigating Electrochemical Reactions** — •Wolfgang Schmickler
O 30.2	Tue	11:10–11:45	R1	**Dynamic Evolution of CO_2 Electroreduction Catalysts** — •Beatriz Roldan Cuenya
O 31.1	Tue	10:30–11:00	R2	**What can we learn from atoms?** — •Alexander Khajetoorians
O 31.3	Tue	11:15–11:45	R2	**Artificial spin chains on superconductor surfaces** — •Jens Wiebe
O 43.1	Tue	13:30–14:05	R1	**Electrocatalysis beyond surface reaction energetics** — •Karen Chan
O 43.2	Tue	14:05–14:40	R1	**Design and application of an ab initio electrochemical cell** — Sudarsan Surendralal, Florian Deissenbeck, Stefan Wippermann, Christoph Freysoldt, Mira Todorova, •Jörg Neugebauer
O 44.1	Tue	13:30–14:00	R2	**Atomic-scale spin sensing with a single molecule at the apex of a STM** — •Laurent Limot
O 44.3	Tue	14:15–14:45	R2	**Quantum sensing and operation of single molecules on the surface** — •Xue Zhang
O 44.4	Tue	14:45–15:15	R2	**Longitudinal and transverse electron paramagnetic resonance in a scanning tunneling microscope** — •Tom S. Seifert, Stepan Kovarik, Dominik Juraschek, Nicola A. Spaldin, Pietro Gambardella, Sebastian Stepanow
O 45.1	Tue	13:30–14:00	R3	**A Superficial Look At Water** — •Olle Björneholm
O 45.4	Tue	14:40–15:10	R3	**Exploring Collisions and Reactions at the Vacuum-Water Interface using Water Microjets** — •Gilbert Nathanson
O 58.1	Wed	10:30–11:00	R1	**Simulating interfacial water with neural network potentials** — •Christoph Dellago, Oliver Wohlfahrt, Marcello Sega
O 58.3	Wed	11:20–11:50	R1	**Surface activity of hydroxide and the hydrated proton** — •Ellen Backus
O 59.1	Wed	10:30–11:00	R2	**TBA** — •Netanel Lindner
O 59.3	Wed	11:15–11:45	R2	**Engineering emergent states in quantum materials with classical and quantum light** — •Michael Sentef
O 60.1	Wed	10:30–11:00	R3	**Rashba effect and chiral magnetism: some insights from density functional theory** — •Gustav Bihlmayer
O 60.2	Wed	11:00–11:30	R3	**Synthetic chiral magnets and domain wall logic circuits** — •Pietro Gambardella
O 60.3	Wed	11:30–12:00	R3	**Zero-field magnetic skyrmions in model-type systems studied with STM** — •Kirsten von Bergmann
O 60.4	Wed	12:00–12:30	R3	**Spin Orbit driven effects in Graphene-FM systems** — •Paolo Perna
O 71.1	Wed	13:45–14:15	R1	**Machine learning for novel functional materials** — •Pascal Friederich
O 71.5	Wed	15:00–15:30	R1	**Theory-informed Machine Learning for Surface and Interface Structure Reconstruction from Experimental Data** — Eric Schwenker, Chaitanya Kolluru, Marcel Chlupsa, Arun Mannodi Kanakkithodi, Richard Hennig, Pierre Darancet, •Maria Chan
O 72.1	Wed	13:30–14:00	R2	**On the survival of Floquet-Bloch states in the presence of scattering** — •Isabella Gierz
O 72.4	Wed	14:30–15:00	R2	**Light-induced anomalous Hall effect in graphene** — •James McIver
O 73.1	Wed	13:30–14:00	R3	**Theoretical insights into Dzyaloshinskii-Moriya interaction in nanostructures based on transition metals, oxides and 2D materials** — •Mairbek Chshiev
O 73.4	Wed	14:40–15:30	R3	**Dzyaloshinskii-Moriya Interaction in magnetic layered systems** — •Albert Fert
O 86.1	Thu	10:30–11:00	R1	**Machine learning for robotic nanofabrication with molecules** — •Christian Wagner
O 86.2	Thu	11:00–11:30	R1	**Chemisorbed or Physisorbed? Resolving surface adsorption with Bayesian inference and atomic force microscopy** — •Milica Todorović
O 87.1	Thu	10:35–11:30	R2	**In-Situ Thin Film Nanoscale Hydrogenography in Magnesium Plasmonics** — •Harald Giessen, Julian Karst, Florian Sterl, Heiko Linnenbank, Mario Hentschel
O 100.1	Thu	13:30–14:15	R2	**Broad spectral tuning of ultra-low-loss polaritons in a van der Waals crystal by intercalation** — •Pablo Alonso-González
O 100.4	Thu	14:45–15:30	R2	**Nanocavities and polaritons in twisted and indirectly nanostructured 2D materials** — •Frank Koppens

Sessions

O 1	Mon	9:45–10:00	R1	**Opening Remarks**
O 2.1–2.1	Mon	10:00–10:30	R1	**Key Note I**
O 3.1–3.5	Mon	10:30–12:30	R1	**Mini-Symposium: Ultrafast surface dynamics at the space-time limit I**
O 4.1–4.6	Mon	10:30–12:30	R2	**Mini-Symposium: Free-standing functional molecular 2D materials I**
O 5.1–5.8	Mon	10:30–12:30	P	**Poster Session I: Metal substrates I**
O 6.1–6.9	Mon	10:30–12:30	P	**Poster Session I: Organic molecules on inorganic substrates: Adsorption and growth I**

O 7.1–7.6	Mon	10:30–12:30	P	**Poster Session I: Heterogeneous catalysis I**
O 8.1–8.9	Mon	10:30–12:30	P	**Poster Session I: Solid-liquid interfaces: Structure, spectroscopy**
O 9.1–9.5	Mon	10:30–12:30	P	**Poster Session I: New methods I**
O 10.1–10.5	Mon	10:30–12:30	P	**Poster Session I: Topological insulators**
O 11.1–11.8	Mon	10:30–12:30	P	**Poster Session I: Plasmonics and nanooptics I**
O 12.1–12.7	Mon	10:30–12:30	P	**Poster Session I: Electronic structure theory: General**
O 13.1–13.8	Mon	10:30–12:30	P	**Poster Session I: Surface magnetism I**
O 14.1–14.9	Mon	10:30–12:30	P	**Poster Session I: Nanostructures at surfaces I**
O 15.1–15.5	Mon	13:30–15:30	R1	**Mini-Symposium: Ultrafast surface dynamics at the space-time limit II**
O 16.1–16.5	Mon	13:30–15:30	R2	**Mini-Symposium: Free-standing functional molecular 2D materials II**
O 17.1–17.4	Mon	13:30–15:30	R3	**Mini-Symposium: Frontiers of electronic-structure theory: Focus on electron-phonon interactions I**
O 18.1–18.8	Mon	13:30–15:30	P	**Poster Session II: Metal substrates II**
O 19.1–19.9	Mon	13:30–15:30	P	**Poster Session II: Organic molecules on inorganic substrates: Adsorption and growth II**
O 20.1–20.5	Mon	13:30–15:30	P	**Poster Session II: Heterogeneous catalysis II**
O 21.1–21.8	Mon	13:30–15:30	P	**Poster Session II: Solid-liquid interfaces: Reactions and electrochemistry I**
O 22.1–22.6	Mon	13:30–15:30	P	**Poster Session II: New methods II**
O 23.1–23.5	Mon	13:30–15:30	P	**Poster Session II: Topology and symmetry-protected materials**
O 24.1–24.7	Mon	13:30–15:30	P	**Poster Session II: Plasmonics and nanooptics II**
O 25.1–25.8	Mon	13:30–15:30	P	**Poster Session II: Surface magnetism II**
O 26.1–26.8	Mon	13:30–15:30	P	**Poster Session II: Nanostructures at surfaces II**
O 27.1–27.4	Mon	13:30–15:30	P	**Poster Session II: Poster to Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces I**
O 28.1–28.1	Mon	15:30–16:00	R1	**Key Note II**
O 29.1–29.1	Tue	10:00–10:30	R1	**Key Note III**
O 30.1–30.5	Tue	10:30–12:30	R1	**Mini-Symposium: Electrified solid-liquid interfaces I**
O 31.1–31.5	Tue	10:30–12:30	R2	**Mini-Symposium: Manipulation and control of spins on functional surfaces I**
O 32	Tue	10:30–12:30	R3	**Mini-Symposium: Frontiers of electronic-structure theory: Focus on electron-phonon interactions II**
O 33.1–33.6	Tue	10:30–12:30	P	**Poster Session III: Semiconductor substrates I**
O 34.1–34.9	Tue	10:30–12:30	P	**Poster Session III: Organic molecules on inorganic substrates: Adsorption and growth III**
O 35.1–35.5	Tue	10:30–12:30	P	**Poster Session III: Surface dynamics I: Phase transitions and elementary processes**
O 36.1–36.7	Tue	10:30–12:30	P	**Poster Session III: Electronic structure of surfaces: Spectroscopy, surface states I**
O 37.1–37.7	Tue	10:30–12:30	P	**Poster Session III: Surface magnetism III**
O 38.1–38.4	Tue	10:30–12:30	P	**Poster Session III: Tribology: Surfaces and nanostructures I**
O 39.1–39.6	Tue	10:30–12:30	P	**Poster Session III: Poster to Mini-Symposium: Free-standing functional molecular 2D materials I**
O 40.1–40.6	Tue	10:30–12:30	P	**Poster Session III: Poster to Mini-Symposium: Infrared nano-optics I**
O 41.1–41.4	Tue	10:30–12:30	P	**Poster Session III: Poster to Mini-Symposium: Ultrafast surface dynamics at the space-time limit I**
O 42.1–42.9	Tue	10:30–12:30	P	**Poster Session III: Poster to Mini-Symposium: Machine learning applications in surface science I**
O 43.1–43.3	Tue	13:30–15:30	R1	**Mini-Symposium: Electrified solid-liquid interfaces II**
O 44.1–44.4	Tue	13:30–15:30	R2	**Mini-Symposium: Manipulation and control of spins on functional surfaces II**
O 45.1–45.5	Tue	13:30–15:30	R3	**Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces I**
O 46.1–46.5	Tue	13:30–15:30	P	**Poster Session IV: Semiconductor substrates II**
O 47.1–47.5	Tue	13:30–15:30	P	**Poster Session IV: Organic molecules on inorganic substrates: networks and overlayers**
O 48.1–48.5	Tue	13:30–15:30	P	**Poster Session IV: Surface dynamics II: Phase transitions and elementary processes**
O 49.1–49.6	Tue	13:30–15:30	P	**Poster Session IV: Electronic structure of surfaces: Spectroscopy, surface states II**
O 50.1–50.3	Tue	13:30–15:30	P	**Poster Session IV: Tribology: Surfaces and nanostructures II**
O 51.1–51.4	Tue	13:30–15:30	P	**Poster Session IV: Poster to Mini-Symposium: Free-standing functional molecular 2D materials II**
O 52.1–52.5	Tue	13:30–15:30	P	**Poster Session IV: Poster to Mini-Symposium: Infrared nano-optics II**
O 53.1–53.7	Tue	13:30–15:30	P	**Poster Session IV: Poster to Mini-Symposium: Frontiers of electronic-structure theory I**
O 54.1–54.4	Tue	13:30–15:30	P	**Poster Session IV: Poster to Mini-Symposium: Ultrafast surface dynamics at the space-time limit II**
O 55.1–55.8	Tue	13:30–15:30	P	**Poster Session IV: Poster to Mini-Symposium: Machine learning applications in surface science II**

O 56.1–56.1	Tue	15:30–16:00	R1	**Key Note IV**
O 57.1–57.1	Wed	10:00–10:30	R1	**Key Note V**
O 58.1–58.5	Wed	10:30–12:30	R1	**Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces II**
O 59.1–59.6	Wed	10:30–12:30	R2	**Mini-Symposium: Coherent band structure engineering with light I**
O 60.1–60.4	Wed	10:30–12:30	R3	**Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems I**
O 61.1–61.9	Wed	10:30–12:30	P	**Poster Session V: Oxide and insulator surfaces: Structure, epitaxy and growth I**
O 62.1–62.9	Wed	10:30–12:30	P	**Poster Session V: Organic molecules on inorganic substrates: electronic, optical and other properties I**
O 63.1–63.5	Wed	10:30–12:30	P	**Poster Session V: Electron-driven processes at surfaces and interfaces**
O 64.1–64.6	Wed	10:30–12:30	P	**Poster Session V: Electronic structure of surfaces: Spectroscopy, surface states III**
O 65.1–65.7	Wed	10:30–12:30	P	**Poster Session V: Solid-liquid interfaces: Reactions and electrochemistry II**
O 66.1–66.13	Wed	10:30–12:30	P	**Poster Session V: 2D Materials: Electronic structure, excitations, etc. I**
O 67.1–67.7	Wed	10:30–12:30	P	**Poster Session V: Ultrafast electron dynamics at surface and interfaces I**
O 68.1–68.7	Wed	10:30–12:30	P	**Poster Session V: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces I**
O 69.1–69.4	Wed	10:30–12:30	P	**Poster Session V: Poster to Mini-Symposium: Infrared nano-optics III**
O 70.1–70.7	Wed	10:30–12:30	P	**Poster Session V: Poster to Mini-Symposium: Frontiers of electronic-structure theory II**
O 71.1–71.5	Wed	13:30–15:30	R1	**Mini-Symposium: Machine learning applications in surface science I**
O 72.1–72.5	Wed	13:30–15:30	R2	**Mini-Symposium: Coherent band structure engineering with light II**
O 73.1–73.4	Wed	13:30–15:30	R3	**Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems II**
O 74.1–74.8	Wed	13:30–15:30	P	**Poster Session VI: Oxide and insulator surfaces: Structure, epitaxy and growth II**
O 75.1–75.8	Wed	13:30–15:30	P	**Poster Session VI: Organic molecules on inorganic substrates: electronic, optical and other properties II**
O 76.1–76.5	Wed	13:30–15:30	P	**Poster Session VI: Supported nanoclusters: structure, reactions, catalysis**
O 77.1–77.6	Wed	13:30–15:30	P	**Poster Session VI: Scanning probe techniques: Method development I**
O 78.1–78.14	Wed	13:30–15:30	P	**Poster Session VI: 2D Materials: Electronic structure, excitations, etc. II**
O 79.1–79.7	Wed	13:30–15:30	P	**Poster Session VI: Ultrafast electron dynamics at surface and interfaces II**
O 80.1–80.7	Wed	13:30–15:30	P	**Poster Session VI: Poster to Mini-Symposium: Electrified solid-liquid interfaces I**
O 81.1–81.7	Wed	13:30–15:30	P	**Poster Session VI: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces II**
O 82.1–82.7	Wed	13:30–15:30	P	**Poster Session VI: Poster to Mini-Symposium: Frontiers of electronic-structure theory III**
O 83.1–83.3	Wed	13:30–15:30	P	**Poster Session VI: Poster to Mini-Symposium: Infrared nano-optics IV**
O 84.1–84.1	Wed	15:30–16:00	R1	**Key Note VI**
O 85.1–85.1	Thu	10:00–10:30	R1	**Key Note VII**
O 86.1–86.6	Thu	10:30–12:30	R1	**Mini-Symposium: Machine learning applications in surface science II**
O 87.1–87.5	Thu	10:30–12:30	R2	**Mini-Symposium: Infrared nano-optics I**
O 88.1–88.8	Thu	10:30–12:30	P	**Poster Session VII: Oxides and insulators: Adsorption and reaction of small molecules I**
O 89.1–89.7	Thu	10:30–12:30	P	**Poster Session VII: Organic molecules on inorganic substrates: electronic, optical and other properties III**
O 90.1–90.8	Thu	10:30–12:30	P	**Poster Session VII: Surface reactions I**
O 91.1–91.7	Thu	10:30–12:30	P	**Poster Session VII: Scanning probe techniques: Method development II**
O 92.1–92.6	Thu	10:30–12:30	P	**Poster Session VII: Ultrafast electron dynamics at surface and interfaces III**
O 93.1–93.14	Thu	10:30–12:30	P	**Poster Session VII: Graphene and beyond I**
O 94.1–94.8	Thu	10:30–12:30	P	**Poster Session VII: Poster to Mini-Symposium: Electrified solid-liquid interfaces II**
O 95.1–95.6	Thu	10:30–12:30	P	**Poster Session VII: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces III**
O 96.1–96.7	Thu	10:30–12:30	P	**Poster Session VII: Poster to Mini-Symposium: Frontiers of electronic-structure theory IV**
O 97.1–97.4	Thu	10:30–12:30	P	**Poster Session VII: Poster to Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces II**
O 98	Thu	13:00–13:30	R1	**Annual Meeting of the Surface Science Division**
O 99.1–99.4	Thu	13:30–15:30	R1	**Gerhard Ertl Young Investigator Award: Finalists session**
O 100.1–100.4	Thu	13:30–15:30	R2	**Mini-Symposium: Infrared nano-optics II**
O 101.1–101.8	Thu	13:30–15:30	P	**Poster Session VIII: Oxides and insulators: Adsorption and reaction of small molecules II**
O 102.1–102.8	Thu	13:30–15:30	P	**Poster Session VIII: Organic molecules on inorganic substrates: electronic, optical and other properties IV**

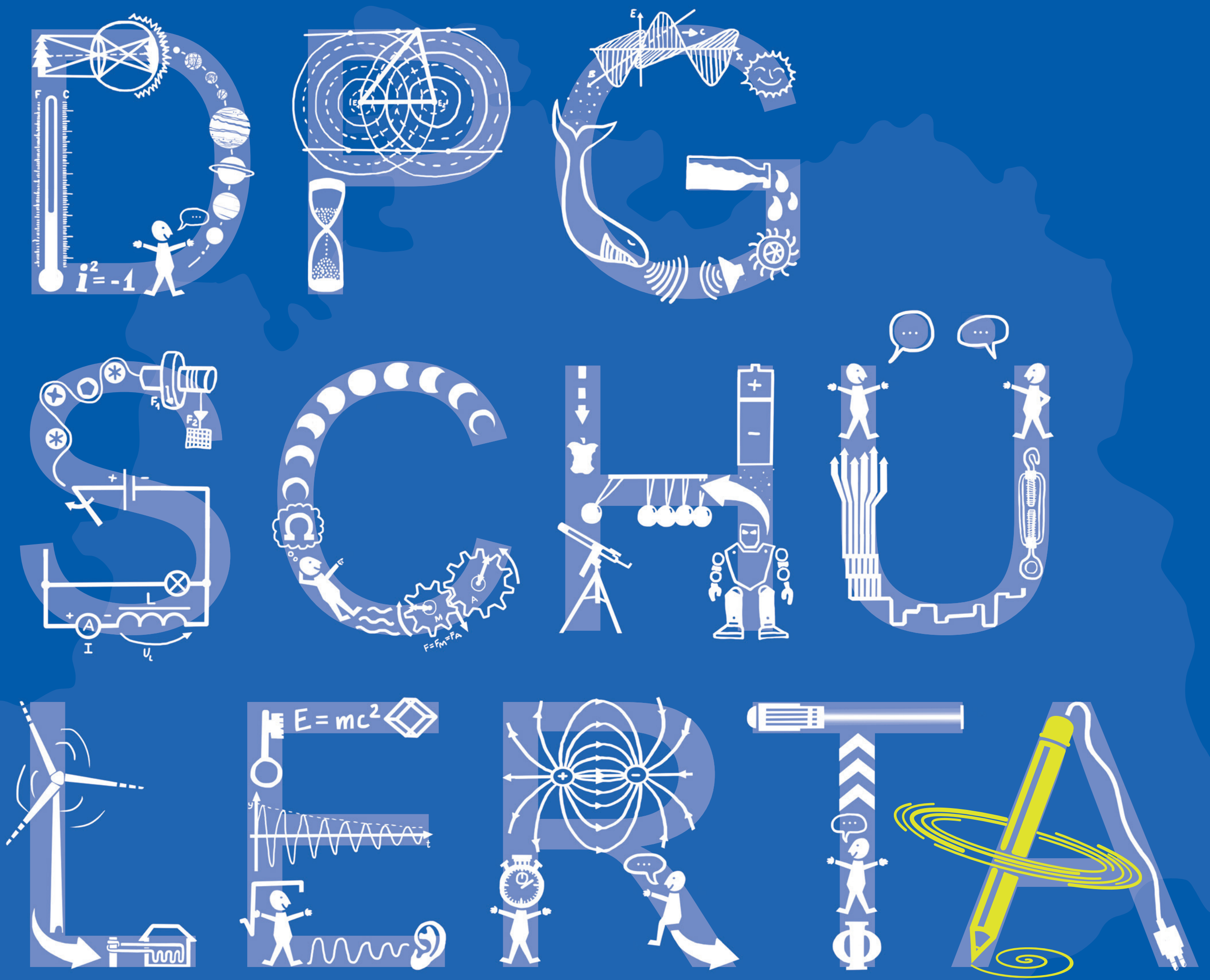
O 103.1–103.7	Thu	13:30–15:30	P	**Poster Session VIII: Surface reactions II**
O 104.1–104.6	Thu	13:30–15:30	P	**Poster Session VIII: Scanning probe techniques: Method development III**
O 105.1–105.13	Thu	13:30–15:30	P	**Poster Session VIII: Graphene and beyond II**
O 106.1–106.7	Thu	13:30–15:30	P	**Poster Session VIII: Poster to Mini-Symposium: Electrified solid-liquid interfaces III**
O 107.1–107.7	Thu	13:30–15:30	P	**Poster Session VIII: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces IV**
O 108.1–108.6	Thu	13:30–15:30	P	**Poster Session VIII: Poster to Mini-Symposium: Frontiers of electronic-structure theory V**
O 109.1–109.8	Thu	13:30–15:30	P	**Poster Session VIII: Poster to Mini-Symposium: Machine learning applications in surface science III**
O 110.1–110.5	Thu	13:30–15:30	P	**Poster Session VIII: Poster to Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems**
O 111.1–111.1	Thu	15:30–16:00	R1	**Key Note VIII**
O 112	Thu	16:00–16:15	R1	**Announcement of Gerhard Ertl Young Investigator Award and Concluding Remarks**

Annual General Meeting of the Surface Science Division

Thursday 13:00–13:30

Deutsche Physikalische Gesellschaft Φ DPG

2021



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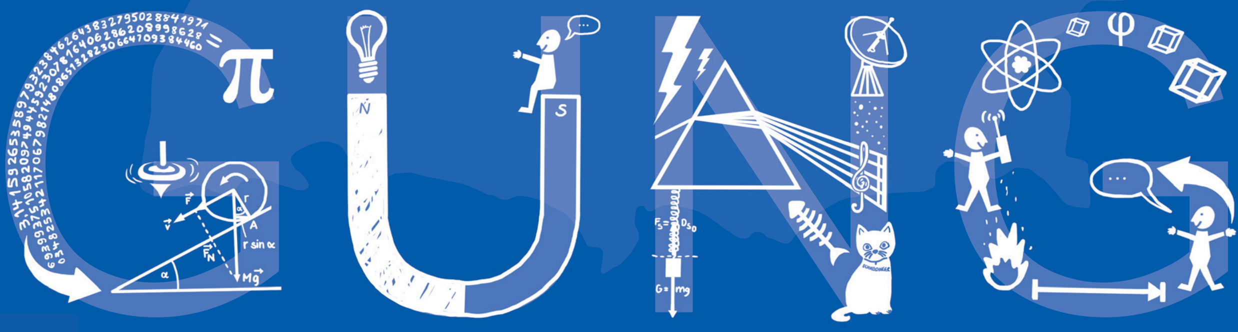

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Sessions

– Plenary Talks, Invited Talks, Paper Discussions, Contributed Talks, and Posters –

O 1: Opening Remarks

Time: Monday 9:45–10:00 Location: R1

Karsten Reuter, Fritz-Haber-Institut der MPG, Chair Surface Science Division

O 2: Key Note I

Time: Monday 10:00–10:30 Location: R1

Plenary Talk O 2.1 Mon 10:00 R1

Chasing excited electrons in energy, momentum space, and time — •Martin Aeschlimann — University of Kaiserslautern (TUK) and Research Center OPTIMAS, Erwin-Schroedinger-Str. 46, 67663 Kaiserslautern, Germany

Optically excited (hot) electrons play a crucial role for many fundamental chemical and physical processes occurring at surfaces, interfaces, and in bulk materials. Despite decades of intense research, however, a complete picture of the hot electrons dynamic in its collective environment is still elusive. In this presentation, I will demonstrate how the latest developments in ultrafast light sources and photoemission detector technology have paved the way towards a completely new generation of time-resolved photoemission experiment based on time-, (and spin-) resolved momentum microscopy [1,2]. With this tool at hand, we can directly watch the temporal evolution of excited carriers in energy, momentum space, and time, which provides an unprecedented view onto the fundamental energy-, and (angular-) momentum-dissipation mechanisms in condensed matter. As exemplary cases, I will focus on the excited state dynamics of low dimensional materials and metal-molecular hybrid systems [3].

[1] B. Yan et al; Nature Communications 6, 10167 (2015)
[2] F. Haag et al, Rev. Sci. Instrum., 90 ,103104 (2019)
[3] F. Haag et al, arXiv:2101.03567 (2020)

O 3: Mini-Symposium: Ultrafast surface dynamics at the space-time limit I

Time: Monday 10:30–12:30 Location: R1

Invited Talk O 3.1 Mon 10:30 R1

Actuating and probing a single-molecule switch at femtosecond timescales — Dominik Peller, Carmen Roelcke, Lukas Z. Kastner, Thomas Buchner, Alexander Neef, Johannes Hayes, Florian Albrecht, Rupert Huber, and •Jascha Repp — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

Combining scanning tunneling microscopy (STM) with lightwave electronics [1] has enabled the simultaneous femtosecond and sub-angstrom resolution in observing matter [2]. We now demonstrate the combined femtosecond and sub-angstrom access in the control of matter. Ultrafast localized electric fields in lightwave STM enable exerting atom-scale femtosecond forces to selected atoms. Utilizing these forces to excite coherent structural dynamics, we can modulate the quantum transitions of a single-molecule switch by up to 39% [3]. Further, we exploit the same single-molecule switch to quantitatively resolve the electromagnetic waveform of the tip-confined near-field transients directly inside the tunneling junction at atomic scales [4].

[1] T. L. Cocker et al., Nature Photon. 7, 620 (2013).
[2] T. L. Cocker et al., Nature 539, 263 (2016).
[3] D. Peller et al., Nature 585, 58 (2020).
[4] D. Peller et al., Nature Photonics (2020).

Invited Talk O 3.2 Mon 11:00 R1

Real space-time imaging of valence electron motion in molecules — •Manish Garg — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Chemical transformations in molecules are a consequence of valence electron motion and its eventual coupling to atomic motion, hence, tracking valence electron motion at the orbital level is the key to understanding and taming such transformations. Scanning tunnelling microscopy (STM) can passively and locally probe the valence electron density in molecules. Contemporary techniques in attosecond science, on the other hand, can generate and track the temporal evolution of a coherent superposition of quantum states of valence electrons by using strong laser fields, which can be probed only non-locally. In absence of the capability to trigger and probe electron dynamics at the single-orbital level, electron motion could only be inferred by reconstruction. Here, we demonstrate that the dynamics of coherent superposition of valence electron states generated by < 6 femtosecond long carrier-envelope-phase (CEP) stable laser pulses, can be locally probed with picometer spatial resolution and 300 attosecond temporal resolution simultaneously, at the single orbital-level with the help of an STM, defying the previously established fundamental space-time limit. We show that near fields of optical pulses confined to the apex of nanotip of an STM enable orbital imaging of electronic levels of molecules with pm resolution. We envisage that it will be possible to see a chemical bond formation dynamics through a transition state at the orbital level in the near future.

Invited Talk O 3.3 Mon 11:15 R1

Ultrafast structural phase transitions probed by low-energy electron diffraction — •Claus Ropers — IV. Phys. Inst., Göttingen, Germany — MPI for biophysical Chemistry

Governed by broken symmetries and an effectively reduced dimensionality, surfaces exhibit a multitude of complex phases and transitions, with prominent examples in metal-to-insulator lattice instabilities. Ultrafast measurement technology has greatly improved our understanding of the formation and non-equilibrium response of such phases, revealing transition pathways and means of optical control.

Despite these advancements, tracking the rapid structural evolution of surfaces has remained challenging. Low-energy electron diffraction (LEED) is an ideal tool to characterize the structure, symmetries and long-range order at surfaces, but it typically lacks ultrafast temporal resolution.

This talk will present the development and first applications of Ultrafast LEED, combining short-pulsed probing with ultimate surface sensitivity. I will give some methodical background on its implementation and will discuss results on optically induced structural phase transitions in charge-density wave systems [1,2].

[1] "Structural dynamics of incommensurate charge-density waves tracked by ultrafast low-energy electron diffraction" G. Storeck et al., Struct. Dyn. 7, 034304 (2020).

[2] "Coherent control of a surface structural phase transition", J.G. Horstmann et al., Nature 583, 232 (2020).

Invited Talk O 3.4 Mon 11:45 R1

Probing the ultrafast electron dynamics in the quantum spin Hall system Bismuthene with time-resolved ARPES — •Julian Maklar[1], Raul Stühler[2], Maciej Dendzik[1,3], Tommaso Pincelli[1], Shuo Dong[1], Samuel Beaulieu[1], Martin Wolf[1], Ralph Ernstorfer[1], Ralph Claessen[2], and Laurenz Rettig[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany — [2]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, D-97070 Würzburg, Germany — [3]Department of Applied Physics, KTH Royal Institute of Technology, Stockholm, Sweden

Quantum spin Hall (QSH) systems are 2D topological insulators with promising device applications due to dissipationless, symmetry-protected spin currents in their edges. A promising high-temperature QSH material is Bismuthene – a 2D honeycomb lattice of bismuth atoms on a silicon carbide substrate – which features a wide bulk band gap and conductive 1D edge states located at substrate steps and domain boundaries.

Here, we investigate the electronic structure of Bismuthene upon ultrafast photoexcitation via time- and angle-resolved photoemission spectroscopy (trARPES). We map out the transiently occupied excited states in the conduction band and additionally observe faint spectral weight within the indirect band gap, which we attribute to metallic edge states. In addition, we observe a surprisingly fast recovery of excited carriers to the ground state – a further hint towards the presence of topological metallic decay channels.

Invited Talk O 3.5 Mon 12:00 R1

Atomic-resolution imaging of THz-driven dynamics on charge-ordered surfaces — •Sebastian Loth — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, 70569 Stuttgart — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

Charge order in correlated-electron materials is intimately linked to fluctuations of charge density that occur at nanometer length scales and at ultrafast speed. Such localized fluctuations are not a simple perturbation but can be the determining factor for the dynamics of phase transitions and the macroscopic response of the electron system. While these fluctuations often remain hidden to ensemble-averaged measurements, the combination of ultrafast THz spectroscopy and scanning tunneling microscopy can both locally excite and probe dynamics with atomic spatial and femtosecond temporal resolution [1]. For the quasi two-dimensional charge density wave state in niobium diselenide we find that the tip-enhanced electric field of the THz pulses excites the sample directly by driving a strong in-plane displacement current in the surface. This leads to a distortion of the charge-density wave in the vicinity of atomic pinning sites that relaxes by emitting a complex pattern of amplitude and phase excitations rather than a uniform collective response. Resolving these fluctuations in real space at the scale of individual impurities provides a new route to unraveling the electronic dynamics of disordered correlated materials.

[1] T. L. Cocker et al., Nature Photon. 7, 620 (2013). & T. L. Cocker et al., Nature 539, 263 (2016).

O 4: Mini-Symposium: Free-standing functional molecular 2D materials I

Time: Monday 10:30–12:30 Location: R2

Invited Talk O 4.1 Mon 10:30 R2

Ion permeation across atomically thin materials — •Marcelo Lozada-Hidalgo — Department of Physics and Astronomy, The University of Manchester

The basal plane of graphene is impermeable to all atoms and molecules - even for helium, the smallest - at ambient conditions. On this basis, it was believed that graphene would be impermeable even to protons, the nuclei of hydrogen atoms. Unexpectedly, we found that graphene is highly permeable to these ions at ambient conditions. Since these early experiments, our research has established that permeation through 2D crystals can be fundamentally different from that in bulk materials. Even basic notions like bulk 3D resistivity need to be considered carefully. Many fundamental questions remain open even for graphene, the most researched of theses crystals - and the vast majority of these materials remain unexplored from this perspective. This talk will provide an overview of this new field of research and discuss some of the recent developments involving new 2D materials.

O 4.2 Mon 11:00 R2

Ultrahigh ionic exclusion through 1-nm-thick carbon nanomembranes — •Yang Yang[1,2], Roland Hillmann[1], Yubo Qi[1], Riko Korzetz[1], Niklas Biere[1], Daniel Emmrich[1], Michael Westphal[1], Björn Büker[1], Andreas Hütten[1], André Beyer[1], Dario Anselmetti[1], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, Germany — [2]Department of Chemical Engineering, Imperial College London, UK

The "single-file" transport of water in natural nanoconduits (i.e., aquaporins) inspires the development of high-performance artificial membranes for water purification. In particular, 2D materials open a path to new filtration processes. However, a key challenge has been finding an effective way to create a large number of narrow channels in the material to realize the desired high water permeance and high ion rejection. Carbon Nanomembranes (CNMs) are 2D carbon sheets fabricated from crosslinking of self-assembled monolayers. This work will show that a ~1.2 nm thick CNM made of terphenylthiol (TPT) precursors possesses a very high density (~10^18 m^2, i.e., 1 sub-nm pore per square nanometer) of sub-nm channels. TPT CNMs let water pass very quickly, but hinder the passing of ions including protons. The membrane resistance in 1 M chloride solutions reaches ~104 Ω cm^2, comparably high to that of lipid bilayers. TPT CNMs show a ~80 times enhancement in water productivity over the commercial forward osmosis membranes. These observations encourage the use of CNMs for producing clean water. The versatile manufacturing process also enables CNM functions to be customized at a molecular level.

O 4.3 Mon 11:15 R2

Atomic-scale carving of nanopores into a van-der-Waals heterostructure with slow highly charged ions — Janine Schwestka[1], Heena Inani[2], Mukesh Tripathi[2], Anna Niggas[1], Niall McEvoy[3], Florian Libisch[4], Friedrich Aumayr[1], Jani Kotakoski[2], and •Richard Wilhelm[1] — [1]TU Wien, Institute of Applied Physics — [2]University Vienna, Faculty of Physics — [3]Trinity College Dublin, AMBER School of Chemistry — [4]TU Wien, Institute for Theoretical Physics

Tailoring the mechanical, electronic and chemical properties of functional 2D materials post-growth demands methods with highest surface sensitivity. Especially in van-der-Waals (vdW) heterostructures a method which only modifies a particular layer in the layer stack is highly beneficial. Here we report on nanoscale perforation of a MoS_2 layer on-top of a single layer of graphene by irradiation with individual slow highly charged ions. While we can perforate the MoS_2 layer with a high efficiency, the graphene stays intact. Even more so, when changing the layer order, the graphene facing the ion beam shields the MoS_2 from damage and the entire vdW heterostructure remains intact. While this monolayer sensitivity is based on different susceptibilities of metals and semiconductors to highly charged ion induced potential sputtering, up to three layers of MoS_2 on-top of graphene also show perforation only in the topmost 1-2 layers. Hence, even a susceptible material can be perforated with monolayer precision. The mechanism of extreme surface sensitive energy deposition is discussed.

Invited Talk O 4.4 Mon 11:30 R2

Macroscopic Two-Dimensional Polymers: Synthesis and Structure Control — •Zhikun Zheng — Key Laboratory for Polymeric Composite and Functional Materials of Ministry of Education, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, P. R. China

At present, one of the key challenges faced by the scientific community is to go beyond graphene, a prototypical two-dimensional polymer (2DP, a laterally infinite, one atom- or monomer-unit thin, free-standing network with long-range order along two orthogonal directions), to synthesize its analogues with structural control at the atomic- or molecular- level under mild conditions. Here we present the rational synthesis of monolayer and multilayer 2DPs at an air-water interface. Such 2DPs are highly crystalline with controlled aggregate structure and microstructure and tunable single-crystal domain size in the range of tens of nanometers to several micrometers. They have a tunable thickness ranges from 0.7 nm to around 1μm and a lateral size up to 4-inch wafer, and can be freely suspended over 40 μm * 40 μm sized holes. They are rigid and flexible, and can be conformed and bonded robustly to nearly any surface, facilitating their integration with target supports or into devices for the extraction of properties. On the basis of the elucidation of their molecular structures, near atomic structures, grain boundaries and edge structures, some preliminary structure-property relationships of the 2DPs were obtained.

O 4.5 Mon 12:00 R2

Low-energy electron irradiation induced synthesis of molecular nanosheets: Influence of the electron beam energy — •Christof Neumann[1], Richard A. Wilhelm[2,3], Maria Küllmer[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Aromatic self-assembled monolayers (SAMs) can be cross-linked into molecular nanosheets - carbon nanomembranes (CNMs) - via low-energy electron irradiation. Due to their favorable mechanical stability and tunable functional properties, they possess a high potential for various applications including nanosensors and separation membranes. Here, we studied the cross-linking of 4'-nitro-1,1'-biphenyl-4-thiol SAM on gold. The SAM samples were irradiated with different electron energies ranging from 2.5 to 100 eV in ultra-high vacuum and subsequently analysed by complementary techniques including X-ray photoelectron spectroscopy (XPS). To demonstrate the formation of CNMs, the formed two-dimensional molecular materials were transferred onto grids and oxidized wafer and analyzed by different microscopy techniques. We found a strong energy dependence for the cross section for the cross-linking process and conducted a comparative analysis of the cross sections for the C-H bond scission via electron impact ionization and dissociative electron attachment. C. Neumann et al., Faraday Discuss. 2020 DOI: 10.1039/C9FD00119K

O 4.6 Mon 12:15 R2

On-surface synthesis of nonbenzenoid planar carbon allotropes — •Qitang Fan[1], Linghao Yan[2], Daniel Martin-Jimenez[3], Daniel Ebeling[3], Matthias W. Tripp[1], Ondřej Krejčí[2], Stefan R. Kachel[1], Claudio K. Krug[1], Adam S. Foster[2], Ulrich Koert[1], André Schirmeisen[3], Peter Liljeroth[2], and J. Michael Gottfried[1] — [1]Department of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany — [2]Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland — [3]Institute of Applied Physics (IAP), Justus Liebig University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

The quest for new carbon allotropes with unusual properties persistently intrigues scientists from various fields. However, the challenge of synthetic carbon allotropes still remains in the limited protocols for their controlled bottom-up construction. To date, no planar sp^2 carbon allotropes other than graphene have been achieved. Here, we show the bottom-up growth of sheets of monoatomically-thick nonbenzenoid carbon allotropes via an Ullmann-type coupling followed by dehydrogenative/dehydrofluorinative C-C coupling reactions on metal surfaces. Such carbon allotropes consist of periodically arrayed non-hexagonal rings of sp^2 carbon atoms, exhibiting electronic properties contrasting those of the benzenoid graphene. We expect that our surface-science based strategy will enrich the bottom-up toolbox for the synthesis of other planar carbon allotropes.

O 5: Poster Session I: Metal substrates I

Time: Monday 10:30–12:30 Location: P

O 5.1 Mon 10:30 P

Multi-method study of trans-DBPen on coinage metal (111)-surfaces — •Felix Otto, Maximilian Schaal, Tobias Huempfner, Falko Sojka, Marco Gruenewald, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, Jena, Germany

Several polycyclic aromatic hydrocarbons (PAHs) become superconducting after the intercalation of alkali metal atoms. The number of promising candidates has increased in the last few years. Among them, $K_{3.45}$1,2:8,9-dibenzopentacene (trans-DBPen, $C_{30}H_{18}$) is the one with the highest critical temperature reported so far. Nevertheless, the microscopic mechanisms of superconductivity in K-doped PAHs are still under debate. One open question is, for example, the effect of structural order in bulk materials as well as two-dimensional layers.

Our work deals with the growth of trans-DBPen on Ag(111), Au(111), and Cu(111) in the monolayer (ML) regime. The self-assembled thin films were prepared using organic molecular beam epitaxy. The structure was characterized by means of low energy electron diffraction (LEED). In the sub-ML range, we observe a 2D gas-like behavior, whereas the first MLs on the different substrates are characterized by highly ordered structures. Photoelectron spectroscopy (PES) including photoelectron momentum maps (PMMs) was used to study the interaction of the molecules with the substrate as well as the influence of the second ML on the electronic structure. The investigated systems exhibit notable differences according to the different interaction strengths with the substrate.

O 5.2 Mon 10:30 P

Scanning tunneling microscopy study of submonolayer growth of Mn_xAu_{1-x} on Cu(001) — •Ismet Gelen[1], Tauqir Shinwari[1], Yasser A. Shokr[1,2], Evangelos Golias[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

Mn_xAu_{1-x} exhibits many antiferromagnetic (AFM) phases. Mn_2Au is one of them that has a high Néel temperature ($\approx$ 1600 K) and, due to its noncentrosymmetric spin structure and metallic nature, is an interesting AFM material for spintronic applications. Here, we study the growth of Mn_xAu_{1-x} in the submonolayer (sub-ML) regime on Cu(001) by medium- and low-energy electron diffraction (MEED, LEED), Auger electron spectroscopy (AES), and scanning tunneling microscopy (STM). Different Mn concentrations ($x \approx 0.7 - 0.9$) and different thicknesses ($\approx 0.2 - 1.1$ ML) were studied, as monitored by AES. Mn and Au were coevaporated by electron bombardment on Cu(001) at room temperature (RT). The growth of thicker films showed MEED intensity oscillations up to around 9 ML. The LEED images display substrate patterns for thicknesses < 0.5 ML, while they display a $c(2 \times 2)$ structure for thicker sub-ML films. We observe Mn_xAu_{1-x} islands on Cu(001) for all sub-ML films with island sizes between $\approx 5 \times 5$ and 30×30 nm^2.

O 5.3 Mon 10:30 P

Submonolayer growth of Te on Cu(111) — •Tilman Kisslinger, Andreas Raabgrund, Maximilian Ammon, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

Tellurium (Te) based alloys play an important role in metallurgy, thermoelectricity and photovoltaics [1]. Thus, an accurate knowledge of the crystallographic surface structure and elemental composition of such systems is the first step to any understanding of their diverse physical properties. We studied the adsorption of Te on Cu(111) for submonolayer coverages with quantitative low-energy-electron diffraction (LEED), scanning tunneling microscopy (STM) and density-functional theory (DFT).

Below Θ =1/12 ML we find Te atoms to form a disordered structure. Above this threshold a $(2\sqrt{3} \times \sqrt{3})R30^\circ$ structure evolves that is fully developed at a coverage of 1/3 ML. STM shows a well-ordered surface phase that is solved by our LEED-analysis (Δ E = 8.9 keV, R = 0.099) to consist of Te_2Cu_2 chains in hcp-sites of the first substrate layer in perfect agreement with the structure calculated by DFT [2].

[1]: Ibers J., Nat. Chem. **1**, 508 (2009)

[2]: Kisslinger T., Phys. Rev. B. **102**, 155422 (2020)

O 5.4 Mon 10:30 P

Inducing and Probing the Rotational Motion of a Single Carbon Monoxide Molecule — •Nicolas Néel and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The control and observation of reactants forming a chemical bond at the single-molecule level is a longstanding challenge in quantum physics and chemistry. Using a single CO molecule adsorbed at the apex of an atomic force microscope tip and a Cu(111) surface at bonding distances, the molecular rotational motion is induced by torques due to van der Waals attraction and Pauli repulsion. As a result, the vertical force exhibits a characteristic dip-hump evolution with the molecule-surface separation, which depends sensitively on the initial tilt angle the CO axis encloses with the microscope tip. The experimental force data are reproduced by model calculations that consider the CO rotational motion in a harmonic potential and the molecular orientation in the Pauli repulsion term of the Lennard-Jones potential.

O 5.5 Mon 10:30 P

First-principles study of the coexistence of a chemisorption and physisorption state of CO on Au(111) — •Svenja M. Janke[1,2] and Reinhard J. Maurer[2] — [1]Institute of Advanced Studies, University of Warwick, Coventry, UK — [2]Department of Chemistry, University of Warwick, Coventry, UK

Accurate representation of the potential energy landscape for a molecule on a metal surface is essential to model energy transfer between the molecule and the surface, but not always straightforward. Recent experiments suggest the presence of a chemisorption and a physisorption state for CO adsorbed on Au(111). Within the all electron electronic structure code FHI-aims, we survey several approximations to Density Functional Theory for their ability to predict the adsorption state of CO on Au(111). In agreement with previous theoretical observations for similar systems, we find that common generalized gradient approximation functionals with van-der-Waals correction lead to overbinding, with the revised Perdew-Burke-Ernzerhof function with van-der-Waals correction coming closest to experimental results. Our results lay the ground work to construct a high-dimensional energy surface to study the nonadiabatic dynamics of carbonyl reactive scattering on Au(111).

O 5.6 Mon 10:30 P

Moving azulene based molecules by STM: The role of dipole moment and field effect — •Tim Kühne[1,2], Kwan Ho Au Yeung[1,2], Frank Eisenhut[1,2], Oumaima Aiboudi[3], Dmitry Ryndyk[2], Gianaurelio Cuniberti[2], Franziska Lissel[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Leibniz Institute of Polymer Research, 01069 Dresden, Germany

Among the different mechanisms that can be used to drive a molecule on a surface by the tip of a scanning tunneling microscope at low temperature, we used voltage pulses to move azulene-based single molecules and nanostructures on Au(111). Upon evaporation, the molecules partially cleave and form metallo-organic dimers while single molecules are very scarce, as confirmed by simulations. By applying voltage pulses to the different structures in similar conditions, we observe that only one type of dimers can be controllably driven on the surface. This has the lowest dipole moment of all investigated structures. Experiments at different bias and tip height conditions reveal that the electric field is the main driving force of the directed motion. We discuss the different observed structures and their movement properties with respect to their dipole moment and charge distribution on the surface.

O 5.7 Mon 10:30 P

LT-STM investigation of transmitting rotation between molecule-gears on Au(111) — •Kwan Ho Au Yeung[1,2], Tim Kühne[1,2], Frank Eisenhut[1,2], Michael Kleinwächter[3], Yohan Gisbert[3], Roberto Robles[4], Nicolas Lorente[4,5], Gianaurelio Cuniberti[2], Christian Joachim[3], Gwénaël Rapenne[3,6], Claire Kammerer[3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany —

[2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]CEMES, Université de Toulouse, CNRS, 31055 Toulouse, France — [4]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [5]Donostia International Physics center, 20018 Donostia-San Sebastian, Spain — [6]Division of Materials Science, Nara Institute of Science and Technology, 8916-5 Takayama, Ikoma, Nara 630-0192, Japan

The realization of a train of molecule-gears working under the tip of a scanning tunneling microscope (STM) requires a stable anchor of each molecule to the surface. Such anchor can be promoted by a radical state of the molecule induced by a dissociation reaction. Our results reveal that such open radical state at the core of star-shaped pentaphenylcyclopentadiene (PPCP) favors the anchoring. Furthermore, to allow the transmission of motion by manipulation, in our case, a tert-butyl group positioned at one tooth end of the gear benefits both the tip-induced manipulation and the monitoring of rotation. With this optimized molecular system, we achieve reproducible rotations of the single gears and transmit rotations up to three interlocked units.

O 5.8 Mon 10:30 P

Fusion of alkyl groups to form phenyl rings: a new on-surface reaction — •Amogh Kinikar[1], Marco Di Giovannantonio[1], Josè Ignacio Urgel[1], Kristjan Eimre[1], Xiao-Ye Wang[2], Zijie Qiu[2], Akimitsu Narita[2], Klaus Müllen[2], Pascal Ruffieux[1], Carlo Antonio Pignedoli[1], and Roman Fasel[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, 8600, Switzerland — [2]Max Planck Institute for Polymer Research, 55128 Mainz (Germany)

On-surface synthesis allows for the design of carbon nanostructures such as graphene nanoribbons with atomic precision. However, the variety of conceivable structures critically depends on the number of available reactions. Here, we present a new surface-assisted reaction allowing for the controlled fusion of two alkyl groups to form a phenyl ring mediated by the activation of alkyl C-H bonds under ultra-high vacuum conditions. Scanning tunneling and non-contact atomic force microscopy images at different stages of the reaction along with DFT simulations allow us to elucidate the reaction mechanism. Furthermore, we study the influence of surface templating by comparing the reaction on Au(111) and Au(110). The selective formation of phenyl rings by the on-surface fusion of alkyl groups is unprecedented, and introduces a powerful new motif for the design of novel carbon nanomaterials while furthering our understanding of the reactive nature of the alkyl C-H bonds.

O 6: Poster Session I: Organic molecules on inorganic substrates: Adsorption and growth I

Time: Monday 10:30–12:30 Location: P

O 6.1 Mon 10:30 P

Graphene as an effective template for tuning the structural and electronic properties of organic-inorganic interfaces — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Controlling the morphological and electronic properties of organic-inorganic interfaces is essential for achieving efficient interface charge injection (or extraction) and transport properties in for example (opto)electronic devices. Here, we present a combined scanning tunneling microscopy and photoelectron spectroscopy study on the adsorption of 5,10,15,20-tetra(4-pyridyl)porphyrin (H2TPyP) on Cu(111) and graphene/Cu(111), respectively. Our experiments showed that for submonolayer coverage, H2TPyP does not form ordered 2D arrangements on Cu(111). Instead, the molecules adsorb randomly and adopt a saddle-shape configuration. However, annealing at 430 K results in short-range, ordered linear and triangular supramolecular arrangements stabilized by Cu-coordination. In contrast, for H2TPyP on graphene/Cu(111) a self-assembled 2D network stabilized by H-bonding forms with unit cell dimensions a = 2.7 nm, b = 1.2 nm and angle = 78°. Furthermore, the work function increases from 3.8 eV for H2TPyP/Cu(111) to 4.1 eV for H2TPyP/graphene/Cu(111), resulting in a considerably different energy level alignment at the hybrid interface. Our experiments demonstrate the feasibility of tuning organic-inorganic interface properties by employing graphene as an intermediate layer.

O 6.2 Mon 10:30 P

An organic electron donor on epitaxial graphene: the role of the metal support — •Joris de la Rie[1], Mihaela Enache[1], Qiankun Wang[1], Wenbo Lu[1], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute for Organic Chemistry, University of Heidelberg, Germany

Graphene has been the first of many 2D materials with excellent electronic properties which make it a material of great interest for future (nano)electronic devices. Implementation of graphene in devices requires interfacing graphene with other materials and tuning of the energy level alignment at the interface. The support on which graphene is placed affects its structural and electronic properties, and further modification is possible through the deposition of thin molecular films which have been shown to modify charge carrier type and concentration. Furthermore, the effect the support has on graphene (corrugation and doping) affects the molecular self-assembly and graphene-molecule interactions. Herein, we compare the self-assembly of an organic triphenylene-based donor (HAT) deposited on graphene on two supports: p doped graphene physisorbed on Ir(111) and n doped graphene chemisorbed on Ni(111). Using scanning tunneling microscopy and low energy electron diffraction we find that on both supports, HAT molecules assemble in a hexagonal network commensurate with the graphene lattice. We used X-ray and ultraviolet photoemission spectroscopy to study modifications of the electronic properties of graphene as well as intermolecular and molecular-graphene interactions.

O 6.3 Mon 10:30 P

Adsorption Behavior of Benzohydroxamic Acid on Rutile TiO_2(110) — •Julia Köbl[1], Elmar Kataev[1], Daniel Wechsler[1], Lisa-Marie Augustin[1], Nataliya Tsud[2], Stefano Franchi[2], Hans-Peter Steinrück[1], and Ole Lytken[1] — [1]University of Erlangen-Nürnberg, Erlangen, Germany — [2]Elettra-Sincrotrone Trieste, Trieste, Italy

Interfaces between organic molecules and oxide surfaces are present in many devices, such as dye-sensitized solar cells and organic field-effect transistors. The organic molecules are often covalently bonded to the oxide surface using specific anchor groups. Using synchrotron-radiation photoelectron spectroscopy, we will focus on how one of these anchor groups, hydroxamic acid, interacts with the rutile TiO_2(110)-(1x1) surface as a function of coverage, temperature, and deposition method. Hydroxamic acid is an interesting anchor group, because it is more stable than carboxylic acid, especially over a wide pH range, and more resistant towards hydrolysis. Benzohydroxamic acid can be evaporated intact in ultrahigh vacuum, and we will compare the behavior of both evaporated and solution-deposited molecules. Supported by the DFG through FOR 1878 (funCOS).

O 6.4 Mon 10:30 P

Chiral Recognition in the Self-Assembly of Trioxa[11]helicene on Metal Surfaces — •Bahaaeddin Irziqat[1], Jan Berger[1,2], Jesús Mendieta-Moreno[2], Mothuku Shyam Sundar[3], Ashutosh V. Bedekar[4], and Karl-Heinz Ernst[1,2] — [1]Surface Science and Coating Technologies, Swiss Federal Laboratories for Materials Science and Technology (EMPA), Dübendorf, Switzerland — [2]Nanosurf Laboratory, Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, The Czech Academy of Sciences, Prague, Czech Republic — [4]Department of Chemistry, The Maharaja Sayajirao University of Baroda, Vadodara, India

Chiral molecules adsorbed on metal surfaces have promising properties for applications in devices based on organic materials, such as chiroptical sensors or electron-spin filters. For this purpose, the two-dimensional (2D) crystallization of trioxa[11]helicene (TO[11]H) on the single crystalline (100) surfaces of Ag and Cu have been studied using scanning probe microscopy techniques (STM/nc-AFM) assisted by molecular dynamics simulations. In similarity to previously reported 2D-crystallization of heptahelicene ([7]H) on Ag(100) and Cu(100) [1,2], TO[11]H on Ag(100) shows a transition from homochiral structural motifs to large heterochiral domains with increasing coverage, whereas on Cu(100), enantiopure mirror domains, forming a 2D conglomerate structure, are observed.

O 6.5 Mon 10:30 P

Layer stability of porphyrin molecules on TiO2(110) — •Maximilian Muth, Alexander Wolfram, Elmar Kataev, Julia Köbl, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen- Nürnberg, Germany

Understanding the adsorption properties of organic molecules to substrate surfaces is of essential importance for applications. Typically, the adsorption energy of a smaller molecule to a surface can be determined by TPD. However, for large organic molecules only desorption of the multilayers is possible while the bottom monolayer in direct proximity to the surface cannot be desorbed without decomposition. But usually, especially the adsorption energies of these directly adsorbed molecules are the ones of the most interest. To overcome this problem we use a method including XPS with which we can determine the binding strength of differently metalated tetraphenyl porphyrins to a rutile TiO2(110) surface comparatively to each other. Therefore, a layer exchange between two differently metalated tetraphenyl porphyrins with subsequent desorption of the multilayers is caused by an annealing ramp. The composition of the residual monolayer is investigated by XPS. By using the ratios of the two porphyrins in the residual monolayer, we can estimate the difference in binding energy between the two porphyrins over a calculation of the equilibrium constant of the layer exchange process.

O 6.6 Mon 10:30 P

Adsorption energies of metalloporphyrins on MgO(100) — •Alexander Wolfram[1], Quratulain Tariq[1], Cynthia Fernandez[2], Bernd Meyer[3], Daniel Wechsler[1], Matthias Franke[1], Hans-Peter Steinrück[1], Federico Williams[2], and Ole Lytken[1] — [1]Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander Universität Errlangen-Nürnberg, GER — [2]Departamento de Química Inorgánica, Analítica y Química Física, Universidad de Buenos Aires, Ciudad Universitaria, ARG — [3]ICMM/CCC, Friedrich-Alexander-Universität Erlangen-Nürnberg, GER

Adsorption energies of large organic molecules on surfaces are often not well known. Experimentally, the large molecules are prone to decomposition before desorption, often ruling out desorption-based techniques. Theoretically, van der Waals interactions, which dominate the interactions between the molecules and the surface, are still challenging. However, for tetraphenylporphyrin adsorbed on MgO(100) desorption of the monolayer is possible, and, using simple Redhead analysis, we have extracted the desorption energies of cobalt, zinc, and magnesium tetraphenylporphyrin. Redhead analysis requires the prefactor for desorption to be known, and we have estimated this prefactor by a combination of transition-state theory and experimentally-derived prefactors from multilayer desorption. The resulting desorption energies are in good agreement with density functional theory calculations. Somewhat unexpectedly, CoTPP exhibits the lowest desorption energy and MgTPP the highest. We suggest the different oxophilicities of the metal centers to be the reason for the trend in adsorption energy.

O 6.7 Mon 10:30 P

Structural Investigation of Caffeine Monolayers on Au(111) — Malte G.H. Schulte[1,2], Andreas Jeindl[3], •Julian A. Hochhaus[1], Ismail Baltaci[1,2], Marie Schmitz[1,2], Ulf Berges[1,2], Oliver T. Hofmann[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, D-44227, Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227, Dortmund, Germany — [3]Institut für Festkörperphysik, NAWI Graz, Technische Universität Graz, Petersgasse 16, A-8010 Graz

In this study, we investigate caffeine monolayers on Au(111). The asymmetric and achiral structure of the caffeine molecule leads to two surface chiralities, which influence the crystal growth of caffeine. Knowledge of these structural properties is of interest because of the in- fluence of caffeine on the human central nervous system.

Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and X-ray photoelectron spectroscopy (XPS) were used to determine the structure of adsorbed caffeine. Additionally performed density functional theory (DFT) calculations allowed a conclusive interpretation of the results. We observed that the caffeine molecules adsorbed in a quasi-hexagonal formation resembling the high-temperature α phase and comprising two domains. The DFT calculations suggest a unit cell containing three molecules. The theoretically calculated structure is in excellent agreement with the experimentally measured LEED, STM and XPS data. The results are published in Phys. Rev. B **101**, 245414 (2020).

O 6.8 Mon 10:30 P

Validation of the inverted adsorption structure for free-base tetraphenyl porphyrin on Cu(111) — Paul TP Ryan[1,2], Paula Laborda Lalaguna[1,3], Felix Haag[4], Mona M Braim[5], Pencheng Ding[5,6], David J Payne[2], Johannes V Barth[4], Tien-Lin Lee[1], D Phil Woodruff[5], Francesco Allegretti[4], and •David A Duncan[1] — [1]Diamond Light Source, Didcot, UK — [2]Imperial College London, UK — [3]University of Glasgow, UK — [4]Technical University of Munich, Germany — [5]University of Warwick, Coventry, UK — [6]Harbin Institute of Technology, China

Utilising normal incidence X-ray standing waves we rigourosly scrutinised the "inverted model" as the adsorption structure of free-base tetraphenyl porphyrin on Cu(111). We demonstrate that the iminic N atoms are anchored at near-bridge sites on the surface, displaced laterally by 1.1*0.2Å in excellent agreement with previously published calculations, thus confirming that this unusual structure is indeed present on the surface.

O 6.9 Mon 10:30 P

Fabrication of high-quality 2-dimensional material single crystal nanoribbon networks — •Muhammad Awais Aslam[1], Markus Kratzer[1], Christian Teichert[1], Raul David Rodriguez[2], and Aleksandar Matković[1] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Tomsk Polytechnic University, Tomsk, Russia

We demonstrate an approach to synthesize 2D material nanoribbon networks. The epitaxially grown organic nanostructures align predominantly in either zigzag or armchair orientation on 2D materials. 1,2 This study demonstrates their usage as a mask. These hybrid heterostructures are plasma etched to form single crystal nanoribbon networks. Raman spectroscopy and atomic force microscopy are employed to verify the quality of the ribbons. Our method opens up a new avenue for straightforward production of 2D material nanoribbon networks on scales relevant to electronic applications. Their high edge-to-surface ratios will also be of technological relevance for the development of future light and chemical sensors.

1.Kratzer, Teichert, 2016. Nanotechnol. 27, 292001.

2.Kratzer, Matkovic, Teichert, 2019 LPD, 52,383001.

O 7: Poster Session I: Heterogeneous catalysis I

Time: Monday 10:30–12:30 Location: P

O 7.1 Mon 10:30 P

Diffusion of oxygen atoms on a highly CO-covered Ru(0001) surface — •Hannah Illner, Ann-Kathrin Henss, and Joost Wintterlin — Chemie Department, Ludwig-Maximilians-Universität München, Deutschland

It was recently shown that oxygen atoms on a Ru(0001) surface covered with 0.33 monolayers (ML) of coadsorbed CO could travel through the CO layer by means of a new diffusion mechanism (Henß et al., Science 2019). The term "door-opening mechanism" indicated that the diffusion of the O atoms was facilitated by fluctuations in the CO layer that frequently opened low-energy paths for the oxygen. Here we report about investigations at higher CO coverages (0.50 ML). The experiments were performed between 239 and 280 K by means of a variable-temperature, high-speed STM that achieves imaging rates of up to 60 frames per second. In the investigated temperature range an ordered $(2\sqrt{3}\ \mathrm{x}\ 2\sqrt{3})\mathrm{R}30^\circ$ CO structure, which was observed at 70 K, had undergone on order-disorder transition. The trajectories of the O atoms through the disordered CO layer were analyzed, and hopping frequencies and an activation energy were extracted. It turned out that the surface diffusion of the O atoms was even faster than at the lower CO coverage and also faster than on the bare surface. We explain this finding by the weakened binding strength of the O atoms to the surface caused by CO.

O 7.2 Mon 10:30 P

Kinetic Monte Carlo simulations of methane and higher oxygenate synthesis over Rh-based catalysts — Martin Deimel[1], Hector Prats Garcia[2], •Michael Seibt[1], Karsten Reuter[1,3], and Mie Andersen[1] — [1]Chair for Theoretical Chemistry, Technical University of Munich, Garching, Germany — [2]Department of Materials Science and Physical Chemistry, University of Barcelona, Spain — [3]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The kinetic Monte Carlo method (KMC) is a powerful tool for microkinetic modeling of heterogeneous catalysis since it provides a statistically correct description of fluctuations and correlations in the coverage and binding sites of adsorbates and allows to take into account lateral interactions between the adsorbates through e.g. cluster expansion methods [1]. However, simulations can become computationally demanding through complexity in the lateral interactions or when processes with highly disparate timescales are present [2]. Here we present some new implementations in our in-house KMC code `kmos` aimed at tackling these challenges and apply these to a highly complex reaction network involving methane and higher oxygenate synthesis over Rh-based catalysts. We carefully analyze how lateral interactions affect the effective barriers in the reaction network and show that their inclusion can lead to mechanistic changes regarding the preferred reaction pathways.

[1] M. Andersen *et al.*, Front. Chem. **7**, 202 (2019)

[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)

O 7.3 Mon 10:30 P

Active Site Representation in First-Principles Microkinetic Models: Data-Enhanced Computational Screening for Improved Methanation Catalysts — •Martin Deimel[1], Karsten Reuter[1,2], and Mie Andersen[1] — [1]Chair for Theoretical Chemistry, Technical University of Munich, Garching, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

In heterogeneous catalysis first-principles microkinetic models have largely contributed to our trend understanding of transition metal (TM) and TM alloy catalysts. Within prevalent screening approaches, the computational costs are kept tractable through the use of reductionist models that only resolve a minimal amount of active site motifs at the surface. This reduces the required input to only a few adsorption energies of key reaction intermediates, while the predictive power might be jeopardized. Here, we scrutinize this common practice by systematically comparing the screening predictions for the CO methanation reaction when using microkinetic models that resolve an increasing number of sites at stepped TM and binary TM alloy catalysts. The excessive amount of predictive-quality adsorption energetics required is obtained from a compressed sensing descriptor that once trained provides these data for a new material from a single DFT calculation of the clean surface.[1] We show that the explicit consideration of hitherto neglected step and terrace sites yields new mechanistic insights and highly active materials.[2]

[1] M. Andersen *et al.*, ACS Catal. **9**, 2752 (2019)

[2] M. Deimel *et al.*, ACS Catal. **10**, 13729 (2020)

O 7.4 Mon 10:30 P

The Water Forming Reaction on Palladium Nanoparticles Studied by Kelvin Probe Force Microscopy — Ali El Barraj, Baptiste Chatelain, and •Clemens Barth — Aix-Marseille University, CNRS, CINaM, 13288 Marseille, France

The adsorption of atomic or molecular species on metal nanoparticles (NP), the absorption of atomic species like carbon, hydrogen or oxygen inside NPs and chemical reactions at NPs are of key interest in heterogeneous catalysis. Such phenomena strongly depend on the NP*s size and shape so that a characterization at the single NP level is desired. A solution is to use Kelvin probe force microscopy (KPFM) and noncontact AFM (nc-AFM) in UHV. Because adsorbed or absorbed species almost always create a surface dipole, their presence can be directly put into evidence by measuring the change of work function (WF) of the NP as recently demonstrated with oxygen and PdNPs [1].

In this contribution, we show that KPFM can be used to monitor the O+H water forming reaction on PdNPs, which is of general importance in astrophysics and for fuel cells. We discuss the reaction itself but also phenomena, which involve possible subsurface oxygen creation and carbon de-activation.

[1] Grönbeck, H.; Barth, C. J. Phys. Chem. C 2019, 123, 24615–24625.

O 7.5 Mon 10:30 P

What we can learn from pushing atoms around: Design of experiment approach to support effects in heterogeneous catalysis — •Frederic Felsen, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut, Berlin, Germany

Intricate interface structures are characteristic for most commonly employed heterogeneous catalysts in industrial applications. Understanding concomitant surface effects is key for a rational improvement and design of future catalysts. Electronic and steric effects of the support material on presumably active metal particles have been shown to interfere with scaling relations for the estimation of adsorption energies in multi-component catalysts[1]. This implies severe limitations for many established screening approaches and points to the need for suitable descriptors in more complex systems.

We present an approach to efficiently characterize solid-solid interface structures by a well defined set of single-point DFT calculations. Instead of brute forcing a full structural relaxation of the complex interface structure we actively introduce geometric distortions using statistical experimental design and evaluate the resulting changes in electronic properties. Encoding information on elementary distortions in a system-specific fingerprint, we introduce a descriptor capable of capturing the main support effects. As a first test case geometric distortions are applied to thin metal films supported on alkaline earth metal oxides.

[1] P. Metha *et al.*, ACS Catal. **7**, 4707 (2017).

O 7.6 Mon 10:30 P

A highly sensitive gas chromatograph for operando STM of catalytic reactions — •Katharina Maria Durner[1], Bernhard Böller[1], Günter Stienen[2], and Joost Wintterlin[1] — [1]Chemie Department, Ludwig-Maximilians-Universität München, Deutschland — [2]S+H Analytik GmbH, Mönchengladbach, Deutschland

Operando STM experiments of catalytic reactions can provide direct correlations between surface structure elements as possible active sites and catalytic activity. However, a major experimental difficulty is the extremely low product concentrations that result from the small size of the single crystal model catalysts and the usually relatively large volumes of STM cells. We present a special gas chromatograph (GC) that has been developed to solve this problem. The setup combines a common GC with a specially designed injection unit. Gas samples, produced at typical experimental pressures between 100 mbar and 1 bar, are compressed to the working pressure of the GC column. In the column the gas samples are condensed in a liquid nitrogen-cooled trap from which they evaporate during the temperature program. In this way the gas sample volumes are strongly enhanced without causing peak broadening. The GC has been used in operando STM experiments on the Fischer-Tropsch synthesis. Hydrocarbons from C1 to C4 produced well separated peaks, and a detection limit of 0.45 ppb was reached.

O 8: Poster Session I: Solid-liquid interfaces: Structure, spectroscopy

Time: Monday 10:30–12:30 Location: P

O 8.1 Mon 10:30 P

Interface Composition of Pure and Mixed Ionic Liquid Films on Metal Surfaces — •Stephen Massicot[1], Tomoya Sasaki[2], Matthias Lexow[1], Sunghwan Shin[1], Florian Maier[1], Susumu Kuwabata[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Japan

Ionic liquids (ILs) are salts with melting points below 100°C and extremely low vapor pressure. Thin films of ILs are of utmost interest in potential applications, e.g. in the fields of catalysis and electrochemistry. In this context, we investigate mixed ultrathin films of two ILs on metal surfaces. The molecular composition of the IL/solid and IL/vacuum interfaces is studied by angle-resolved and temperature-programmed X-ray photoelectron spectroscopy on the molecular scale. We observe phenomena of ion exchange and preferential enrichment at the interfaces, and selective desorption which opens pathways for on surface formation of new ILs by metathesis at IL/metal interfaces. In particular, we address mixtures of the protic IL diethylmethylammonium trifluoromethanesulfonate ([dema][TfO]) and the aprotic IL 1-methyl-3-octylimidazolium hexafluorophosphate ([C8C1Im][PF6]).

Supported by the European Research Council (ERC) through an Advanced Investigator Grant (ILID 693398) to HPS.

O 8.2 Mon 10:30 P

bias- and concentration- dependent switching of supramolecular nanostructures at the solid-liquid interface — •Baoxin Jia[1], Mihaela Enache[1], Sandra Miguez-Lago[2], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute of Organic Chemistry, University of Heidelberg, Germany

Research into the controlled switching between different molecular phases at the solid-liquid interface induced by an external trigger has gained increasing attention over the past years, also in view of application as smart surfaces. Here we discuss the bias- and concentration-dependent switching of a carboxy-functionalized triarylamine derivative at the HOPG/nonanoic interface studied by scanning tunneling microscopy. For a fully saturated solution, a porous phase (chickenwire) was observed for negative sample bias and a close-packed phase was observed for positive sample bias. For a 50% saturated solution, a second porous phase (flower) coexisted with the chickenwire phase at negative sample bias, while the close-packed phase was still observed at positive sample bias. For a 20% saturated solution, the two porous phases and the close-packed phase coexisted at positive sample bias because of the low molecule concentration in the solution. By changing the sample bias from negative to positive, an electric field-induced phase transition from the porous phases to the close-packed phase was accomplished, which was fully reversible by changing the bias back. Our study demonstrates that switching can be accomplished by changing the polarity of the applied external electric field.

O 8.3 Mon 10:30 P

Stability and Exchange Processes in Ionic Liquid/Porphyrin Composite Films on Metal Surfaces — •Matthias Lexow, Stephen Massicot, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In the context of organic-organic multicomponent heterostructures on metals, we studied prototypical composite systems of ultrathin porphyrin and ionic liquid (IL) films on metallic supports – Ag(111) and Au(111) – by means of angle-resolved X-ray photoelectron spectroscopy under well-defined ultrahigh vacuum conditions. After deposition of an IL on top of a monolayer of porphyrin, we observe changes in the growth behavior and thermal stability of the IL compared to deposition directly on the metals. Upon adsorption of a porphyrin layer on top of a frozen IL film at around 90 K, the porphyrin molecules replace the IL at the IL/metal interface upon heating above 240 K, a process likely driven by a larger adsorption energy of the porphyrin molecules on the Ag(111) and Au(111) surfaces.

Supported by the European Research Council (ERC) through an Advanced Investigator Grant to HPS (No. 693398-ILID).

Lexow *et al.*, *J. Phys. Chem. C*, **2019**, 123, 29708.

O 8.4 Mon 10:30 P

Chemistry and phase transition of pyridine derivatives on a gold electrode probed by vibrational sum frequency generation — Xin Gong[1], Martin Wolf[1], R. Kramer Campen[1], and •Yujin Tong[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Fakultät für Physik Universität Duisburg-Essen, 47057 Duisburg, Germany

Pyridine and its derivatives are of both practical and fundamental importance in electrochemistry. While the flat to vertical phase transition has been extensively studied and well understood, knowledge on the deprotonation and protonation chemistry at the electrode/solution interface in aqueous solution is still very limited. In the current study, we employed vibrational sum frequency generation (VSFG) to monitor both the structral and chemical evolution of 4-(dimethylamino)pyridine (DMAP) adsorbed on a gold electrode as a function of external bias. Significant spectral changes are observed as a function of the applied bias voltage in the cyclic voltammetry. These features can be unambiguously assigned to the protonation/deprotonation and orientational changes respectively. The information revealed by this study is essential for the application of pyridine derivatives in nanoparticle manipulation, enhancement of CO_2 reduction, formic acid electro-oxidation, etc.

O 8.5 Mon 10:30 P

Water structure at Pb(100) and (111) surfaces studied with the interface force field — •Oskar Cheong[1,3], Michael H. Eikerling[1,2], and Piotr M. Kowalski[1,2] — [1]Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance, JARA-CSD and JARA-ENERGY, 52425 Jülich, Germany — [3]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

The activity and selectivity of vital electrochemical reactions such as the oxygen evolution reaction or the CO2 reduction reaction strongly depend on the solvent structure at the metal-electrolyte interface. In this realm, ab initio as well as classical molecular dynamics (AIMD and CMD) simulations are harnessed to study the structure and dynamics of water at metal surfaces. AIMD provides high accuracy but is restricted to short time- and length-scales. CMD allows simulating larger scales. However, the accuracy of CMD depends on the force field applied to describe interatomic interactions. We present results of CMD investigation of water structures on Pb metal surfaces performed with the interface force field [1]. On comparable time- and length-scales, AIMD water structures were reproduced. However, on much larger scales CMD yields different, more stable and better equilibrated water structures [2]. This clearly shows the large potential of CMD for efficient statistical sampling of atomic structures at the interfaces. [1] Heinz et al., Langmuir. 29, 1754 (2013). [2] Cheong et al. submitted (2021).

O 8.6 Mon 10:30 P

Solving Catalyst Degradation: Platinum Stability for Fuel Cell Operation — •Francesc Valls Mascaró[1], Marc T. M. Koper[1], and Marcel J. Rost[2] — [1]Leiden Institute of Chemistry, Leiden University — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University

The longevity of a catalyst plays a crucial role for many industrial scale applications. Platinum is the best candidate to be used in electrochemical energy conversion systems due to its high activity. However, platinum suffers from degradation during fuel cell operation. This degradation is caused by the nucleation and growth of nanoislands, which roughen the surface [1, 2]. It is known that the extend of this roughening can be tuned by including additives, changing the electrolyte pH or working within different potential windows [3, 4]. In this work, we study the degradation of different platinum stepped surfaces under potential cycling to oxidative potentials. Interestingly, we quantify significantly less degradation for the surfaces with shorter terraces: Pt(111) > Pt(15 15 14) > Pt(554). We present here a model that explains this trend, in which steps act like sinks for both adatoms and vacancies, slowering down the nucleation and growth of the mentioned nanoislands. Finally, we do not observe roughening at all for platinum surfaces with only four atoms terrace width: Pt(553) and Pt(533).

[1] Jacobse, L. et al., ACS Cent. Sci. 5 (12), 1920 (2019)

[2] Rost, M.J. et al., Nat. Commun. 10, 5233 (2019)

[3] Topalov, A. et al., J. Chem. Sci., 5, 631 (2014)

[4] Ruge, M. et al., J. Am. Chem. Soc., 139, 4532 (2017)

O 8.7 Mon 10:30 P

TiO_2(110) in Liquid Water, Air, and Solution — •Jan Balajka[1,2], Melissa Hines[2], William DeBenedetti[2], Jiri Pavelec[1], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Department of Chemistry and Chemical Biology, Cornell University, Ithaca NY, USA

Our understanding of metal oxide surface chemistry arises from studies under highly idealized ultrahigh vacuum (UHV) conditions, that cannot be extrapolated to the complex reaction environments of real industrial processes. Material properties, such as chemical reactivity, are determined by the nature of individual surface sites and thus related to the detailed atomic configuration. Yet, the interfacial structure under application conditions remains largely unexplored.

I will review our work on the prototypical TiO_2(110) surface in ambient and aqueous environments. Using a UHV-compatible dispenser of ultrapure liquid water, we demonstrated that the TiO_2(110) surface is not altered upon contact with clean liquid water. However, when exposed to air, low-concentration atmospheric species, such as carboxylic acids, adsorb with high affinity and form an ordered overlayer at the surface, effectively passivating the undercoordinated Ti surface sites.[1]

I will further discuss a chemical functionalization of the TiO_2(110) surface by a monolayer of terephthalic acid (1,4-benzenedicarboxylic acid) deposited from solution and intended to serve as a growth template for three-dimensional metal-organic networks (MOFs).

[1] J. Balajka, *et. al.*, Science 361, 786 (2018)

O 8.8 Mon 10:30 P

How surface oxides determine the activity of Mo_2C electrocatalysts — •Christoph Griesser[1], Haobo Li[2], Eva-Maria Wernig[1], Daniel Winkler[1], David Egger[2,3], Christoph Scheurer[2,3], Karsten Reuter[2,3], and Julia Kunze Liebhäuser[1] — [1]Department of Physical Chemistry, Universität Innsbruck, Austria — [2]Chair of Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Transition metal (TM) compounds are widely applicable as materials in heterogeneous catalysis, due to their compositional and structural diversity. TM carbide compounds are praised as electrocatalysts for the CO_2 reduction reaction (CO_2RR), due to a possible break of key adsorption energy scaling relations, predicted by density-functional theory studies. Mo_2C was classified as highly suitable for the CO_2RR in an active-site computational screening study. Here we assess the activity of hexagonal Mo_2C towards the CO_2RR in aqueous electrolyte by a multimethod experiment and theory approach. We find, that an ultrathin oxide film persists at the surface of this catalyst material and completely suppresses any CO_2RR activity. The one monolayer thin oxide films are stable down to -1.9 V_{SHE}, and exclusively the hydrogen reduction reaction is found to take place. This points to the necessity of considering the true interface, forming under operando conditions, in computational screenings for catalyst materials. Preliminary experiments performed under protection of Mo_2C from ambient air in non-aqueous electrolyte indeed reveal CO_2RR activity.

O 8.9 Mon 10:30 P

Hydration of Polyvinyl Alcohol Surfaces Mediated by Ammonia — Takahiko Ikarashi[1], Takumi Yoshino[1], Naoki Nakajima[1], Kazuki Miyata[1], Keisuke Miyazawa[1], •Ygor Morais Jaques[2], Adam S. Foster[2], Megumi Uno[3], Chikako Takatoh[3], and Takeshi Fukuma[1] — [1]Kanazawa University, Japan — [2]Aalto University, Finland — [3]EBARA Corporation, Japan

Chemical mechanical planarization (CMP) is a process that smooths silicon wafers surface for their efficient use in electronics. This procedure results in the surfaces being covered by silica nanoparticles. An effective way of removing these debris is by scrubbing polyvinyl alcohol (PVA) brushes on the wafer's surface in an aqueous solution. However, this can cause cross-contamination between wafers due to debris adhesion into the PVA surface. Thus, for an optimal technical setup, the interactions between silica nanoparticles and PVA as well as PVA's hydration in different liquids have to be properly addressed. Here, we investigate the hydration of PVA in NH_3 aq. and pure water. Using atomic force microscopy, we found that the adhesion force between a silica tip and a PVA surface in NH_3 aq. is drastically reduced when compared to the system immersed in water. Using molecular dynamics simulations, we have found that this happens because the NH_3 molecules perturb the hydrogen bond networks formed between water and the PVA hydroxyl groups, promoting faster interactions and diffusion. This central role of ammonia in the inhibition of nanoparticle adhesion can further improve post CMP cleaning processes.

O 9: Poster Session I: New methods I

Time: Monday 10:30–12:30 Location: P

O 9.1 Mon 10:30 P

Deterministic quantum mechanics: simulation of chemical reactions — •Irmgard Frank — Leibniz University Hannover, Hannover, Germany

Roberto Car and Michele Parrinello had the great idea to describe electronic structure using the Schrödinger equation and nuclear motion using Newton dynamics. Over the years it turned out, that with this approach it is possible to describe arbitrary chemical reactions. We observe classical chaos: Starting from identical initial conditions, we will always get the same reaction pathway. If, however, slightly changing the initial conditions, it is possible to observe completely different reactions. Both electronic cloud and nuclear positions are moved using differential equations, hence we have very clearly a deterministic picture. The general idea is similar to Bohm mechanics, with the difference that we use classical Newton dynamics for the nuclei instead of a guiding equation. An apparent difference is that there is no zero-point energy in nuclear motion. This facilitates the description of potential energy surfaces and of motion on these surfaces.

O 9.2 Mon 10:30 P

How to train a Gaussian Approximation Potential for metal oxides: A three stage process towards fast surface sampling — •Carsten Staacke[1,2], Jakob Timmermann[1,2], Yonghyuk Lee[1,2], Christoph Scheurer[1,2], and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der MPG — [2]Technische Universität München

Surface orientation and termination play a decisive role for the chemical and physical behavior of catalysts and functional materials. *Ab initio* thermodynamics comparing the stability of different density-functional theory computed trial structures has emerged as a standard tool to determine surface structures under working conditions. However, limited by the high computational cost, these trial structures are up to now typically derived manually, reflecting the researcher's ability to imagine possible structural models. Efficient and accurate machine-learned (ML) interatomic potentials promise to replace this state-of-the-art by systematic global optimization methods. To this end, we have developed a protocol to train short-ranged ML potentials for metal oxides based on the Gaussian Approximation Potential and Smooth Overlap of Atomic Positions (SOAP) descriptors to capture atomic environments.[1,2] We will present a systematic three-stage training process. For various rutile type metal oxides the role of all three stages will be exemplified and critically evaluated. [1] J. Timmermann *et al.*, Phys. Rev. Lett. **125**, 206101 (2020). [2] A.P. Bartók *et al.*, Phys. Rev. Lett. **104**, 136403 (2010).

O 9.3 Mon 10:30 P

Biaxial atomically resolved force microscopy based on a qPlus sensor operated simultaneously in the first flexural and length extensional modes — •Dominik Kirpal[1], Jinglan Qiu[1,2], Korbinian Pürckhauer[1], Alfred J. Weymouth[1], Michael Metz[1], and Franz J. Giessibl[1] — [1]Institute of experimental and applied physics, University of Regensburg, Regensburg, Germany — [2]College of Physics and Hebei Key Laboratory of Photophysics Research and Application, Hebei Normal University, Shijiazhuang, Hebei, China

In frequency-modulation atomic force microscopy typically the tip is driven to oscillate vertically, giving a measure of the vertical force component. However, for many systems the lateral force component of force provides valuable information about the sample. Measuring lateral and vertical force components simultaneously by oscillating vertically and laterally has so far only been demonstrated with relatively soft silicon cantilevers and optical detection. Here, we show that the qPlus sensor can be used in biaxial mode with electrical detection by making use of the first flexural mode and the length extension mode. We describe the necessary electrode configuration as well as the electrical detection circuit, and compare the length extension mode to the needle sensor. Finally, we show atomic resolution in ambient conditions of a mica surface and in ultra-high vacuum of a silicon surface. With this, we show how any qPlus AFM setup can be modified to work as a biaxial sensor, allowing two independent force components to be recorded.

O 9.4 Mon 10:30 P

Design of an IRAS Setup to Investigate Adsorbates on Metal-Oxide Single Crystals — •David Rath, Jiri Pavelec, Gareth Parkinson, Michael Schmid, and Ulrike Diebold — Institut für Angewandte Physik, Technische Universität Wien, A-1040 Wien, Austria

The IRAS system GRISU (**GR**azing incident **I**nfrared absorption **S**pectroscopy **U**nit) was developed for investigations in the research field of single atom catalysis [1]. It combines the commercially available FTIR spectrometer Bruker Vertex 80v with an UHV chamber [2]. GRISU features five mirrors for beam guidance placed in HV and UHV environment. The development was concentrated to optimise the system's performance, flexibility and usability resulting in a small controllable focal-spot diameter (3 mm) on the sample, different optical apertures, and motorised optical components. The simulated system (done with a ray tracing program and a simplified spectrometer model) shows an efficiency of 13 %, i.e. 13 % of the radiation passing through the first aperture (Ø 6 mm) after the IR source in the FTIR spectrometer reaches the detector after being reflected from the molecular beam spot on the sample. Compared to a commercially available system with two parabolic mirrors with a focal length of 500 mm, this is higher by a factor of about 60. All the optical components are mounted precisely in respect to each other to ensure the high performance requirement also after long term use.

[1] G. S. Parkinson, Catal. Lett. 149, 1137 (2019)
[2] J. Pavelec, et al., J. Chem. Phys. 146, 014701 (2017).

O 9.5 Mon 10:30 P

Vienna Package for TensErLEED: A new environment for analysis and calculation of LEED *I(V)* data — •Florian Kraushofer[1], Michael Schmid[1], Tilman Kisslinger[2], Ulrike Diebold[1], Lutz Hammer[2], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]FAU Erlangen-Nürnberg, Erlangen, Germany

Low-Energy Electron Diffraction (LEED) is a structure-sensitive technique commonly available in most surface science laboratories. Beyond the usual application as a tool to determine periodicity and degree of order of a surface phase, the method also gives access to the surface's crystallographic structure via a quantitative analysis of the modulation of beam intensities as a function of electron energy (LEED *I(V)*). This, however, requires complex full-dynamical intensity calculations as well as a time-consuming optimization of structural parameters minimizing the deviation between experimental and calculated *I(V)* curves. The Erlangen program package TensErLEED [1] readily performs this task, but its required user input is almost prohibitively complex.

We show that for most cases, the necessary TensErLEED input can be generated automatically by combining a handful of user parameters and a structure file in a standard format. Based on this, we introduce the new "Vienna Package for TensErLEED" (ViPErLEED), which greatly simplifies the code application and substantially reduces the amount of work and potential for errors, even for experienced users. The package is completed by a versatile utility for extracting experimental *I(V)* spectra from a LEED video or stack of images.

[1] V. Blum, and K. Heinz, Comput. Phys. Commun. **134**, 392 (2001).

O 10: Poster Session I: Topological insulators

Time: Monday 10:30–12:30 Location: P

O 10.1 Mon 10:30 P

Topologization of beta-antimonene on Bi2Se3 via proximity effects — •Kris Holtgrewe[1], Conor Hogan[2], and Simone Sanna[1] — [1]Justus-Liebig-Universität, Gießen, Germany — [2]Institute of Structure of Matter (ISM-CNR), Rome, Italy

Thin antimony (Sb) layers adsorbed on bismuth selenide (Bi_2Se_3) are an exciting van der Waals heterostructure system. While the substrate is a topological insulator (TI), thin sheets of the β-phase of antimony are topologically trivial (CI). So, the question arises whether the topological surface states form at the substrate-adlayer interface or whether the TI/CI boundary shifts downwards (trivialization of the substrate) or upwards (topologization of the adlayer). In this theoretical work, we apply density functional theory to model heterostructures of single and double bilayers of antimonene on a bismuth selenide substrate. After investigating the structural details, we analyse the space- and spin-resolved electronic band structure. We show that the topological surface states of the pristine Bi_2Se_3 substrate migrate to the top antimony bilayer, while their unique helical spin texture is preserved. The topologization of the Sb sheets is a consequence of the complex hybridization process between the bands of the substrate and the sheets.

O 10.2 Mon 10:30 P

Dirac Fermions in a Two-Dimensional Triangular Indium Layer on SiC(0001) — •Maximilian Bauernfeind[1,3], Jonas Erhardt[1,3], Philipp Eck[2,3], Jörg Schäfer[1,3], Simon Moser[1,3], Domenico Di Sante[2,3], Ralph Claessen[1,3], and Giorgio Sangiovanni[2,3] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

— [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

The Kane-Mele model provides an intuitive strategy to realize nontrivial topology in two-dimensional honeycomb lattices. Graphene, the most prominent representative of this class, lacks spin-orbit coupling (SOC), which prevents the formation of a sizeable bulk band gap and the utilization of the topological phase at reasonable temperatures. By enriching the orbital subspace and concomitantly switching to a triangular lattice, new possibilities arise. Here, we demonstrate by angle-resolved photoelectron spectroscopy that a triangular indium lattice grown on SiC(0001) - indenene - hosts massive, i.e., gapped Dirac Fermions at the K-point. The opening of this topologically non-trivial gap of approx. 100 meV relies on the strong local SOC. The in-plane inversion symmetry breaking induced by the substrate counteracts the topology but produces on the other hand a distinctive charge localization that directly reflects the non-trivial topological character of indenene, which allowed us to identify this new quantum spin Hall insulator by scanning tunneling microscopy.

O 10.3 Mon 10:30 P

Lifting topological protection in a quantum spin Hall insulator — •Raul Stühler[1], André Kowalewski[1], Felix Reis[1], Dimitri Jungblut[1], Fernando Dominguez Tijero[1,2], Johannes Weis[1], Benedikt Scharf[1], Werner R. Hanke[1], Gang Li[3], Joerg Schaefer[1], Ewelina M. Hankiewicz[1], and Ralph Claessen[1] — [1]Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [2]Technische Universität Braunschweig, Germany — [3]ShanghaiTech University, China

The recently discovered monolayer system bismuthene/SiC(0001) is a promising candidate for the realization of a room-temperature quantum spin Hall (QSH) effect [1]. As expected for a QSH insulator, the electronic edge channels do not show any signs of backscattering from kinky edge sections that would manifest in interference phenomena [2]. Notwithstanding, topological protection against defect scattering may become lifted when two helical edge channels are brought into direct proximity, resulting in quantum interference. By scanning tunneling microscopy we study phase-slip domain boundaries (DB) with limited longitudinal extent. By spectroscopic means we scrutinize quasi-particle interference along these one-dimensional topographic defects that points towards a linear electronic dispersion. We discuss our findings as possible quantum interference between coupled helical edge states formed in the vicinity of a DB, accompanied by lifting the topological protection via hybridization.

[1] F. Reis et al., Science **357**, 287–290 (2017).
[2] R. Stühler et al., Nature Physics **16**, 47–51 (2020).

O 10.4 Mon 10:30 P

2D to 3D crossover in topological insulators — •Corentin Morice[1], Thilo Kopp[2], and Arno Kampf[3] — [1]Institute for Theoretical Physics Amsterdam and Delta Institute for Theoretical Physics,University of Amsterdam, 1098 XH Amsterdam, The Netherlands — [2]Center for Electronic Correlations and Magnetism, Experimental Physics VI,Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Center for Electronic Correlations and Magnetism, Theoretical Physics III,Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

At the heart of the study of topological insulators lies a fundamental dichotomy: topological invariants are defined in infinite systems, but their main footprint, surface states, only exists in finite systems. In systems in the slab geometry, namely infinite in two dimensions and finite in one, the 2D topological invariant was shown to display three different types of behaviours. In the limit of zero Dirac velocity along z, these behaviours extrapolate to the three 3D topological phases: trivial, weak and strong topological insulators. We show analytically that the boundaries of these regions are topological phase transitions of particular significance, and allow one to fully predict the 3D topological invariants from finite-thickness information. Away from this limit, we show that a new phase arises, which displays surface states but no band inversion at any finite thickness, disentangling these two concepts closely linked in 3D.

O 10.5 Mon 10:30 P

Temperature Evolution of the Magnetic Gap in the Ferromagnetic Topological Insulator MnSb$_2$Te$_4$ **probed by Scanning Tunneling Spectroscopy** — •Philipp Küppers[1], Stefan Wimmer[2], Andreas Ney[2], Jannik Zenner[1], Marcus Liebmann[1], Markus Morgenstern[1], Günther Bauer[2], and Gunther Springholz[2] — [1]II. Institute of Physics B and JARA-FIT, RWTH Aachen Unversity, 52074 Aachen, Germany — [2]Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität, Altenberger Straße 69, 4040 Linz, Austria

MnSb$_2$Te$_4$ has recently been established as a ferromagnetic topological insulator with out-of-plane anisotropy and large Curie temperature T$_C$ = 40-50 K [1]. Here, we show that it exhibits a band gap at the Fermi level that closes rather precisely at T$_C$ using scanning tunneling spectroscopy (STS) down to 4 K. At 4K, the gap has an average size of 17 meV exhibiting spatial fluctuations due to disorder with strength 11 meV and correlation length 2nm. We also applied in-plane magnetic fields in order to close the gap by changing of the magnetic orientation.

[1] Wimmer et al., arXiv:2011.07052 (2020)

O 11: Poster Session I: Plasmonics and nanooptics I

Time: Monday 10:30–12:30 Location: P

O 11.1 Mon 10:30 P

Fabrication and transfer of hexagonal gold nano-pyramid arrays on PDMS for SERS — •Peter Christian Simo[1], Florian Laible[1], Anke Horneber[1], Claus Burkhardt[2], and Monika Fleischer[1] — [1]Institute for Applied Physics, University of Tuebingen, Germany — [2]Natural and Medical Sciences Institute at the University of Tuebingen, Reutlingen, Germany

Surface enhanced Raman scattering (SERS) with pyramidal nanostructures increases the signal of Raman active analytes, since hotspots form at the edges and tip of a nano-pyramid under illumination. 2D hexagonal arrays of pyramidal nanostructures with a quadratic base are fabricated through cost-effective nanosphere lithography and transferred onto PDMS. Under varying uniaxial strain the localized surface plasmon resonances (LSPRs) of the nanostructures on the PDMS can also be analysed. By making use of the (111) crystal plane of a silicon (100) wafer, an inverted pyramidal array is etched, which serves as the complementary negative for the gold nanostructures. Either a continuous gold thin-film with protruding pyramids or separate isolated nano-pyramids are produced. The use of a linker molecule between the PDMS and the gold is mandatory to increase the weak Au-PDMS adhesion. (3-Mercaptopropyl)triethoxysilane (MPTS) is able to bind to both PDMS and to the gold structures, thus strongly increasing stability for mechano-optical experiments. The SERS enhancement is verified by Raman mapping of 4-Mercaptobenzoic acid molecules.

O 11.2 Mon 10:30 P

Fabricating ultra-narrow gaps in bow-ties utilizing strain junctions — •Florian Laible[1], Kai Braun[2], Martin Eberle[2], Dieter P. Kern[1], Alfred J. Meixner[2], and Monika Fleischer[1] — [1]Institute for Applied Physics and Center LISA+, University of Tübingen, 72076, Tübingen, Germany — [2]Institute for Physical and Theoretical Chemistry and Center LISA+, University of Tübingen, 72076, Tübingen, Germany

Mechanically controllable break junctions (MCBJs) are widely used to create sub-1 nm gaps between two metal contacts. In this regime, the width of the gap can be controlled with Angstrom precision using the tunnel effect. The ability to create ultra-narrow gaps in bow-tie antennas is desirable for investigations on the interplay of localized plasmonics and electron tunneling, as well as for SERS applications since ultra-narrow gaps are promising highly enhanced near fields. The integration of nanoantennas into MCBJs is challenging since the localization of the plasmon and the mechanical properties of the break junction have to be preserved simultaneously. We present an approach to reach ultra-narrow gaps between two nanoantennas in the focus of a confocal microscope. A gapless bow-tie antenna is integrated into a mechanically controllable break junction. The nanostructure is optically decoupled from the electrical leads. The gap is created by bending the substrate, causing the nanoantenna to break at its thinnest point. The gap size is measured using electron tunneling and controlled by changing the bend of the substrate. Combined electrical and optical measurements will be presented alongside the fabrication process.

O 11.3 Mon 10:30 P

Ab-Initio study of plasmonic properties of metallic magnesium nanoclusters — •Oscar A. Douglas-Gallardo, Connor L. Box and, and Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, United Kingdom

The study of optical, electronic and catalytic properties of nanostructured plasmonic materials has been traditionally focused on gold and silver. In recent years, however, the plasmonic properties of a set of Earth-abundant materials (Al, Mg) have gradually gained increasing interest in the plasmonic area. These new plasmonic materials can potentially extend the application areas of standard plasmonic material (Au, Ag and Cu) adding more chemical variety whilst simultaneously reducing the production cost associated with coinage metals. In this context, the optical and electronic properties of a set of nanostructured metallic magnesium particles and surfaces have been explored by means of time-dependent density functional tight-binding (TD-DFTB) approach along with molecular dynamics with electronic friction (MDEF) simulation. The hot carrier distributions produced when Mg nanoclusters are exposed to light were computed and compared against silver nanoclusters. Finally, chemical interface damping due to molecular hydrogen/atomic hydrogen adsorption was also considered. The results obtained here represent the first step toward full characterization and assessment of this new variety of plasmonic material made of Earth-abundant elements.

O 11.4 Mon 10:30 P

Dramatic Enhancement of Tip-Enhanced Raman Scattering Mediated by Atomic Point Contact Formation — •Shuyi Liu[1], Borja Cirera[1], Yang Sun[2], Ikutaro Hamada[2], Melanie Muller[1], Adnan Hammud[3], Martin Wolf[1], and Takashi Kumagai[1,4] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]GREEN, National Institute for Materials Science, Ibaraki, Japan — [3]Department of Inorganic Chemistry, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [4]Center for Mesoscopic Sciences, Institute for Molecular Science, Okazaki, Japan

Tip-enhanced Raman scattering (TERS) in ångström-scale plasmonic cavities has drawn increasing attention. However, Raman scattering at vanishing cavity distances remains unexplored. In this presentation, I show the evolution of TERS in transition from the tunneling regime to atomic point contact (APC). A stable APC is reversibly formed in the junction between an Ag tip and ultrathin ZnO or NaCl films on the Ag(111) surface at 10 K. An abrupt increase of the TERS intensity occurs upon APC formation for ZnO, but not for NaCl. This remarkable observation is rationalized by a difference in hybridization between the Ag tip and these films, which determines the contribution of charge transfer enhancement in the fused plasmonic junction. The strong hybridization between the Ag tip and ZnO is corroborated by the appearance of a new vibrational mode upon APC formation, whereas it is not observed for the chemically inert NaCl.

O 11.5 Mon 10:30 P

Dipolar coupling of nanoparticle-molecule assemblies: An efficient approach for studying strong coupling — •Jakub Fojt[1], Tuomas P Rossi[2], Tomasz J Antosiewicz[3], Mikael Kuisma[4], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Faculty of Physics, University of Warsaw, Warsaw, Poland — [4]Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland

Strong light-matter interactions facilitate not only emerging applications in quantum and non-linear optics but also modifications of materials properties. In particular the latter possibility has spurred the development of advanced theoretical techniques that can accurately capture both quantum optical and quantum chemical degrees of freedom. These methods are, however, computationally very demanding, which limits their application range. Here, we demonstrate that the optical spectra of nanoparticle-molecule assemblies, including strong coupling effects, can be predicted with good accuracy using a subsystem approach, in which the response functions of the different units are coupled only at the dipolar level. We demonstrate this approach by comparison with previous time-dependent density functional theory calculations for fully coupled systems of Al nanoparticles and benzene molecules. While the present study only considers few-particle systems, the approach can be readily extended to much larger systems and to include explicit optical-cavity modes.

O 11.6 Mon 10:30 P

Boosting Light Emission from Single Hydrogen Phthalocyanine Molecules by Charging — •Vibhuti Rai[1], Lukas Gerhard[1], Qing Sun[1], Christof Holzer[2], Taavi Repaen[3], Marjan Krstic[2], Liang Yang[3], Martin Wegener[3], Carsten Rockstuhl[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

The aspect of light emission from single molecules on insulating layers studied by scanning tunneling microscopy induced luminescence (STML) has made considerable progress. Many fundamental aspects of light emission, however, remain unclear for the future prospect of device applications. Here, we used STML to investigate light emission from individual Hydrogen-Phthalocyanine (H_2Pc) molecules thermally evaporated onto bi- and trilayers of NaCl on Au(111). Combining STML measurements, full-wave electrodynamics, and quantum chemical calculations, we show that the emitted light from a charged H_2Pc couples more efficiently to the far-field than its neutral form [1]. This boost can be explained by the development of a vertical dipole moment normal to the substrate, facilitating out-coupling of the local excitation to the far-field. Since this effect is not related to the specific molecule, it provides a general pathway for enhancing the quantum efficiency of light emission from a molecular junction.

[1] Rai et al. Nano Letters 2020, 20 (10), 7600-7605.

O 11.7 Mon 10:30 P

Design of periodic structures by surface plasmon polaritons excitation — •Pavel N. Terekhin[1], Jens Oltmanns[2], Andreas Blumenstein[2], Dmitry S. Ivanov[1,3,4], Frederick Kleinwort[2], Martin E. Garcia[3], Baerbel Rethfeld[1], Juergen Ihlemann[2], and Peter Simon[2] — [1]Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institut für Nanophotonik Göttingen e.V., 37077 Göttingen, Germany — [3]Theoretical Physics Department, University of Kassel, 34132 Kassel, Germany — [4]Quantum Electronics Division, Lebedev Physical Institute, 119991 Moscow, Russia

Laser irradiation of solids can lead to the spontaneous formation of periodic structures on the surface. They are known as laser-induced periodic surface structures (LIPSS) and have unique properties with a broad spectrum of applications. For their controlled fabrication, it is essential to understand the basic governing mechanisms of energy deposition.

We demonstrate the influence of surface plasmon polaritons (SPP) on the process of LIPSS formation after irradiation of a step edge structure in a single-pulse experiment. The absorption of laser energy is described by an analytical source term, which considers the excitation of SPP. The further surface structures development is traced by a hybrid atomistic-continuum model. The theoretical predictions are fully confirmed by experimental observations. The developed method can be used to study the mechanisms of laser energy absorption and to design surface structures under controlled conditions.

O 11.8 Mon 10:30 P

Dependency of aggregate absorption on near field polarization — •Sidhartha Nayak[1], Fulu Zheng[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany

Strong interaction between transition dipoles of molecules leads to the formation of delocalized excitonic eigenstates of molecular aggregates. To understand their optical and transfer properties, knowledge of these eigenstates is required. Using near-field radiation stemming from a metallic tip which is scanned over the aggregate one can record position-dependent absorption spectra [1]. From these spectra, it is possible to reconstruct excitonic wavefunction [2]. In this contribution, we focus on the situation when the tip is irradiated by linear polarized light. We show that there is a strong dependence of the near field spectra on the polarization and propagation direction of the incident light, which can be used to facilitate the wavefunction reconstruction. Finally, we explain this orientation dependency using three basic functions which depend on tip position and eigenfunctions but not on the orientation of the incoming radiation.

[1] X. Gao and A. Eisfeld, *J. Phys. Chem. Lett.* 9, 6003 (2018)
[2] F. Zheng, X. Gao and A. Eisfeld, *Phys. Rev. Lett.* 123, 163202 (2019)

O 12: Poster Session I: Electronic structure theory: General

Time: Monday 10:30–12:30 Location: P

O 12.1 Mon 10:30 P

Electronic Structure of Cesium-based Photocathode Materials from Density Functional Theory — •Holger-Dietrich Sassnick[1] and Caterina Cocchi[1,2] — [1]Institut für Physik - Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]Institut für Physik - Humboldt-Universität zu Berlin und IRIS Adlershof, 12489 Berlin, Germany

The development of novel materials for vacuum electron sources is an active field of research that can greatly benefit from the results of *ab initio* calculations [1]. Density functional theory offers a good compromise between accuracy and computational feasibility, however, its results crucially depend on the choice of the exchange-correlation potential, v_{xc}. To address this point, we systematically analyze the performance of three popular approximations of v_{xc} (PBE, SCAN and HSE06) on the structural and electronic properties of bulk Cs_3Sb and Cs_2Te, two representative Cs-based semiconductors employed in photocathode applications. We find that PBE shows expectedly the largest discrepancies from the target, while both SCAN and HSE06 perform remarkably well in reproducing the materials properties. Additionally, we study the effect of spin-orbit coupling which mainly impacts the valence region of both materials inducing a band splitting of about 150 meV. Our results indicate SCAN as the best trade-off between accuracy and computational costs, outperforming the considerably more expensive HSE06 [2].

[1] Cocchi et al, *J. Phys.: Condens. Matter* **2019**, 31, 014002
[2] Saßnick & Cocchi, *submitted* **2020**, arXiv:2101.04596

O 12.2 Mon 10:30 P

Solvated Electrons in Alkali Metal Doped Zeolites: Insights from *Ab-initio* Atomistic Thermodynamics — •Debalaya Sarker[1,2], Maria Troppenz[3], Santiago Rigamonti[3], Claudia Draxl[3], Sergey V Levchenko[1,2], and Matthias Scheffler[2] — [1]Skoltech, Moscow, RU — [2]Fritz-Haber-Institut der MPG, DE — [3]Humboldt-Universität zu Berlin, DE

Doping nanoporous aluminosilicate zeolites viz. faujasite Y, with alkali metal atoms (M) is a promising way of producing outstanding catalysts. The dopants, along with extra-framework M atoms, often form M_4^{3+}, clusters inside zeolite pores, leaving the valence electron of the dopant solvated and available for catalysis. Despite extensive experimental efforts[1], the distribution of the dopants and solvated electrons remains debated to date. Combining a cluster-expansion model, parameterized with density-functional theory calculations, with *ab-initio* thermodynamics, we address this issue. The electronic structure for low-energy configurations is calculated with the hybrid functional HSE06. We find that even at room temperature, Na atoms in NaY zeolites with 2 extra-framework atoms/unit cell on average redistribute such that areas with lower and higher local concentrations emerge. The redistribution is driven by increased configurational disorder, mainly at higher concentrations. This explains why solvated electrons can be located inside both small and large cages in NaY, reconciling experiments that assign the solvated electrons to a particular pore type.

[1] A. R. Armstrong *et al.*, J. Am. Chem. Soc. **117**, 9087 (1995).

O 12.3 Mon 10:30 P

Hole mobility response through gas adsorption at the inner surface of the iron (1,2,3)-triazolate metal-organic framework — •Christoph Muschielok[1], Alexander Reiner[2], Richard Röss-Ohlenroth[2], Andreas Kalytta-Mewes[2], Dirk Volkmer[2], Achim Wixforth[2], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Universität Augsburg

Metal-organic frameworks (MOFs) are hybrid network materials, built from metal centers interconnected by organic linker molecules. Often they exhibit pores, into which atoms or small molecules may be absorbed, and a select few of them even display some electronic conductivity. Utilizing both, we investigate the response of the hole mobility in the iron (1,2,3)-triazolate MOF to guest atoms for a possible use as a trace gas sensor. To deepen our understanding of the material, we employ our adapted variant of Bardeen and Shockley's deformation potential theory to analyze the impact of the guest atoms' presence on the corresponding material properties: the effective mass, the bulk modulus, and the deformation potential of the MOF crystal. We find significant influence of guest atom absorption on the hole mobility, consistent with first experimental results.

O 12.4 Mon 10:30 P

First-Principles Study of Lead-free Halide Double Perovskites for Photovoltaic Applications — •Elisabetta Landini[1,2], Harald Oberhofer[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Gremany — [2]Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, D-85747 Garching, Germany

Metal halide perovskites, such as methylammonium lead iodide [1], are promising materials in the field of optoelectronics. However, the toxicity of lead, hysteresis effects, and the sensitivity of the structures to moisture and heat prevent this technology to become technologically viable. To overcome these limitations, heterovalent substitution of Pb forming the double perovskite structure $A_2BB'X_6$, has been suggested.

In this context theoretical modeling is a valuable tool to develop a comprehensive picture of the electronic structure of different double perovskites. Density-functional theory calculations have been carried out using semi-local and screened hybrid functionals and including spin-orbit coupling corrections. Experimentally studied Cs_2AgBiX_6 (X=Br,Cl) [2] are chosen as a starting point. Native point defects and incremental substitutions are then created to systematically study their effect on the band structure and charge carrier mobility.

[1] D. Zhao *et al.*, ACS Eng. Lett. **3**, 305 (2018).

[2] X. Zhao *et al.*, J. Am. Chem. Soc. **139**, 2630 (2017).

O 12.5 Mon 10:30 P

Electronic Structure of Self-assembly Crystalline Perylene in Metal-Organic Frameworks Thin Film — •Yohanes Pramudya, Mariana Kozlowska, Shahriar Heidrich, Marius Jakoby, Liuyang Pan, Bryce Richard, Christof Wöll, Ritesh Haldar, and Wolfgang Wenzel — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Metal organic frameworks (MOFs) are a very versatile platform for exploring nearly unlimited chemical space of organic components linkers connected by the metal centers or vertices in various topologies and their self-assembly for device optimization. Here, we demonstrated the impact of interchromophore interactions in the photophysical properties of a surface-anchored MOF (SURMOF) based on 3,9-perylenedicarboxylicacid linkers. We predicted the structural assembly of the perylene molecules in the MOF via robust periodic density functional theory calculations and described the impact of unit topology and $\pi^*\pi$ interaction patterns on spectroscopic and semiconducting properties of the MOF films. We elaborated the dual nature of excited states in the perylene MOF, where strong temperature-modulated excimer emission, enhanced by the formation of perylene J-aggregates, and low stable monomer emission was observed. We used band transport and hopping transport mechanisms to predict the semiconducting properties of perylene SURMOF-2 films as a function of inter-linker interactions and the resulting both p-type and n-type electronic transport mechanisms.

O 12.6 Mon 10:30 P

Optical and X-ray absorption spectra of oxides: Theoretical description including many-body effects — •Vijaya Begum[1], Markus E. Gruner[1], Christian Vorwerk[2], Claudia Draxl[2], and Rossitza Pentcheva[1] — [1]Faculty of Physics and Centre for Nanointegration, University of Duisburg-Essen, Duisburg. — [2]Institute für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany.

We present a comprehensive study of the optical and x-ray absorption spectra (XAS) in two paradigmatic oxides – $SrTiO_3$ (STO) and MgO, from first-principles calculations. Many-body effects were taken into account by a single step G_0W_0, followed by the excitonic effects by solving the Bethe-Salpeter Equation (BSE). The results demonstrate that the inclusion of the excitonic/electron-(core)hole (e-h) interactions is integral to describe the spectra accurately. For the optical spectra, the influence of different starting exchange-correlation functionals [1,2] is discussed, and the best correspondence with experiment is achieved using a hybrid functional for MgO [2]. The simulated XAS spectra for the O and Mg K-edge (MgO), and O K-edge (STO) are in excellent agreement with experiment w.r.t. the spectral shape and peak positions. We also analyze the origin of prominent peaks in the spectra and identify the orbital character of the relevant contributions by projecting the e-h coupling coefficients from the BSE eigenvectors on the band structure. The real-space projection of the respective wave functions in MgO shows a Wannier-Mott type lowest energy exciton for the optical spectrum, and a strong localization for the O K-edge.

[1] Phys. Rev. Materials **3**, 065004 (2019), [2] arXiv:2012.08960v1

O 12.7 Mon 10:30 P

Self-energy self-consistent density functional theory plus dynamical mean field theory — •Sumanta Bhandary[1] and Karsten Held[2] — [1]School of Physics and CRANN Institute, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria

We propose a hybrid approach which employs the dynamical mean-field theory (DMFT) self-energy for the correlated, typically rather localized orbitals and a conventional density functional theory (DFT) exchange-correlation potential for the less correlated, less localized orbitals. We implement this self-energy self-consistent DFT+DMFT scheme[1], in addition to charge self-consistency[2], in a basis of maximally localized Wannier orbitals using Wien2K, wien2wannier, and the DMFT impurity solver w2dynamics. We apply the method to SrVO3 and report a significant improvement as compared to previous d+p calculations. In particular the position of the oxygen p bands is reproduced correctly, which has been a persistent problem in DFT+DMFT before, and has unwelcome consequences for the d-p hybridization as well as for the correlation strength. Taking the (linearized) DMFT self-energy also in the Kohn-Sham equation bypasses the uncertainty of the "double-counting" problem of DFT+DMFT and yields very similar quasiparticle renormalized bands on the "DFT" and "DMFT" side. [1] S. Bhandary and K. Held, arXiv:1904.02967 (2020). [2] S. Bhandary, E. Assmann, M. Aichhorn, and K. Held, Phys. Rev. B 94, 155131 (2016).

O 13: Poster Session I: Surface magnetism I

Time: Monday 10:30–12:30 Location: P

O 13.1 Mon 10:30 P

Scaling Information Technology to the Atomic Limits — •Brian Kiraly, Elze J. Knol, Werner M.J. van Weerdenburg, Daniel Wegner, and Alexander A. Khajetoorians — Radboud University, Nijmegen, The Netherlands

The end of the scaling era in microelectronics and the expanding demand for computational resources will require new fundamental approaches to energy-efficient computing. The successes of software-based artificial intelligence are promising in this direction, yet the big payoffs promised from hardware implementations are much rarer, as they require the development of dynamic physical systems with tunable, memory-bearing coupling. In this talk, I will discuss our efforts to connect these computational requirements to the physics of single atoms on the surface of the semiconductor black phosphorus. I will show how the screening characteristics of the surface play an important role in stabilizing multiple orbital configurations, or valencies, and how these valencies realize robust non-volatile memory. I will then discuss the valency dynamics in coupled cobalt ensembles on black phosphorus. After revealing how the anisotropic surface- mediated interactions enable tunable atomic coupling, I will demonstrate that a fully functional atomic scale neural network, or so-called Boltzmann machine, can be derived from just seven cobalt atoms on black phosphorus. With two naturally separated time scales, one for computation and one for learning, this atomic Boltzmann machine further presents the possibility for autonomous learning based on the response of the system to external stimuli.

O 13.2 Mon 10:30 P

Chiral spin coupling arising from step edges in ultrathin magnetic films — Anika Schlenhoff, •Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Germany

Step edges represent a local break of lateral symmetry in ultrathin magnetic films. In our experiments, we investigate the spin coupling across atomic step edges on Fe/W(110) by means of spin-polarized scanning tunneling microscopy and spectroscopy.

As we show in our experiments, atomic step edges induce a chiral spin coupling, with outreaching consequences on the local spin texture in the film [1]. Local modifications of the spin texture toward step edges separating double from single layer areas of Fe on W(110) are observed, and selection rules indicate a chiral spin coupling that significantly changes with the propagation along different crystallographic directions. The experimental results will be presented, and the findings are explained in terms of anisotropic Dzyaloshinskii-Moriya interaction arising from the broken lateral symmetry at atomic step edges.

Our experiments strongly indicate that surface roughness and interface quality on the atomic scale is of high relevance for spin manipulation and transmission in terms of tailored magnetic coupling for future spintronic applications.

[1] A. Schlenhoff, S. Krause, and R. Wiesendanger, Phys. Rev. Lett. **123**, 037201 (2019).

O 13.3 Mon 10:30 P

Trends of higher-order exchange interactions in transition metal trilayers — •Mara Gutzeit, Soumyajyoti Haldar, Sebastian Meyer, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Higher-order exchange interactions (HOI) beyond the pair-wise Heisenberg exchange can play a crucial role in the formation of the magnetic ground state of a system. Prominent examples are both Rh/Fe atomic bilayers on Ir(111) [1] and a monolayer Fe on Rh(111) [2] which are shown to exhibit a double-row-wise antiferromagnetic (↑↑↓↓) ground state stabilized by HOI. Here, employing density functional theory as implemented in the FLEUR and VASP code, we investigate the behaviour of HOI in magnetic trilayer systems. Choosing the above-mentioned Rh/Fe/Ir system as a starting point, we systematically study how the HOI change not only with the band filling as Rh (Ir) is replaced by other elements of the 4*d* (5*d*) series but also how they are affected by different stackings of the involved transition metals. Additionally, trends for HOI parameters are presented for the case that the central 3*d* element Fe is replaced by Co. Finally, the values obtained for the biquadratic exchange, the four-site-four-spin term and the three-site-four-spin interaction of the trilayers are compared with values calculated for respective ultrathin film systems.

[1] Romming *et al.* PRL 120, 207201 (2018)

[2] Krönlein *et al.* PRL 120, 207202 (2018)

O 13.4 Mon 10:30 P

Evidence of topological Shiba bands in artificial spin chains on superconductors — •Lucas Schneider[1], Philip Beck[1], Thore Posske[2,3], Daniel Crawford[4], Eric Mascot[5], Stephan Rachel[4], Roland Wiesendanger[1], and Jens Wiebe[1] — [1]Department of Physics, Hamburg University — [2]I. Institute for Theoretical Physics, Hamburg University — [3]Centre for Ultrafast Imaging Hamburg — [4]School of Physics, University of Melbourne — [5]Department of Physics, University of Illinois at Chicago

Magnetic chains on superconducting substrates are a promising system to realize topological superconductivity and Majorana states [1-3]. In this study, we use the tip of a scanning tunneling microscope to assemble magnetic chains atom-by-atom on the surface of an elemental superconductor. We analyze Bogoliubov quasiparticle interference, reveal the formation of multiple in-gap bands and access momentum information about the band dispersions. Using this information, we find evidence that one of the bands is topologically non-trivial and gapped by effective *p*-wave correlations. This work features an important step towards the distinct experimental determination of topological phases from bulk properties only. We acknowledge funding by the ERC via the Advanced Grant ADMIRE (No. 786020), by the Cluster of Excellence 'Advanced Imaging of Matter' (EXC 2056 - project ID 390715994) and by the DFG (SFB-925 - project 170620586). [1] J. Li *et al.* PRB **90**, 235433 (2014). [2] S. Nadj-Perge *et al.*, Science **346**, 6209 (2014). [3] H. Kim *et al.*, Science Advances **4**, eaar5251 (2018).

O 13.5 Mon 10:30 P

Epitaxial growth of Fe on Be(0001) studied by STM — •Karoline Oetker, Hermann Osterhage, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Structural and magnetic properties of Fe thin films can be tuned by the choice of substrate material and lattice structure [1]. Under high pressure, bulk Fe is known to undergo a phase transition to the hexagonal close-packed (hcp) structure [2]. Despite experimental and theoretical efforts, the magnetism of hcp Fe remains unclear [3]. Utilizing substrates with hcp structure as hosts for pseudomorphic growth potentially forces Fe films into the hcp phase, which may then be investigated by spin-polarized scanning tunneling microscopy (SP-STM) [1].

In preparation for such studies, Fe growth on clean Be(0001) surfaces has been investigated in dependence of coverage and substrate temperature during deposition. High resolution STM images and Auger electron spectroscopy will be presented and discussed in terms of growth behavior and chemical composition of the films at room temperature and at elevated temperatures.

[1] R. Wiesendanger, Rev. Mod. Phys. **81**, 1495 (2009).

[2] I. Leonov *et al.*, Phys. Rev. Lett. **106**, 106405 (2011).

[3] R. Lizárraga *et al.*, Phys. Rev. B **78**, 064410 (2008).

O 13.6 Mon 10:30 P

Temperature and magnetic field dependent behavior of atomic-scale skyrmions in Pd/Fe/Ir(111) nanoislands — •Philipp Lindner, Lennart Bargsten, Stepan Kovaric, Johannes Friedlein, Jonas Harm, Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Jungiusstraße 11A, 20355 Hamburg, Germany

The thermal stability of atomic-scale skyrmions is of high relevance for potential spintronics applications and validation of theoretical models, but atomic-scale skyrmion observation was hitherto limited to very low temperatures.

In our recent study [1], we employed our unique experimental setup [2] to systematically explore the thermomagnetic phase space of Pd/Fe nanoislands on an Ir(111) substrate in an external magnetic field up to 3 T within the temperature range between 1 K and 100 K via scanning tunneling microscopy and spectroscopy.

Evidence is found for the spin spiral, field-polarized and fluctuating disordered magnetic phases. Irrespective of considerable thermally driven magnetization dynamics, evidence for skyrmions is found at up to approximately 80 K. This critical temperature is almost tripled compared to the Fe/Ir(111) system without Pd capping [3], thereby demonstrating the stabilization of atomic-scale skyrmions against thermal agitation by highly polarizable adlayers.

[1] P. Lindner *et al.*, Phys. Rev. B **101**, 214445 (2020).

[2] J. Friedlein *et al.*, Rev. Sci. Instrum. **90**, 123705 (2019).

[3] A. Sonntag *et al.*, Phys. Rev. Lett. **113**, 077202 (2014).

O 13.7 Mon 10:30 P

Bloch-type spin helix in bilayer Fe islands on Ir(110) measured by spin-polarized STM — •Jeison A. Fischer[1], Timo Knispel[1], Vasily Tseplyaev[2], Markus Hoffmann[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Most work on interfacial chiral spin textures focused on films exhibiting C_{3v} symmetry and isotropic Dzyaloshinskii-Moriya interaction (DMI), known to only support Néel-type spin helices and skyrmions [1]. In contrast, C_{2v} symmetry systems such as the (110) surface of an fcc crystal are predicted to show anisotropic DMI, leading to various scenarios of topological pattern formation [2]. Fully unexpectedly, our spin-polarized STM/STS study reveals a magnetic stripe phase, due to a spin helix with a period of 1.2 nm along the $[\bar{1}10]$ direction in bilayer Fe islands on unreconstructed Ir(110). Based on detailed field dependent measurements with a vector magnet, we conclude that the chirality of the spin helix is of Bloch-type, where the rotation is perpendicular with the propagation direction. This contradicts the assumption of the spin helix being induced by an interface in-plane DMI vector. Combined with theoretical insights, we discuss our findings in terms of the formation energy in systems with C_{2v} symmetry.

[1] S. Heinze et al. Nat. Phys. Vol.7, p.713 (2011).
[2] M. Hoffmann et al. Nat. Commun. Vol.8, p.308 (2017).

O 13.8 Mon 10:30 P

Efficient Ab-initio Multiplet Calculations for Magnetic Adatoms on MgO — •Christoph Wolf[1], Fernando Delgado[2], Jose Reina[3], and Nicolas Lorente[3] — [1]Center for Quantum Nanoscience, Seoul, Korea — [2]Universidad de La Laguna, Spain — [3]Centro de Fisica de Materiales CFM/MPC, Spain

Scanning probe microscopy and spectroscopy, and more recently in combination with electron spin resonance, have allowed the direct observation of electron dynamics on the single-atom limit. The interpretation of data is strongly depending on model Hamiltonians. However, fitting effective spin Hamiltonians to experimental data lacks the ability to explore a vast number of potential systems of interest. By using plane-wave density functional theory (DFT) as starting point, we build a multiplet Hamiltonian making use of maximallylocalized Wannier functions. The Hamiltonian contains spinorbit and electron-electron interactions needed to obtain the relevant spin dynamics. The resulting reduced Hamiltonian is solved by exact diagonalization. We compare three prototypical cases of 3d transition metals Mn (total spin S=5/2), Fe (S=2) and Co (S=3/2) on MgO with experimental data and find that our calculations can accurately predict the spin orientation and anisotropy of the magnetic adatom. Our method does not rely on experimental input and permits us to explore and predict the fundamental magnetic properties of adatoms on surfaces.

O 14: Poster Session I: Nanostructures at surfaces I

Time: Monday 10:30–12:30 Location: P

O 14.1 Mon 10:30 P

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747AG Groningen, the Netherlands — [2]Strating Institute for Chemistry, University of Groningen, 9747AG Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material due to their excellent and tunable electronic properties. For instance, GNRs with armchair edge possess a width-dependent band gap, whereas zigzag GNRs are expected to host spin-polarized edge states and be semimetallic [1]. Previously, narrow chevron-like GNRs, which host a combination of zigzag and armchair edge terminations, were fabricated on a Au(111) substrate from the prochiral precursor 6,12-dibromochrysene through a combination of Ullmann-type coupling and cyclodehydrogenation [2]. Depending on the number of monomer units the ribbons are made of, an even and an odd number lead to a mirror and a point symmetric ribbon. Using scanning tunneling spectroscopy we investigated the potential effect of this length dependent symmetry on the electronic properties. In addition, we observed that through a common coupling defect bends are formed in the ribbons. We characterized these bends using a combination of high-resolution scanning tunneling microscopy and spectroscopy. It turned out the bends are based on the formation of both a five- and six-membered ring and that their electronic properties are altered. [1] K. Nakada et al., Phys. Rev. B 54, 17954 (1996) [2] T.A. Pham et al., Small 13, 1603675 (2017)

O 14.2 Mon 10:30 P

Thermally vs. Light-Induced On-Surface Polymerization — •Christophe Nacci and Leonhard Grill — Department of Physical Chemistry, University of Graz, Austria

Covalent on-surface polymerization via Ullmann coupling is one of the preferred chemical reactions to produce novel, and potentially functional, structures in the two-dimensional confinement of a surface. The dissociation of specific substituents and the formation of new covalent bonds can be induced by using different external stimuli, for instance heat, light and inelastic electron scattering. While plenty of examples exist on the thermal control of the reaction, only very few studies have reported a photochemical approach to form polymers at single-crystal surfaces. We compare the reaction pathways of individual molecular species to one-dimensional polymers by driving the reaction of the same precursor on Au(111) either by heat or by illumination with UV light. The results obtained by low-temperature scanning tunneling microscopy under ultrahigh vacuum conditions show that both stimuli are successful to induce the desired reaction on the surface. However, very different polymer length distributions are found, which will be discussed in view of the experimental conditions. Interestingly, under UV illumination the molecular coverage changes across the surface as it increases at the position of laser spot on the sample.

O 14.3 Mon 10:30 P

Adsorption Geometry and Intramolecular Reactions of 9-bromo-10- (1,1':3',1"-terphenyl-5'-yl)anthracene on Au(111) and Cu(111) — •Alexander Ihle[1], Daniel Ebeling[1], Doreen Mollenhauer[2], Hermann A. Wegner[3], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

On-surface chemistry is a powerful tool for building covalent molecular structures such as chains or graphene nanoribbons [1, 2]. Such tailored materials are interesting for future applications since their optical and electronic properties are controllable via their structure [3]. Furthermore, their main component carbon is environmentally friendly and sustainable. In addition to the structure of the precursors, the chemical properties of the substrate direct the reaction pathway. Using low-temperature atomic force microscopy with CO-functionalized tips, we identify the precise adsorption geometry of the pristine molecules, intermediates, and reaction products after subsequent heating steps. While the pristine molecules show similar features on both surfaces and adsorb quasi-planar, the adsorption geometry of the intermediates differs after heating depending on the substrate material. We suspect that different molecule-substrate interactions lead to this observation.

[1] Grill, L. et al. Nature Nanotechnology 2, 687-691 (2007)
[2] Cai, J. et al. Nature 466, 470-473 (2010)
[3] Zhong, Q. et al. J. Am. Chem. Soc. 141, 7399-7406 (2019)

O 14.4 Mon 10:30 P

Kinetically controlled on-surface playground of nanostructure growth — •Aisha Ahsan[1], Fatemeh Mousavi Mousavi[1], Thomas Nijs[1], Sylwia Nowakowska[1], Olha Popova[1], Aneliia Wäckerlin[1], Jonas Björk[2], Lutz Gade[3], and Thomas Jung[1,4] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, Linköping 581 83, Sweden — [3]Anorganisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany — [4]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Rare gases on metals serve as models for understanding mass transport and crystal growth of adsorbates on surfaces, while LT-STM studies enriched our knowledge how rare gases behave at atomic level. Deep insight has been gained into the diffusion mechanisms of van der Waals adsorbates on a complex energy landscape defined by an on-surface coordination network architecture. Using Xe as the model case, a complex re-distribution/re-nucleation and coarsening/growth phenomena has been investigated where the adsorbate can be evaporated/recaptured into/from *gas phases* or *lattice gas phases* between 5K and 50K showing hopping motion between different confinements (0D), along boundaries of network (1D) and across whole network backbone (2D). After heating to ~50K then back to 5K, atoms are exclusively found in the thermally minimal state of 12 Xe atoms filling one pore, a process which we assign to the analogon of Ostwald ripening/coarsening transition which clearly limited in size.

O 14.5 Mon 10:30 P

Electrospray Ion Beam Deposition of Biological Molecules — •Henrik Siboni[1,2], Andreas Zimmer[2], and Leonhard Grill[1] — [1]Single-Molecule Chemistry, Institute of Chemistry, University of Graz, Austria — [2]Pharmaceutical Technology & Biopharmacy, Institute of Pharmaceutical Sciences, University of Graz, Austria

Scanning Tunneling Microscopy under Ultra-High Vacuum (UHV) conditions is a powerful method to image single molecules. However, its application in biophysics and pharmacy is limited by the fact that thermal sublimation, which is the common deposition method under UHV, requires rather high temperatures, due to the large molecular mass and thus low vapour pressures. This typically leads to molecular fragmentation before they can adsorb on a surface. Drop casting, on the other hand, can leave too much solvent contamination. In this poster, electrospray ion beam deposition of biological molecules will be presented where the molecules are gently transferred from solution under atmospheric pressure to a single-crystal metal surface at UHV pressure.

O 14.6 Mon 10:30 P

Defect-mediated *ab initio* thermodynamics of metastable γ-MoN(001) — •Giyeok Lee[1], Hojun Lee[1], Taehun Lee[1,2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Chemistry, Princeton University, Princeton, New Jersey 08540, United States

Refractory transition metal nitrides exhibit a plethora of polymorphic expressions and chemical stoichiometries. To afford a better understanding of how defects may play a role in the structural and thermodynamics of these nitrides, using density-functional theory calculations, we investigate the influence of point and pair defects in bulk metastable γ-MoN and its (001) surface. We report favorable formation of Schottky defect pairs of neighboring Mo and N vacancies in bulk γ-MoN and apply this as a defect-mediated energy correction term to the surface energy of γ-MoN(001) within the *ab initio* atomistic thermodynamics approach. We also inspect the structural distortions in both bulk and surfaces of γ-MoN by using the partial radial distribution function, $g(r)$ of Mo-N bond lengths. Large atomic displacements are found in both cases, leading to a broad spread of Mo-N bond length values when compared to their idealized bulk values. We propose that these structural and thermodynamic analysis may provide some insight to a better understanding of metastable materials and their surfaces.

O 14.7 Mon 10:30 P

Completing the Picture of Embryonic Oxidation on Copper — •Yun-Jae Lee[1], Trinh Thi Ly[2], Taehun Lee[1], Krisztián Palotás[3], Se Young Jeong[4], Jungdae Kim[2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, and EHSRC, University of Ulsan, Ulsan 44610, Republic of Korea — [3]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, 1525 Budapest, Hungary — [4]Department of Optics and Mechatronics Engineering, Pusan National University, Busan 46241, Republic of Korea

The oxidation of copper surfaces has been studied extensively in the literature – from simple oxygen chemisorption to the formation of complex surface oxides. Having an accurate atomistic model for this metal/oxide interface plays a pivotal role in determining interfacial processes in many copper-based technologies. The “29” and “44” complex surface oxides represent two of the most classical embryonic oxides on Cu(111). Although many attempts have been made to offer a detailed atomistic model of these surface oxides, their atomic structures remain ambiguous. In this work, we address this open question via *ab initio* scanning tunneling microscopy simulations that go beyond the simplistic Tersoff-Hamann approach where the (functionalized) metal tips are explicitly included, and are corroborated by high-resolution STM experiments. In particular, we reexamine the “29” structure and elucidate a complete atomistic model for the “44” structure.

O 14.8 Mon 10:30 P

Nano-hillock formation on CaF_2 due to individual slow Au-cluster impacts — •Gabriel L. Szabo[1], Markus Lehner[1], Lothar Bischoff[2], Wolfgang Pilz[2], Ulrich Kentsch[2], Friedrich Aumayr[1], Nico Klingner[2], and Richard A. Wilhelm[1] — [1]TU Wien, Institute of Applied Physics, 1040 Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Ion-irradiation of surfaces was found to be a very powerful technique for surface modifications on a large amount of technologically relevant materials. Especially the formation of nanostructures, such as iontracks and nano-hillocks, which are mediated by electronic excitation induced by slow highly charged ions and swift heavy ions received lots of interest in recent years. For those experiments, the ionic crystal CaF_2 was a model system for the underlying processes. We use the same model system here, but a more direct way of creating nanohillocks by heavy cluster irradiation. In our investigations we show the formation of nanohillocks by slow individual Au-cluster-irradiation on CaF_2(111) surface that are very similar to hillocks iobserved previously with highly charged ions. We show that the size of the hillocks can be tuned by the cluster size.

O 14.9 Mon 10:30 P

A molecular quantum ring formed from a π-conjugated macrocycle — Chris J. Judd[1], Anton S. Nizovtsev[2,3,4], Rikke Plougmann[1], Dmitry V. Kondratuk[5], Harry L. Anderson[5], Elena Besley[2], and •Alex Saywell[1] — [1]School of Physics & Astronomy, University of Nottingham, UK. — [2]School of Chemistry, University of Nottingham, UK. — [3]Nikolaev Institute of Inorganic Chemistry, Russian Academy of Sciences, Russian Federation. — [4]Novosibirsk State University, Russian Federation. — [5]Department of Chemistry, University of Oxford, UK.

Quantum rings are structures that facilitate phase-coherent electron motion around a closed path and exhibit quantum phenomena; e.g. persistent currents and the Aharonov-Bohm effect. Our approach utilises cyclic porphyrin polymers, possessing a delocalised π-conjugated electronic structure [1], as molecular quantum rings.

We present details from our recent work [2] where the electronic structure of a molecular quantum ring (a 40 unit cyclic porphyrin polymer within stacks of 2-3 rings supported on a Ag(111) substrate) is characterised via scanning tunnelling microscopy (STM) and scanning tunnelling spectroscopy (STS). Combining density functional theory and tight binding calculations, in concert with experimental data, we interpret the experimentally obtained electronic structure in terms of quantum states confined around the π-conjugated macrocycle.

[1]M.D. Peeks,et al., Nature 541, 200 (2017).[2]C.J. Judd, et al., Phys.Rev.Lett. 125, 206803 (2020).

O 15: Mini-Symposium: Ultrafast surface dynamics at the space-time limit II

Time: Monday 13:30–15:30 Location: R1

Invited Talk O 15.1 Mon 13:30 R1

The ultrafast Einstein-de Haas effect triggered by ultrafast demagnetization — •Steven L. Johnson[1,4], Christian Dornes[1], Yves Acremann[2], Matteo Savoini[1], Martin Kubli[1], Martin J. Neugebauer[1], Elsa Abreu[1], Lucas Huber[1], Gabriel Lantz[1], Carlos A. F. Vaz[3], Henrik Lemke[4], Elizabeth M. Bothschafter[3], Michael Porer[3], Vincent Esposito[3], Laurenz Rettig[3,5], Michael Buzzi[3,6], Aurora Alberca[3], Yoav W. Windsor[3,5], Paul Beaud[4], Urs Staub[3], Diling Zhu[7], Sanghoon Song[7], and James M. Glownia[7] — [1]Institute for Quantum Electronics, Physics Department, ETH Zurich, Zurich, Switzerland — [2]Laboratory for Solid State Physics, Physics Department, ETH Zurich, Zurich, Switzerland — [3]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland — [4]SwissFEL, Paul Scherrer Institute, Villigen, Switzerland — [5]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [6]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [7]Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, Menlo Park, CA, USA

The Einstein-de Haas effect is a historically important experiment that demonstrated clearly the equivalence between spin angular momentum and mechanical angular momentum. Here I discuss an experiment where ultrafast demagnetization driven by laser excitation of a thin film of iron drives transverse atomic displacement waves from the interfaces of the film, a direct consequence of subpicosecond angular momentum transfer from electronic spins to the lattice.

Round Table Discussion and introduction of panel members:

All following contributed talks will be presented in form of a round table discussion with expert panel members Prof. Martin Aeschlimann (TU Kaiserslautern), Prof. Michael Horn-von-Hoegen (U Duisburg) and Prof. Julia Stähler (HU Berlin)

O 15.2 Mon 14:05 R1

Structural Dynamics at Surfaces: Current State and Prospects of tr-RHEED — •Christian Brand, Jonas Fortmann, Thorben Groven, Tobias Witte, Fabian Thiemann, Bernd Hafke, Mohammad Tajik, and Michael Horn-von Hoegen — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg

Ultrafast time-resolved reflection high energy electron diffraction (tr-RHEED) is employed to follow structural dynamics at surfaces upon fs-laser excitation. We measure the transient changes of intensity, profile and position of diffraction spots in a pump-probe setup with a temporal resolution of 350 fs. We demonstrate the broad capabilities of this technique through three examples: Electron phonon coupling and nanoscale heat transport is studied for ultrathin epitaxial Pb and Bi films through the Debye-Waller effect [1,2]. Ultrafast dynamics in the In atomic wire system on Si(111) serves as an example for a strongly driven first order phase transition (PT) [3]. The dynamics of a second order PT are observed through the order-disorder transition in the Si spin chain system on the Si(553)-Au surface [4]. We discuss future developments of this technique for improving the temporal resolution below 200 fs at increased brightness of the electron pulses, the perspectives of mode specific excitation with reduced photon energy or with THz radiation, and the combination of electron and optical probes to access transient changes of electronic properties. [1] T. Witte *et al.*, Appl. Phys. Lett. **110**, 243103 (2017); [2] V. Tinnemann *et al.*, Structural Dynamics **6**, 035101 & 065101 (2019); [3] T. Frigge *et al.*, Nature **544**, 207 (2017); [4] B. Hafke *et al.*, PRL **124**, 016102 (2020).

O 15.3 Mon 14:25 R1

Towards understanding the time evolution of metastable charge-ordered states — •Yaroslav A. Gerasimenko[1,2], Jan Ravnik[1,3], Jaka Vodeb[1], Michele Diego[1], Yevhenii Vaskivskyi[1], Viktor V. Kabanov[1], Igor Vaskivskyi[4], Tomaz Mertelj[1,4], and Dragan Mihailovic[1,4,5] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]University of Regensburg, Regensburg, Germany — [3]Paul Scherrer Institute, Villigen, Switzerland — [4]CENN Nanocenter, Ljubljana, Slovenia — [5]University of Ljubljana, Ljubljana, Slovenia

Metastable self-organized electronic states in quantum materials are emergent states of matter[1] typically formed through phase transitions under non-equilibrium conditions. It is of fundamental importance to understand the process of their formation that can involve multiple mechanisms[1,2] spanning a large range of timescales.

Here we combine multiple techniques to map the evolution of metastable states in 1T-TaS_2, a prototypical charge-ordered quantum material, using the photon density and temperature as control parameters on timescales ranging from 10^{-12} to 10^3s. The combination of STM and in situ ultrafast excitation allows us to observe explicitly both parametric stability and nanoscale relaxation of the light-induced metastable states on the scale of seconds, while time-resolved optical techniques and electrical measurements allow us to study the ordering and relaxation processes down to a few picoseconds. [3]

[1] Ya. A. Gerasimenko et al., Nature Materials 18, 1078-1083 (2019)

[2] Ya. A. Gerasimenko et al., npj Quantum Materials 4, 1-9 (2019)

[3] J. Ravnik et al., arXiv:2011.00930

O 15.4 Mon 14:45 R1

Ultrafast atomic and electronic dynamics at the molecule-$TiSe_2$ interface — •Markus Scholz[1], Kiana Baumgärtner[2], Nils Wind[3], Christian Metzger[2], Dmytro Kutnyakhov[4], Michael Heber[4], Lukas Wenthaus[4], Friedrich Roth[5], Kai Rossnagel[6], Friedrich Reinert[2], and Serguei Molodtsov[1] — [1]European X-Ray Free-Electron Laser Facility, Schenefeld — [2]Experimentelle Physik 7, Julius-Maximilians-Universität, Würzburg — [3]Universität Hamburg — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg — [5]TU Bergakademie Freiberg — [6]Christian-Albrechts-Universität zu Kiel

In recent years layered transition-metal dichalcogenides (TMDCs) have been extensively investigated due to their intriguing electronic phenomena ranging from Mott localization to charge-density-wave (CDW) formation [1] as well as their potential for novel electronic and optical devices. First studies of adsorbed molecules on the TMDC surface have revealed a rich potential to tailor optical, electronic, and magnetic properties of organic-TMDC devices. However, very few studies have been carried out on understanding fundamental interactions at the molecule-TMDC interface. Time-resolved imaging of orbitals with time-resolved photoelectron spectroscopy (trPES) will not only allow us to separate the molecular contribution to the trPES signal but also to determine the ultrafast charge-transfer dynamics at the interface. In order to probe structural changes at the interface, we also perform time-resolved XPD at FLASH FEL.

[1] Rossnagel K, et. al., J Phys Cond Matter 23:213001 (2011)

O 15.5 Mon 15:05 R1

Tracing orbital images on ultrafast time scales — •Robert Wallauer[1], Miriam Raths[2,3], Klaus Stallberg[1], Lasse Münster[1], Dominik Brandstetter[4], Xiaosheng Yang[2,3], Jens Güdde[1], Peter Puschnig[4], Sergey Soubatch[2], Christian Kumpf[2,3], Francois C. Bocquet[2], Frank Stefan Tautz[2,3], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Peter Grünberg Institut, PGI-3, Forschungszentrum Jülich, Germany — [3]Jülich Aachen Research Alliance (JARA), Jülich, Germany — [4]Insititute of Physics, Universität Graz, Austria

Photoemission tomography is a powerful tool to image the electron distribution in molecular orbitals in momentum space. Unoccupied molecular orbitals, however, have not been accessed until now. In our experiment, we combine time-resolved photoemission using high laser harmonics and a momentum microscope to establish a tomographic, femtosecond pump-probe experiment of unoccupied molecular orbitals. We measure the full momentum-space distribution of transiently excited electrons within a single molecular layer of PTCDA on an oxygen-passivated Cu(001) surface.

Beside the identification of the lowest unoccupied molecular orbital and its lifetime, we were able to link the excited state dynamics to real-space excitation pathways. Electron transfer from the substrate to the molecule and intramolecular excitation lead to distinct signatures in the time evolution of the respective momentum map. Our results show the potential of this technique to identify electron excitation and transfer processes at molecular surfaces and interfaces.

Concluding remarks

O 16: Mini-Symposium: Free-standing functional molecular 2D materials II

Time: Monday 13:30–15:30 Location: R2

Invited Talk O 16.1 Mon 13:30 R2

Combining 2D materials and optical metasurfaces — •Isabelle Staude — Institute of Solid State Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, 07743 Jena, Germany

Optical metasurfaces, two-dimensional arrangements of designed nanoresonators, offer unique opportunities for controlling light fields and for tailoring the interaction of light with nanoscale matter. Due to their flat nature, their integration with two-dimensional materials consisting of only a single molecular layer is particularly interesting [1]. This talk reviews our recent and ongoing activities in hybridizing optical metasurfaces composed of resonant metallic or dielectric building blocks with different types of two-dimensional materials, including monolayer transition metal dichalcogenides (2D-TMDs) and carbon nanomembranes (CNMs). On the one hand, we will show that CNMs can serve as mechanically stable substrates for free-standing metasurface architectures of nanoscale thickness [2]. On the other hand, we will demonstrate that the ability of the nanoresonators to concentrate light into nanoscale volumes can be utilized to carefully control the properties, such as pattern and polarization, of light emitted by 2D-TMDs via photoluminescence or nonlinear processes [3,4]. [1] R. Mupparapu et al., Advances in Physics: X 5, 1734083 (2020). [2] Y. D. Sirmaci et al., ACS Photonics 7, 1060 (2020). [3] T. Bucher et al., ACS Photonics 6, 1002 (2019). [4] F. J.F. Löchner et al., ACS Photonics, https://doi.org/10.1021/acsphotonics.0c01375 (2020).

O 16.2 Mon 14:00 R2

Towards atomic-resolution HRTEM imaging of organic 2D materials — •Haoyuan Qi, Baokun Liang, David Mücke, and Ute Kaiser — Electron Microscopy Group of Materials Science, Universität Ulm, 89081 Ulm, Germany

Organic two-dimensional materials (O2DMs), such as 2D polymers, 2D covalent-organic frameworks (COFs), and 2D metal-organic frameworks (MOFs), open up the exciting possibility of crystal engineering tailored for next-generation applications. However, structural characterization of O2DMs via transmission electron microscopy (TEM) remains a formidable task. The main challenge arises from the strong interaction between incident electrons and the bonded hydrogen atoms. During TEM imaging, the incident electrons transfer kinetic energy to the atoms (i.e., knock-on damage) and may trigger bond dissociation and various chemical reactions degrading the structural integrity of O2DMs.

Here, we will present a comprehensive illustration of experimental techniques that are dedicated to enhancing achievable image resolution. For instance, through low-dose HRTEM imaging, a near-atomic resolution has been achieved on 2D polyimine under 300 kV. We further demonstrate that, by applying a mid-range acceleration voltage, i.e., 120 kV, the useful structural information per unit damage can be enhanced in several COFs, resulting in higher S/N ratio in the experimental images as compared to 300 kV. Besides, through a hydrogen-free structural design, MOFs' intrinsic stability can be significantly increased, allowing direct observation down to atomic scale.

O 16.3 Mon 14:15 R2

Mechanics of free-standing inorganic and molecular 2D materials — •Xianghui Zhang, André Beyer, Florian Paneff, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

The discovery of graphene has triggered a great interest in inorganic as well as molecular two-dimensional (2D) materials. In this contribution, we summarize recent progress in the mechanical characterization of free-standing 2D materials, such as graphene, hexagonal boron nitride (hBN), transition metal-dichalcogenides, MXenes, black phosphor, carbon nanomembranes (CNMs), 2D polymers, 2D metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). Elastic, fracture, bending and interfacial properties of these materials have been determined using a variety of experimental techniques including AFM-based nanoindentation, in situ tensile/fracture testing, bulge testing, Raman spectroscopy, Brillouin light scattering, and buckling-based metrology. Additionally, we address recent advances of 2D materials in mechanical applications, including resonators, microphones, and nanoelectromechanical sensors.

Invited Talk O 16.4 Mon 14:30 R2

Electronic properties of freestanding ultra-thin small-molecular and multilayer graphene films — •Thomas Weitz — I. Physics Institute, Faculty of Physics, Georg-August-University Göttingen, Germany — AG Physics of Nanosystems, Faculty of Physics, LMU Munich, Germany

Suspension of thin functional films allows to investigate their electronic properties in vacuum - a low-dielectric (low-k) environment free from contaminants. Two examples of our recent work in this direction will be discussed: 1.) Highly-crystalline, two molecule thin organic semiconducting films composed of an electron-conductive perylene-diimide have been investigated by temperature-dependent charge transport and have shown a small density of charge traps due to the inert surrounding. [1] 2.) Enabled by the low-k surrounding, dually-gated, suspended bi- and trilayer graphene films show exchange-driven quantum phases such as the quantum anomalous Hall effect. [2-4]

[1] L.S. Schaffroth, J. Lenz, V. Geigold, M. Kögl, A. Hartschuh, R.T. Weitz, Adv. Mat. 31, 1808309 (2019) [2] R.T. Weitz, M.T. Allen, B.E. Feldman, J. Martin, and A. Yacoby, Science 330, 812 (2010) [3] F.R. Geisenhof, R.T. Weitz et al. In preparation (2021) [4] F. Winterer, R.T. Weitz et al. In preparation (2021)

O 16.5 Mon 15:00 R2

Sensitive detection of biomarkers in clinical samples based on van der Waals heterostructures of carbon nanomembrane and graphene — •David Kaiser[1], Nikolaus Meyerbroeker[2], Werner Purschke[3], Simone Sell[3], Christof Neumann[1], Andreas Winter[1], Zian Tang[1], Daniel Hüger[1], Gerben Ferwerda[4], Thomas Weimann[5], Marien de Jonge[4], Albert Schnieders[2], Axel Vater[3], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Germany — [2]CNM Technologies GmbH, Germany — [3]APTARION biotech AG, Germany — [4]Radboud University, The Netherlands — [5]Physikalisch-Technische Bundesanstalt, Germany

Due to their low surface charge in aqueous electrolytes, almost direct contact with the analyte and special electronic properties, graphene field-effect transistors (GFETs) are promising for ultrasensitive biodetection. However, challenges with their reliable biochemical functionalization have hindered their use with real clinical samples so far. Here, we employ 1 nm thick carbon nanomembranes (CNMs) to functionalize GFETs via van der Waals assembly of the CNM/graphene heterostructures. The aptamers grafted on the CNMs result in specific adsorption of the relevant biomarkes on the GFET surface. Using clinical samples, we demonstrate the detection of the biomarker CXCL8 with a very low concentration (5 pg/ml). We support our experimental findings by a detailed modelling of the device performance.

Final discussion with all speakers

O 17: Mini-Symposium: Frontiers of electronic-structure theory: Focus on electron-phonon interactions I

Time: Monday 13:30–15:30 Location: R3

Invited Talk O 17.1 Mon 13:30 R3

Predominance of non-adiabatic effects in zero-point renormalization of electronic energies — •Xavier Gonze[1,2], Anna Miglio[1], Véronique Brousseau-Couture[3], Gabriel Antonius[4,5], Yang-Hao Chan[4], Steven Louie[4], Bogdan Guster[1], Matteo Giantomassi[1], and Michel Côté[3] — [1]UCLouvain, Belgium — [2]Skoltech, Moscow, Russia — [3]U. de Montréal, Canada — [4]U. California at Berkeley, USA and NBNL, Berkeley, USA — [5]U. Québec à Trois-Rivières, Canada

Electronic and optical properties of materials are affected by atomic motion through electron-phonon interaction: not only band gaps change with temperature, but even at zero K, zero-point motion causes band-gap renormalization. We present a large-scale first-principles evaluation of the zero-point renormalization beyond the adiabatic approximation [1]. For materials with light elements, the band gap renormalization is often larger than 0.3 eV, and up to 0.7 eV. This effect cannot be ignored if accurate band gaps are sought. For infrared-active materials, global agreement with available experimental data is obtained only when non-adiabatic effects are taken into account. They even dominate zero-point renormalization for many materials, as shown by a generalized Fröhlich model that includes multiple phonon branches, anisotropic and degenerate electronic extrema, whose range of validity is established by comparison with first-principles results. We also investigate effective mass changes in such generalized Fröhlich model. [1] A. Miglio et al. npj Computational Materials, 6, 167 (2020).

Invited Talk O 17.2 Mon 14:00 R3

Huge quantum effects on the 250 K superconducting lan- thanum hydride — •Ion Errea — University of the Basque Country, San Sebastian, Spain

The discovery of superconductivity at 200 K in the hydrogen sulfide system at large pressures was a clear demonstration that hydrogen-rich materials can be high-temperature superconductors. The recent syn- thesis of LaH10 with a superconducting critical temperature (Tc) of 250 K place these materials at the verge of reaching the long-dreamed room-temperature superconductivity. Here we show that quantum atomic fluctuations stabilize in the superconducting pressure range a high-symmetry Fm-3m crystal structure consistent with experiments, which has a colossal electron-phonon coupling of 3.5. Even if ab initio classical calculations predict this structure to distort below 230 GPa yielding a complex energy landscape, the inclusion of quantum effects evidences the Fm-3m as the true ground state. The agreement be- tween the calculated and experimental Tc values further supports this phase as responsible for the 250 K superconductivity. The relevance of quantum fluctuations questions many of the crystal structure predic- tions made for hydrides within a classical approach that at the moment guide the experimental quest for room-temperature superconductivity. Furthermore, quantum effects are revealed to be crucial to stabilize solids with extraordinary electron-phonon coupling, which may other- wise be destabilized by the large electron-phonon interaction, reducing the pressures needed for their synthesis.

Invited Talk O 17.3 Mon 14:30 R3

Out-of-equilibrium lattice dynamics in two-dimensional materials — •Fabio Caruso — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

The coupling between electronic and vibrational degrees of freedom influences profoundly the ultrafast dynamics of electrons [1] and phonons [2]. We conducted first-principles calculations of the coupled electron-phonon dynamics to investigate the characteristic fingerprints of crystal-lattice vibrations in systems driven out of equilibrium by the interaction with ultra-short light pulses. The relaxation of photo-excited carriers via phonon emission exhibits a striking selectivity in momentum space, and it underpins the emergence of a non-thermal vibrational state of the lattice. These vibrational excited states are characterized by a highly anisotropic population of different phonons and persist for up to 10 ps, until thermal equilibrium is re-established by phonon-phonon scattering. For the prototypical layered semiconductors black phosphorus and MoS2, these findings are corroborated by femto-second electron diffuse scattering (FEDS) experiments [3]. The control of non-thermal vibrational states may provide unexplored opportunities to selectively enhance the phonon population and, thereby, transiently tailor electron-phonon interactions over picosecond time scales.

[1] Caruso, Novko, Draxl, Phys. Rev. B 101, 035128 (2020). [2] Novko, Caruso, Draxl, Cappelluti, Phys. Rev. Lett. 124, 077001 (2020). [3] Seiler, Zahn, Zacharias, Hildebrandt, Vasileiadis, Windsor, Qi, Carbogno, Draxl, Caruso, Ernstorfer, arXiv:2006.12873 (2020).

Invited Talk O 17.4 Mon 15:00 R3

Ultrafast optical control of complex oxide functional properties: New insights from theory and first-principles calculations — •Nicole Benedek — Cornell University, Ithaca, NY USA

Recent experiments have demonstrated the potential for ultrafast changes in the functional properties of materials upon selective optical excitation of particular phonon modes. The chemical diversity of complex oxides, and their strong lattice-properties coupling, have made them ideal test systems for new experimental approaches that exploit anharmonic phonon couplings to induce and modify magnetism, superconductivity and ferroelectricity with light. In this talk, I will describe our recent theoretical efforts exploring ultrafast optical control of the functional properties of perovskite oxides. First, I will describe the theoretical framework that we have developed, and the role of electronic structure calculations in that framework. I will then focus on an example of our framework in action: dynamical stabilization of a non-equilibrium magnetic phase in $GdTiO_3$. Finally, I will consider how to identify materials that may exhibit a large dynamical response and present our results of a systematic exploration of intrinsic materials factors that may contribute to the nonlinear phononics response in $LaAlO_3$. Our work highlights the importance of understanding the contributions of small structural distortions to the optical response in perovskites (in contrast with large-amplitude distortions, such as octahedral rotations), and illustrates how anharmonic mode coupling strengths may not be the most important factor in which materials exhibit large or unusual responses, as has generally been assumed.

O 18: Poster Session II: Metal substrates II

Time: Monday 13:30–15:30 Location: P

O 18.1 Mon 13:30 P

Atom exchange and registry shift upon formation of surface tellurides on Ag(111) and Cu(111) — •Andreas Raabgrund, Maximilian Ammon, Tilman Kisslinger, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The formation of (surface) metal alloys using Te achieved a lot attention lately, e.g. for photovoltaics or thermoelectrics [1]. In this work, we study the initial stages of Te surface alloy formation on Ag(111) and Cu(111) by STM, STS, LEED, and DFT. For coverages below 0.14 ML tellurium is readily incorporated into the topmost substrate layer via local atomic exchange. The process occurs already at or below room temperature and eventually leads to a $(\sqrt{7}\times\sqrt{7})$R19.1° short-range order. Increasing the Te coverage leads to coexisting islands of a $(\sqrt{3}\times\sqrt{3})$R30° superstructure on Ag(111) [2] and a $(2\sqrt{3}\times\sqrt{3})$R30° superstructure on Cu(111) [3], which are well-ordered and fully developed at $\Theta = 1/3$ ML Te. In these two phases, the top layer has $1:1$ stoichiometry in hcp registry to the substrate and only 2/3 of the surface sites are occupied. The Te atoms are only threefold coordinated in-plane. STS data shows that the substitutional Te phases have a distinctly different electronic structure from that of the well-ordered phases at $\Theta = 1/3$ ML. Notably, the unoccupied dispersing states with sp_z character are not found anymore in the range E_F to $E_F + 2.5$ eV. [1] Ibers J., Nat. Chem. **1**, 508 (2009) [2] Ünzelmann et al, Phys. Rev. Lett. **124**, 176401 (2020) [3] Kisslinger T., Phys. Rev. B. **102**, 155422 (2020)

O 18.2 Mon 13:30 P

Growth of samarium thin films and subsequent oxidation on polycrystalline copper — •Emilia Pozarowska, Carlos Morales, and Jan Ingo Flege — BTU Cottbus-Senftenberg, Konrad-Zuse-Str. 1, 03046 Cottbus, Germany

The growth of samaria thin films on copper sheets has been chemically studied by in situ X-ray photoelectron spectroscopy (XPS). The early stages of growth (0.1-14 ML) were studied by consecutive evaporations of Sm by chemical vapor deposition followed by XPS measurements. Subsequently, samaria films of different thicknesses, namely 0.1, 1, and 14 ML, were oxidized at room temperature (RT). The evolution of the sample morphology was determined through inelastic peak shape analysis (IPSA) using the QUASES software as an indirect method to study the relationship between Sm oxidation state and its surface arrangement. Our results show that samarium grows as 2D islands up to 2ML, which is followed by 3D growth. Chemical analysis indicates that at low coverages (<0.5ML) Sm is already oxidized, leading to the appearance of Sm3+ as the only oxidation state. The increase in the intensity of the O1s peak with time and the absence of spectral changes in the Cu2p and LMM Auger (substrate) indicate that the transformation is mainly due to adventitious oxidation of the layer. With further deposition at RT the metallic state Sm0 appears at higher coverages, which is readily postoxidized by subsequent exposure to molecular oxygen, leading to complete oxidation. No intermediate oxidation states (Sm2+) were observed, in contrast to the reported prevalence of Sm2+ on single crystal surfaces during the early stages of growth.

O 18.3 Mon 13:30 P

The influence of charge transfer on molecular structure and conformation at surfaces: TCNQ on metals — •Luke Rochford[1], David Duncan[1], Phil Woodruff[2], and Reinhard Maurer[2] — [1]Diamond Light Source, UK — [2]Warwick University, UK

Electron acceptors such as TCNQ are believed, based on previous studies, to adopt bent conformations when adsorbed on metal surfaces due to electron transfer. Our recent, quantitative, structural experiments show definitively that this is not the case on a variety of metal surfaces.

Our experimental work has combined powerful complimentary surface science techniques in the home lab with synchrotron light-based techniques, mainly synchrotron x-ray photoelectron spectroscopy (S-XPS) and x-ray standing waves (XSW). XSW has been central here, as it allows quantitative measurement out-of-plane structure of molecules with chemical specificity and sub-bond-length precision.

These data are supported by DFT calculations which show that dispersion force corrections are vital to properly reproduce our observed structures. The explicit inclusion of metal adatoms in structural models is also of key importance to explain our experimental observations.

This fundamental understanding has allowed us to understand the lateral charge transfer at work between native metal adatoms and electron acceptor molecules. We have applied this knowledge to design and create two-dimensional charge transfer salts using low concentrations of alkali metal atoms.

O 18.4 Mon 13:30 P

Heat of Adsorption on Single Crystals: Microcalorimetry — •Ann-Katrin Baumann and Swetlana Schauermann — Max-Eyth-Str.2, 24118 Kiel

Rational design of new heterogeneous catalysts requires detailed understanding of the bonding interactions between the gaseous species and the catalytic surface. One of the crucial parameters in this interaction is the adsorption enthalpy of the involved surface species.

Adsorption enthalpies can be determined with high level of accuracy by a direct method of single crystal adsorption calorimetry (SCAC), which has a number of advantages over the commonly used indirect method of temperature programmed desorption. In contrast to indirect methods, SCAC provides heats of adsorption without relying on assumptions on the details of the desorption kinetics or reversibility of the desorption processes.

In this work, an improved experimental setup of SCAC is presented. In ultra high vacuum, a pulsed molecular beam is employed to dose a known amount of molecules on a well-defined thin metal single crystal (1-2 μm) or nanostructured model surfaces containing supported metallic nanoparticles. The arising heat of adsorption is detected by a pyroelectric material (β-PVDF) pressed against the back of the thin metal crystal. Simultaneously, the sticking coefficient of the molecules is recorded in order to determine the amount of molecules contributing to the signal (short-term sticking) and the total amount of molecules remaining permanently adsorbed on the surface (long-term sticking).

O 18.5 Mon 13:30 P

Dynamics of Adsorption and Desorption on Chiral Surfaces — •Sabine Charlotte Matysik and Stephen John Jenkins — Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

The relationship between structural chirality and chiral motion is not well understood and often involves different length scales for both phenomena. In this dispersion-corrected density functional theory study, we focus on the dissociative adsorption of small achiral molecules on both chiral and achiral surfaces. The interplay between chirality and surface dynamics is explored by using the transition state of the dissociation reaction as a starting point for ab initio molecular dynamics simulations. Special focus in the analysis of these reactive trajectories lies on the time evolution of rotational momenta.

O 18.6 Mon 13:30 P

Study of tritium uptake in thin palladium-titanium-gold films by Beta-Induced X-ray Spectrometry — •Max Aker[1], Sonja Schneidewind[2], Sebastian Vetter[1], Chirstian Goffing[1], and Magnus Schlösser[1] — [1]Institute for Astroparticle Physics, Karlsruhe Institute of Technology — [2]Institute of Nuclear Physics, University of Münster

Metallic multilayer-systems are promising materials for tritium storage utilizable for passive tritium pumps, dedicated radioisotope heat sources, or calibration standards for the analysis of tritium in solids. Beta-Induced X-ray Spectrometry (BIXS) is a technique for tritium activity measurements and depth profiling in solids.

BIXS was used for activity measurements on Pd/Ti/Au multilayers in air which were tritiated at T_2 pressures up to 0.7 mbar. The measurements were complemented by activity quantifications using liquid scintillation counting. Combined with GEANT4 simulations the activity determination in samples consisting of three different metals with total thicknesses up to 300 nm and activities of 10^4 Bq to 10^8 Bq was accomplished. Pd/Ti/Au systems are interesting for tritium capture studies since Ti allows a quasi-irreversible tritium capture at room temperature, Pd prevents the formation of an oxide barrier on the Ti, and Au has low permeation to tritium, but increases the BIXS detection efficiency due to high stopping power. The findings on the influence of T_2 pressure, Pd layer thickness and bake-out on the final activity and its stability in the sample are reported in this poster.

O 18.7 Mon 13:30 P

Tritium adsorption on a gold surface from a gaseous tritium source — Max Aker and •Frank Hermann — Institute for Astroparticle Physics and Institute of Experimental Particle Physics, Karlsruhe Institute of Technology

The KATRIN collaboration aims to determine the neutrino mass with a sensitivity of 0.2 eV/c^2 (90 % CL). This will be achieved by measuring the endpoint region of the β-electron spectrum of gaseous tritium. A gold-coated stainless steel disk defines the physical limit of the tritium source. This so-called rear wall and any potential adlayer on it are exposed to impinging β-electrons, tritium cluster ions and neutral tritium molecules which allows ad- and absorbing tritium.

The beta-spectrum from tritium decays on or below the rear wall surface differs from that of the gaseous tritium source. This leads to a spectral distortion which needs to be considered in the neutrino mass determination. Investigations with regard to spectral shape, radial distribution and temporal evolution will be presented in this poster. Also first models predicting its future increase and hypotheses for the state of the surface-near bound tritium will be discussed.

This work is supported by the Helmholtz Association (HGF), the Ministry for Education and Research BMBF (05A17PM3, 05A17PX3, 05A17VK2, and 05A17WO3), the Helmholtz Alliance for Astroparticle Physics (HAP), and the Helmholtz Young Investigator Group (VH-NG-1055).

O 18.8 Mon 13:30 P

Adsorption and reactivity of monodispersed silver clusters stabilized by an organic network — •Vishkaya Jayalatharachchi[1], Elizabeth Graham[1,2], Jennifer MacLeod[1], and Josh Lipton-Duffin[1,2] — [1]Queensland University of Technology, Brisbane,Australia — [2]Central Analytical Research Facility (CARF)

In this study, we investigate the chemical and electronic structures of Ag metal clusters coordinated by deprotonated 1,3,5-benzenetricarboxylic acid (TMA) molecules on Ag(111) using soft x-ray spectroscopy techniques. Deprotonation was examined by X-ray photoemission spectroscopy (XPS) and scanning tunnelling microscopy (STM). We used Near edge X-ray absorption fine structure spectroscopy (NEXAFS) in these experiments to study the molecular geometry after deprotonation of the carboxylic/ carboxylate groups via C-K edge/ O-K edge measurements. Evolution of HOMO-LUMO levels has been studied using combination of Valence band spectra and Resonant photoemission spectroscopy (RESPES) and compared with the calculated density of states with corresponding charge distribution of intact TMA and deprotonated TMA molecules.

Careful study of the chemical and electronic structure of these clusters will allow us to better understand how to use organic molecules to engineer arrays of single-atom catalysts on surfaces, with the goal of tailoring these 2D materials systems for reactivity and selectivity in targeted catalysed reaction.

O 19: Poster Session II: Organic molecules on inorganic substrates: Adsorption and growth II

Time: Monday 13:30–15:30 Location: P

O 19.1 Mon 13:30 P

Stereoselective cyclodehydrogenetion of bishelicenes: preservation of handedness from helical to planar chirality — Bahaaeddin Irziqat[1,2], •Aleksandra Cebrat[1,2], Miloš Baljozović[1], Kevin Martin[3], Manfred Parschau[1], Narcis Avarvari[3], and Karl-Heinz Ernst[1,2,4] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [2]Department of Chemistry, University of Zurich, 8057 Zürich, Switzerland — [3]Laboratoire Moltech-Anjou, CNRS-Université d'Angers, 49045 Angers, France — [4]Nanosurf Laboratory, Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, Prague 6, Czechia

Here, we report the 2D chiral crystallization of 2,2'-bispentahelicene on Au(111) and its thermal-induced dehydrogenation studied with scanning tunneling microscopy. The low coverage deposition on Au(111) kept at 400 K, leads to formation of heterochiral zigzag chains of the (M,M)- and (P,P)-enantiomers along the herringbone reconstruction pattern. In the closed-packed monolayer, both enantiomers self-assemble into racemic phase. Due to its strong sterical overcrowding in its adsorbate state, the (P,M)-meso form was not observed on the surface. Upon annealing and subsequent cooling of the substrate, the characteristic twisted shape of bis[5]helicenes can no longer be observed and only 2D homochiral conglomerate domains of planar Sp- and Rp-coronocoronene can be distinguished. The transformation from helical to planar chiral molecules via dehydrogenation and loss of eight hydrogen atoms was confirmed by secondary ion mass spectrometry.

O 19.2 Mon 13:30 P

Identifying Surface Adsorbate Structures with Bayesian Inference and Atomic Force Microscopy — •Jari Järvi, Benjamin Alldritt, Ondřej Krejčí, Milica Todorović, Peter Liljeroth, and Patrick Rinke — Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Espoo, Finland

Determining stable structures of organic molecular adsorbates on inorganic substrates requires both quantum mechanics and thorough exploration of the potential energy surface (PES). This is prohibitively expensive with density-functional theory (DFT). Bayesian Optimization Structure Search (BOSS) [1] is a new tool that combines DFT with Bayesian inference for accurate global structure search. BOSS applies strategic sampling to compute the complete PES with a small number of expensive DFT simulations. This allows a clear identification of stable structures and their energy barriers.

We apply BOSS to study the adsorption of (1*S*)-camphor on the Cu(111) surface as a function of molecular orientation and translations [2]. We identify 8 unique adsorbate types, in which camphor chemisorbs or physisorbs to the Cu(111) surface. We employ the most stable structures to produce simulated atomic force microscopy (AFM) images, which we use to identify adsorbate configurations in AFM experiments [3]. This study demonstrates the power of cross-disciplinary tools in detecting complex interface structures.

[1] M. Todorović et al., npj Comput. Mater. 2019, 5, 35.
[2] J. Järvi et al., Beilstein J. Nanotechnol. 2020, 11, 1577-1589.
[3] J. Järvi et al., in preparation. doi:10.21203/rs.3.rs-50783/v1.

O 19.3 Mon 13:30 P

On-surface Synthesis of Porphyrin-GNR Hybrid Chains — •Joel Deyerling[1], Mathias Pörtner[1], Luka Dordević[2], Alexander Riss[1], Davide Bonifazi[3], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]The School of Chemistry, Cardiff University, UK-CF10 3AT Cardiff, United Kingdom — [3]Institute of Organic Chemistry, Faculty of Chemistry, University of Vienna, Austria

In recent years, the on-surface formation of hybrid structures combining porphyrins and graphene nanoribbons (GNRs) attracted increasing interest due to their potential for electronic, optoelectronic and spintronic applications [1-3]. A control on the precise atomic structure of such covalently linked porphyrin-based heterosystems is highly relevant for the tuning of their electronic and functional properties. Here, we address dehalogenative coupling reactions of a bromo-naphthalene functionalized Zn-porphyrin derivative on Ag(111) and Au(111). This precursor, its reaction steps, and different coupling motifs are characterized by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) with CO functionalized tips. Porphyrin-GNR hybrid chains with lengths exceeding 20 nm are achieved. Our experiments reveal atomistic details of different coexisting coupling motifs and give first insights into the electronic structure of this porphyrin-GNR system.

[1] J. Li *et al.*, Sci. Adv. 4, eaaq0582 (2018)
[2] L.M. Mateo *et al.*, Chem. Sci. (2021)
[3] F. Bischoff *et al.*, Angew. Chem. Int. Ed., 57, 16030 (2018)

O 19.4 Mon 13:30 P

Guiding molecular self-assembly by molecule-surface interaction — Ole Bunjes[1], Lucas A. Paul[2], Xinyue Dai[3], •Alexandra Rittmeier[1], Tobias Claus[1], Feng Ding[3], Inke Siewert[2], and Martin Wenderoth[1] — [1]IV. Physical Institute, University of Göttingen, Germany — [2]Institute of Inorganic Chemistry, University of Göttingen, Germany — [3]Ulsan National Institute of Science and Technology, Korea

One strategy for the generation of renewable fuels is the reduction of CO_2 to CO. Hence, the development of new hybrid systems catalyzing involved reaction steps is in the focus of current research. In this study the anchoring of the CO_2 reduction catalyst *fac*-Re(bpy)CO_3Cl (bpy = 2,2′-bipyridine) on the clean Ag(001) surface is investigated by means of scanning tunneling microscopy (STM) and density functional theory (DFT). Sub-monolayer films of the complex were deposited with the substrate held at 300K. STM measurements at 77K show that the beginning of cluster formation takes place at steps with a geometric orientation along the crystal axes <110>. The interaction between cluster and step leads to a restructuring of the surrounding step segments thereby promoting further cluster growth. Well-aligned decorated steps are found to be the nucleation point for higher dimensional growth. Comparing high resolution STM data to DFT calculations we get access to the local structural arrangement of the self-assembled complexes. Taking into account the calculated energies we develop a comprehensive growth model. This work was funded by the DFG - 217133147/SFB 1073, projects C1, C4, C7.

O 19.5 Mon 13:30 P

Surface-controlled reversal of the selectivity of halogen bonds — Jalmar Tschakert[1], Qigang Zhong[1], Daniel Martin-Jimenez[1], Jaime Carracedo-Cosme[2], Carlos Romero Muniz[2], Pascal Henkel[3], Tobias Schlöder[3], Sebastian Ahles[4], Doreen Mollenhauer[3], Hermann A. Wegner[4], Pablo Puo[2], Ruben Perez[2], Andre Schirmeisen[1], and •Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany — [4]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

Halogen bonds are ideally suited for designing molecular assemblies because of their strong directionality and the possibility of tuning the interactions by using different types of halogens or molecular moieties. This is interesting for applications in supramolecular chemistry, crystal engineering, or drug design. Here, we present an approach for tuning the 2D self-assembly process of organic molecules by adsorption to reactive vs. inert metal surfaces. **[1]** Therewith, the order of halogen bond strengths that is known from gas phase or liquids can be reversed. Our approach relies on adjusting the molecular charge distribution, i.e., the σ -hole, by molecule-substrate interactions. The polarizability of the halogen and the reactiveness of the metal substrate are serving as control parameters. Our results establish the surface as a control knob for tuning molecular assemblies by reversing the selectivity of bonding sites. **[1]** Tschakert et al. *Nature Communications* 11, 5630 (2020)

O 19.6 Mon 13:30 P

Adsorption of organic molecules on the Cu(110)-(2x1)O stripe phase — •Ilias Gazizullin, Christophe Nacci, and Leonhard Grill — Physical Chemistry Department, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

The deposition of molecules onto single-crystal surfaces allows their investigation at the single-molecule level by scanning tunneling microscopy (STM), in particular for planar molecular structures. Here, we have studied flat dibromoanthracene (DBA) molecules on the Cu(110)-(2x1)O stripe phase under ultra-high vacuum conditions with low-temperature STM. The Cu(110)-(2x1)O stripe phase is of particular interest since it offers alternating stripes of (metallic) Cu(110) areas and of oxygen-covered copper areas where the molecules are slightly decoupled from the metal substrate. The focus of our study is first on the preferred adsorption configuration and orientation of the linear molecules on the surface. It turns out that the molecules form organometallic chains on the copper areas, oriented in two surface directions. Second, we have attempted to investigate the electronic structure of the molecules by comparing their adsorption when they are on the metallic areas or on the oxide stripes. The results are compared with calculations of the molecular orbital structure.

O 19.7 Mon 13:30 P

Monodispersed graphene nanoribbons on Ag(111) by electrospray controlled ion beam deposition: their self-assembly and on-surface extension visited by STM — •Wei Ran[1], Andreas Walz[1], Karolina Stoiber[1], Peter Knecht[1], Anthoula C. Papageorgiou[1], Annette Huettig[1], Diego Cortizo-Lacalle[2], Juan P. Mora-Fuentes[2], Aurelio Mateo-Alonso[2,3], Hartmut Schlichting[1], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]POLYMAT, University of the Basque Country UPV/EHU, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Graphene nanoribbons (GNRs) are of interest due to their potential in electronics, energy conversion, and storage. For atomically precise GNRs, elaborate bottom-up fabrication protocols have been developed, utilising the reactivity of a metallic support.1) However this approach often results in GNR arrays with a variety of lengths. Here we employ a different approach for the preparation and study of GNRs on surfaces: chemical synthesis and purification of well-defined nanoribbons 2) followed by processing with electrospray controlled ion beam deposition (ES-CIBD). With this method, we can deposit well-defined GNRs on any solid support under ultra-high vacuum conditions. The quality of the films produced is exemplified for a 3 nm GNR on Ag(111). We explore their self-assembly and thermally activated polymerisation reactions by means of scanning tunnelling microscopy.

1) Fasel et al. Adv. Mater. 2016, 28, 6222. 2) Mateo-Alonso et al. Angew. Chem., Int. Ed. 2018, 57, 703.

O 19.8 Mon 13:30 P

Structural Details of a Prototypical Organic-Inorganic Interface: CuPc on In_2O_3(111) — •Matthias A. Blatnik[1,3], Peter Jacobson[2], Michael Schmid[1], Jan Cechal[3], Ulrike Diebold[1], and Margareta Wagner[1] — [1]Institut f. Angew. Physik, TU Wien, Austria — [2]School of Mathematics and Physics, University of Queensland, Australia — [3]CEITEC, Brno University of Technology, Czech Republic

Indium oxide (In_2O_3) is a ubiquitous material in OLEDs and photovoltaics due to an ideally matched optical transmission window and metal-like conductivity at room temperature when doped with Sn (as ITO). When In_2O_3 is paired with organic materials, a nearly universal fabrication step is the introduction of a thin organic buffer layer to improve the charge injection efficiency from In_2O_3 to the organic active layers. Using a combination of STM, nc-AFM and local spectroscopy (STS), we probe the adsorption structure and density of states (DOS) at the prototypical copper phthalocyanine (CuPc)-In_2O_3 interface. We focus on the stoichiometric (111) surface but also investigate the effects of dissociated water coadsorbed in UHV. STM/AFM imaging reveals single CuPc molecules adsorb in a flat, slightly tilted geometry in three symmetry-equivalent orientations. Increasing the coverage leads to (densely packed) 1D chains oriented along the <$1\bar{1}0$> directions. With increasing coverage up to 1 ML, first a (2×2) and then a (1×1) superstructure is found. Finally, differential conductance (dI/dV) measurements reveal the energetic positions of the HOMO and LUMO states which are critical for improving charge injection.

O 19.9 Mon 13:30 P

Elucidating the bonding of 2-mercaptobenzimidazole on Cu(111) by STM and DFT — •Marion van Midden, Matic Lozinšek, Tone Kokalj, and Erik Zupanič — Jožef Stefan Institute, Ljubljana, Slovenia

While organic corrosion inhibitors such as 2-mercaptobenzimidazole are widely used to protect the surface of copper, their bonding mechanism on the atomic scale remains elusive. DFT calculations have shown that different bonding configurations have comparable energies when considering the binding of a single molecule to the surface. In the case of larger coverages, which are common in real-life applications, various inter-molecular interactions have to be considered as well, further complicating calculations. To determine which interactions are most significant for the bonding and self-assembly of 2-mercaptobenzimidazole on the surface of Cu(111) we prepared samples in ultra high vacuum and imaged them using STM. Varying the evaporation rate and time as well as the substrate temperature allowed us to control the coverage and limit the energy the molecules have available to self assemble. Surprisingly the molecules formed ordered self-assembled structures even when depositing on samples cooled to approximately 50 K, which opposes the idea that strong binding to specific sites on the surface is crucial for corrosion prevention. The large variety of obtained self-assembled structures at different deposition parameters suggests, that the energy scales of competing interactions must be similar.

O 20: Poster Session II: Heterogeneous catalysis II

Time: Monday 13:30–15:30 Location: P

O 20.1 Mon 13:30 P

Data-Driven Descriptor Engineering and Refined Scaling Relations for Predicting Transition Metal Oxide Reactivity — •Wenbin Xu[1], Mie Andersen[1], and Karsten Reuter[1,2] — [1]Chair for Theoretical Chemistry, Technical University of Munich, Garching, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Screening of transition metal (TM) and TM alloy catalysts is often carried out using the comparatively simple d-band model and related scaling relations to predict adsorption enthalpies. Unfortunately, these methodologies do not extend to TM oxides due to their more localized and intricate electronic structure. Multiple geometric and electronic properties could in principle govern the adsorption enthalpies at these more complex compound materials. Given the immense number of candidates, we here apply a data-driven compressed sensing method[1] to tackle the search for best-performing multidimensional descriptors expressed as nonlinear functions of intrinsic properties of the clean surface. Our descriptors largely outperform previously highlighted descriptors in terms of accuracy and computational cost. Furthermore, we identify properties related to the local charge transfer to be the missing ingredient in standard scaling relations and show that their inclusion is crucial for the correct identification of promising catalyst materials for the oxygen evolution reaction.[2]

[1]R. Ouyang *et al.*, Phys. Rev. Mater. **2**, 083802 (2018)

[2]W. Xu *et al.*, ACS Catal. **11**, 734 (2021)

O 20.2 Mon 13:30 P

Microscopy of Gold Oxide Formation on TiO_2/Au(111) Model Catalysts for CO Oxidation — •Sabine Wenzel and Irene M. N. Groot — Leiden Institute of Chemistry, The Netherlands

Hydrogen produced from methanol has to be cleaned from traces of CO for its use in fuel cells [1]. Gold-based catalysts have been shown to selectively oxidize CO in H_2 environment at low temperatures [2]. There is ample evidence for strong interactions between gold and typically used supports such as TiO_2 [3]. However, the exact oxidation state of the active phase of gold as well as the role of oxide supports and water remain under debate [4,5,6]. Our set-up [7] allows for the controlled preparation and characterization of model catalyst surfaces in ultra-high vacuum combined with scanning tunneling microscopy at atmospheric pressures. A TiO_2/Au(111) model catalyst was prepared via physical vapor deposition and exposed to CO oxidation reaction conditions. We present evidence for the formation of a surface gold oxide in this environment. Our findings suggest that transfer of atomic oxygen from the titania nanoparticles to the gold substrate does not occur but that contaminants can promote the oxidation of gold.

References: [1] Dhar et al., J. Electrochem. Soc. 1987, 134, 12, 3021 [2] Haruta, The Chemical Record 2003, 3, 75 [3] Palomina et al., ACS Sustainable Chem. Eng. 2017, 5, 10783 [4] Min et al., Chem. Rev. 2007, 107, 2709 [5] Klyushin et al., ACS Catal. 2016 6 , 3372 [6] Kettemann et al., ACS Catal. 2017, 7, 8247 [7] Herbschleb et al., Rev. Sci. Instrum. 2014, 85, 083703

O 20.3 Mon 13:30 P

surface structure and stoichiometry of PdZn alloys under realistic (T, p) conditions — •yuanyuan zhou[1], lara kabalan[2], igor kowalec[2], luca m.ghiringhelli[1], sergey levchenko[1], andrew logsdail[2], richard catlow[2], and matthias scheffler[1] — [1]NOMAD Laboratory, Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]School of Chemistry, Cardiff University, Cardiff, United Kingdom

PdZn is known to efficiently catalyze CO_2 to methanol.[1] However, the microscopic understanding of the underlying chemical reactions at the surface is lacking, for example, the stoichiometry and structure of the surface under catalytic T, p conditions. The talk will, address the first and crucial step for achieving an improved understanding needed for predicting better catalysts in the family of bi- and tri-metallic materials. Specifically, we will analyze the composition and structure of PdZn(101) in a constrained thermal equilibrium with CO_2 and H_2 gases using density-functional theory and *ab initio* atomistic thermodynamics [2], considering a bulk composition of 1:1. Exposure to H_2 induces a restructuring of the surface and an enhancement of the Pd concentration. This is understood in terms of the stronger Pd-H bonds compared to Zn-H. Importantly, the adsorption of CO_2 is stronger in the presence of surface hydrogen. We discuss the various restructurings, order/disorder adsorbate phases, and the possibility of the formation of a surface hydride.

[1]H. Bahruji, *et al.*, J. Catal. 343, 133 (2016).

[2]K. Reuter and M. Scheffler, Phys. Rev. B. 65, 035406 (2001).

O 20.4 Mon 13:30 P

Performance and predictions of kinetic models for MgO-catalyzed ethanol conversion to butadiene — •Astrid Boje[1], William E. Taifan[2], Henrik Ström[1], Tomáš Bučko[3,4], Jonas Baltrusaitis[2], and Anders Hellman[1] — [1]Chalmers University of Technology, Göteborg, Sweden. — [2]Lehigh University, Bethlehem, USA. — [3]Comenius University in Bratislava, Bratislava, Slovak Republic. — [4]Slovak Academy of Sciences, Bratislava, Slovak Republic.

Formation of 1,3-butadiene from ethanol is a sustainable alternative to conventional synthesis; however, selectivity is challenging and there is significant sensitivity to catalyst composition and conditions. We employ a combination of first-principles-informed energetic span and microkinetic models to interrogate the kinetic behavior of this system on a model MgO catalyst, demonstrating the utility and limitations of both perspectives. The microkinetic model was developed based on the extensive DFT mechanism of Taifan *et al.* [1], comprising several possible pathways. Both models allow quantification of rate-determining states and turnover, with the microkinetic model characterizing kinetic limitations due to coverage and adsorption/desorption effects. The dominance of the pathways varied with temperature. We considered the impact of uncertainty in the free energy landscape on kinetic predictions by sampling from a correlated error model, finding that the microkinetic model was less robust but both models predicted similar median outcomes. The two models thus provide valuable and complementary insights into the operation of a complex, selectivity-limited process. [1] Taifan, W. E., *et al.*, J. Catal. **346**, 78 (2017).

O 20.5 Mon 13:30 P

Interfacial catalysis over well-defined Cu2O nanostructures — •Fan Yang — School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China

The catalytic properties of nano-oxides are increasingly recognized and currently explored for a wide range of applications. However, the nature of the active sites of these nano-oxides, as well as their catalytic chemistry, remain poorly understood, because of the difficulties to access these surface/interfacial sites at the atomic level. Using molecular beam epitaxy, we construct well-defined oxide nanostructures (NSs) on planar metal or oxide surfaces, which serve as the model systems for understanding the catalytic chemistry of the metal-oxide interface and nano-oxides. In this talk, we report our recent progress in the studies of low temperature CO oxidation using supported Cu2O NSs as the model catalyst. The Cu2O-M interface has been suggested as catalytic active sites for low temperature CO oxidation and a series of selective oxidation reactions. Combining microscopic and spectroscopic methods, CO oxidation was investigated at the Cu2O-M interface, to understand the mechanism of low temperature CO oxidation and the catalytic properties of the metal-oxide interface. A highly dynamic behavior of the catalytically active interfacial sites were observed, which accounts for the enhanced activities and stability of supported oxide NSs for oxidation reactions. Overall, we wish to demonstrate that the control over supported oxide NSs could enable a wide range of catalytic properties for the rational design of highly efficient catalysts.

O 21: Poster Session II: Solid-liquid interfaces: Reactions and electrochemistry I

Time: Monday 13:30–15:30 Location: P

O 21.1 Mon 13:30 P

Stable and cost-efficient core-shell catalysts for enhanced acidic oxygen evolution–a first principles approach — •Yonghyuk Lee[1,2], Christoph Scheurer[1,2], and Karsten Reuter[1,2] — [1]Technical University Munich, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

Most commercial oxygen evolution reaction (OER) catalysts in proton exchange membrane electrolyzers contain precious IrO_2 due to its high catalytic activity and favorable stability in acidic electrolytes. IrO_2 supported on rutile TiO_2 has been utilized in order to reduce the price without sacrificing activity. However, thin IrO_2 films seem generally not stable on titania and a gradual dewetting of the film takes place.

In the present work, we use density-functional theory (DFT) calculations to further scrutinize the feasibility of encapsulating a cheap rutile TiO_2 core with thin coherent IrO_2 or RuO_2 films as potentially stable catalyst materials for water electrolysis. We calculate facet-resolved interface formation energies and works of adhesion to quantify the effect of interfacial strain, the stability of the oxide interfaces and their strong directional dependence. A wetting tendency results only for some low-index facets under experimental gas-phase synthesis conditions. Surprisingly, *ab initio* thermodynamics indicates a significantly better wetting stability for lattice-matched RuO_2 films in more oxidizing conditions such as under OER operation. The calculations also predict an enhanced OER activity of epitaxial RuO_2/TiO_2 core-shell particles. [1] D. Opalka *et al.*, ACS Catal. **9**, 4944 (2019).

O 21.2 Mon 13:30 P

Interaction of Small Alcohols with TiO_2 studied by Vibrational Sum Frequency Spectroscopy — •Anupam Bera, Denise Bullert, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

The interaction of alcohols with oxide surfaces such as TiO_2 attracts interest as the oxidation of these species is of large industrial relevance. The interaction of TiO_2 with alcohols has attracted less interest although oxidation of the latter is of large industrial relevance.Surface-sensitive vibrational sum frequency spectroscopy (vSFS) has been utilised to study the adsorption chemistry of small alcohols namely methanol, ethanol, 1-propanol and 2-propanol on TiO_2 thin films under vapour pressure conditions at which a condensed molecular film is maintained. The vSF spectra in the C-H region reveal that methanol and ethanol adsorb both molecularly and dissociatively, while 1-propanol and 2-propanol are solely detected in molecular form. The different adsorption behaviour suggests that the extend of dissociation decreases from methanol to propanol. Moreover, polarisation analysis of the spectra reveals that the methyl groups are preferentially oriented with their symmetry axis pointing in a direction close to the surface normal for methanol, ethanol and 1-propanol. That seems not to be the case for 2-propanol.

O 21.3 Mon 13:30 P

Cooperative Effect of Carbonaceous Material with Water Enhances the Growth of SiOx on Si — •Rémi Dupuy[1], Clemens Richter[1], Pip CJ Clark[2], Rossella Yivlialin[2], Michael J Sear[2], Marco Favaro[2], Robert Schlögl[1], David E Starr[2], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, D-14195 Berlin, Germany — [2]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-14109 Berlin, Germany

We have investigated the influence of carbonaceous materials on the growth of SiOx layers on Si under dry conditions and in the presence of water and/or water vapor. Dip-and-pull experiments were carried out using the SpAnTeX endstation using tender X-rays (3 keV) from the KMC-1 beamline at BESSY II. Si wafers (n-doped) cleaned using the RCA-method exhibited initially a uniform SiOx film thickness of the order of 1 nm, as determined from Si 2p and Si 1s spectra.

In the dip-and-pull experiments the Si wafers were partly immersed into pure water or octanoic acid, as well as mixtures of water and stearic or octanoic acid. The XPS data clearly show a correlation between the thickness of the SiOx layer and the amount of carbon present at the surface. However, this effect is only observed in experiments where the Si wafer was exposed to both water and carbonaceous species. Oxide growth was not observed for experimental conditions where the SiOx/Si surface was exposed to only either water or carbonaceous material. These results thus point to a cooperative effect between water and carbonaceous species that induces SiOx growth.

O 21.4 Mon 13:30 P

2D water structures on low index Pt surfaces — •Alexandra C. Dávila[1], Nicolas G. Hörmann[1,2], Thorben Eggert[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany — [2]Chair of Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Germany

It is a common approximation in *ab initio* calculations of electrocatalytic metal-water interfaces, to use static ice-like water adlayers to represent the first solvent shell on the electrode [1,2]. To date, these ice-like layers are typically created manually and in an *ad-hoc* fashion. To extend this to a better defined protocol that also allows to generate a larger statistical ensemble of ice-like adlayers, we here develop a versatile construction recipe leveraging lattice-matching algorithms in combination with a database of metastable 2D water polymorphs. We illustrate the approach for Pt (100), (110) and (111) surfaces, and systematically compute the energetics, as well as geometric and electronic properties of the created structures using density-functional theory. Comparison to corresponding literature data from full *ab initio* molecular dynamics simulations allows to gauge the accuracy of the prevalent single ice-adlayer approximation and assess ice-ensemble averaging as a controlled and cost-efficient proxy.

[1] S. Schnur *et al.*, New J. Phys. **11**, 125003 (2009).

[2] J. Rossmeisl *et al.*, Chem. Phys. Lett **466**, 68 (2008).

O 21.5 Mon 13:30 P

Ni modified Fe3O4(001) surface as a simple model system for understanding the Oxygen Evolution Reaction — •Francesca Mirabella[1,2], Matthias Müllner[2], Thomas Touzalin[3], Michael Schmid[2], Marc Koper[3], Gareth Parkinson[2], and Ulrike Diebold[2] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [2]TU Wien, Vienna, Austria — [3]Leiden Institute of Chemistry, Leiden University, The Netherlands

Electrochemical water splitting is an environmentally friendly technology to store renewable energy in the form of chemical fuels. Among the Earth-abundant first-row transition metal-based catalysts, mixed Ni-Fe oxides have shown promising performance for effective and low-cost catalysis of the oxygen evolution reaction (OER) in alkaline media, but the synergistic roles of Fe and Ni cations in the OER mechanism remain unclear. In this work, we report how the Ni-modification changes the reactivity of a model iron oxide catalyst using a combination of surface science techniques in ultra-high-vacuum (LEED, XPS, LEIS, STM), AFM in air, and electrochemical methods (CV and EIS) in alkaline media. A significant improvement in the OER activity is observed when the surface presents an Fe:Ni ratio in the range 20-40%, which is in good agreement with what has been observed for powder catalysts. EIS suggests that the OER precursor species observed on the clean and Ni-modified surfaces are similar, but form at lower overpotentials when the surface Fe:Ni ratio is optimized. We propose that the well-defined Fe3O4(001) surface can serve as a model system for understanding the OER mechanism on mixed Fe/Ni oxides.

O 21.6 Mon 13:30 P

Active-Site Computational Screening: Role of Structural and Compositional Diversity for the Electrochemical CO2 Reduction at Mo Carbide Catalysts — •Haobo Li[1] and Karsten Reuter[1,2] — [1]Technical University of Munich, Lichtenbergstr. 4, D-85747 Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

The surfaces of compound catalyst materials generally exhibit a wide range of geometric and compositional motives that could act as active sites. We address this inherent complexity by extending computational materials screening over a diverse set of such sites. For the electrochemical CO2 reduction reaction (CO2RR) at molybdenum carbides, extensive density functional theory (DFT) calculations for key reaction intermediates at these sites show that differing adsorption modes break many of the scaling relations known to hold across transition metals. Despite the resulting inherently rich reduction chemistry, clear trends emerge. Notably, this includes a product selectivity governed by the metal/carbon ratio of the active site. The trend toward methanol formation for C-containing active sites mirrors thermal heterogeneous CO2 activation and suggests a shift of focus toward more C-rich carbides for CO2RR to methanol [1].

[1] H. Li and K. Reuter, ACS Catal. 10, 11814 (2020).

O 21.7 Mon 13:30 P

When to stop the count? - Time scales of liquid water on metal substrates — •Thorben Eggert, Nicolas G. Hörmann, and Karsten Reuter — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The detailed arrangement of water layers at a metal surface plays a crucial role for a plethora of different properties concerning the solid-liquid interface like the work function or the adsorption energy [1]. However, reliably determining this arrangement through predictive-quality simulations generally requires computationally most demanding *ab initio* molecular dynamics (MD) simulations with explicit water. In practice, the high costs then often allow to acquire trajectories only over limited simulation times and in simulation cells of limited size.

We examine this problem with reactive force field MD simulations, collecting data over extended time scales of a few nanoseconds. As a test system, we study water films on Pt(111) for various thicknesses. While running averages look highly converged on the limited time scale of *ab initio* MD simulations, significant differences are found when comparing them to results obtained on the nanosecond time scale. This showcases the difficulty of generating a representative subset of the relevant configurational space in a controlled fashion.

[1] A. Groß *et al.*, J. Electrochem. Soc. **161**, E3015-E3020 (2014).

O 21.8 Mon 13:30 P

Boosting Hydrogen Evolution Reaction Activity by Lateral Electrode Structuring — •Thomas L. Maier[1], Matthias Golibrzuch[2], Tina Angerer[1], Markus Becherer[2], and Katharina Krischer[1] — [1]Nonequilibrium Chemical Physics, Technical University of Munich, Garching, Germany — [2]Nanoelectronics, Technical University of Munich, Munich, Germany

Producing solar fuels with devices based on metal-insulator-semiconductor (MIS) interfaces is a very promising future technology for a renewable energy economy. The semiconductor part of such hybrid devices can provide efficient light absorption while the metal part facilitates fast reaction kinetics. However, in order to fulfil these two functionalities, the device requires patterning of the MIS interface.

We show that lateral structuring of silicon-based electrodes with well-defined gold arrays exhibits cooperative effects, i.e. strongly altered catalytic activities compared to bare metal surfaces. We demonstrate this with the hydrogen evolution reaction (HER) in acidic and alkaline medium and show that the HER rate scales with the interfacial area between the metal catalyst and the adjacent silicon oxide support. The rate of alkaline HER can be enhanced by an order of magnitude, which results in a very similar HER activity in alkaline and acidic medium. We explain this increase by a bifunctional mechanism at the metal/silicon oxide interface and argue that the lateral structuring changes locally the electric field, which increases the reaction rate of alkaline HER at the interface compared to the rate at the metal bulk.

O 22: Poster Session II: New methods II

Time: Monday 13:30–15:30 Location: P

O 22.1 Mon 13:30 P

Enabling size convergence for surface calculations of materials exhibiting spontaneous polarization — •Su-Hyun Yoo[1], Mira Todorova[1], Liverios Lymperakis[1], Chris Van de Walle[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Materials Department, UCSB, USA

The most common approach to describe surfaces in density-functional theory is the repeated slab geometry based on periodic boundary conditions. A common strategy to avoid artificial charge transfer from one side of the slab to the other when modelling semiconductor surfaces is to passivate partially filled surface dangling bonds at the backside of the slab. Using the example of wurtzite (0001) surfaces we demonstrate that conventionally used passivation schemes (e.g. pseudo H or surface reconstructions) break down for materials exhibiting spontaneous polarization. We have therefore developed a generalized passivation method that accounts for the effect of spontaneous polarization and correctly describes the asymptotic bulk limit for pyroelectric materials. It is robust and ensures quick convergence of total energies and electronic structure with respect to system size. The performance of our approach will be demonstrated using the example of wurtzite ZnO polar [1] and wurtzite GaN semi-polar surfaces [2].

[1] S. Yoo, M. Todorova, D. Wickramaratne, L. Weston, C. Van de Walle, and J. Neugebauer, NPJ Computational Materials (submitted).

[2] S. Yoo, L. Lymperakis, and J. Neugebauer (in preparation).

O 22.2 Mon 13:30 P

WannierBerri code - a fast python code for Wannier interpolation. — •Stepan Tsirkin[1], Xiaoxiong Liu[1], Minsu Ghim[2], Patrick Lenggenhager[2,3,6], Iñigo Robredo[4], Miguel Ángel Jiménez Herrera[5], Ji Hoon Ryoo[2], Jae-Mo Lihm[2], Cheol-Hwan Park[2], and Ivo Souza[5] — [1]University of Zurich — [2]Seoul National University — [3]ETH Zurich — [4]Donostia International Physics Center, Spain — [5]CFM, Universidad del País Vasco, Spain — [6]Paul Scherrer Institute, Villigen PSI, Switzerland

We present WannierBerri (WB) [1] - a new Python code for Wannier interpolation, which is close in spirit to the postprocessing module of the well-known

Wannier90 code [2] (postw90.x), but improves over it by implementing a number of methodological advances [3], which boost the speed of computations by orders of magnitude, enabling to study more complex materials with higher accuracy without demanding enormous computational resources. A plethora of quantities are implemented, such as anomalous Hall conductivity, orbital magnetization, Berry curvature dipole, and spin Hall conductivity, among many others. WB is also capable of evaluating analytical covariant derivatives of the Berry curvature and orbital moment, which allows to study different magnetotransport phenomena, and also to implement Fermi-sea formulations of Berry dipole.

[1] http://wannier-berri.org
[2] http://wannier.org
[3] https://arxiv.org/abs/2008.07992

O 22.3 Mon 13:30 P

Frequency and momentum-resolved detection of non-thermal gigahertz phonons with Fano coupling to charge carriers — •Thomas Vasileiadis[1], Heng Zhang[2], Hai Wang[2], Mischa Bonn[2], George Fytas[2], and Bartlomiej Graczykowski[1] — [1]Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznanskiego 2, 61-614 Poznan, Poland. — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany.

Spontaneous micro-Brillouin light scattering (μ-BLS) can probe gigahertz acoustic phonons in nano-confined materials with momentum and spatial resolution. However, the downsizing of the scattering volume implies weak BLS signals, sample overheating, and damage [1]. In this work, we present pumped-BLS [2], an all-optical technique that generates non-thermal acoustic phonons with ultrashort laser pulses and probes them with frequency- and momentum-resolution. Using pumped-BLS we show: (i) a hundred-fold enhancement of BLS spectra, compared to equilibrium, of 260 nm thick Si membranes due to photoexcited non-thermal gigahertz phonons, (ii) Stokes / anti-Stokes asymmetry due to asymmetric non-thermal phonon propagation and (iii) strongly asymmetric Fano resonances due to coupling between the electron-hole pairs and the phonons. This project is funded from NCN (UMO-2018/31/D/ST3/03882), ERC (grant no. 694977) and FNP (POIR.04.04.00-00-5D1B/18). TV acknowledges funding from the European Union's Horizon 2020 research and innovation programme. [1] M. Sledzinska, et al. Adv. Funct. Mater. 30 (8), 2020. [2] Th. Vasileiadis et al. Science Advances 6 (51), eabd4540, 2020.

O 22.4 Mon 13:30 P

Bound in the continuum modes in indirectly-patterned hyperbolic media — •Hanan Herzig Sheinfux[1], Lorenzo Orsini[1], Minwoo Jung[2], Iacopo Torre[1], Matteo Ceccanti[1], Eli Janzen[3], James Edgar[3], Gennady Shvets[2], and Frank H Koppens[1] — [1]ICFO, Spain — [2]Cornell university, USA — [3]Kansas state university, USA

Conventional optical cavities support one or more modes, which are unable to leak out of the cavity. Bound state in continuum (BIC) cavities are an unconventional alternative, where there are available channels for the mode to leak through, but it remains confined due to destructive interferences. BICs are a general wave phenomenon. It is interesting to consider BICs in the context of hyperbolic media (HyM), as a way to produce cavties with extremely small mode volume and enhanced light matter interaction. However a hyperbolic BIC cavity presents a fundamental challenge, since the cavity's HyM cladding supports an infinite number of modes which would need to interfere. Here, we introduce hyperbolic BICs (hBICs) and construct the first BIC-based nanocavities. These hBICs are formed through a novel multimodal reflection spatial mechanism, to do with the vanishing spatial overlap between ray-like excitations in a HyM and all leakage channels. Using near-field microscopy, we directly observe this asymmetrically enhanced reflection and demonstrate mid-IR nanocavities with volumes down as small as 15x15x3nm and quality factors reaching above 100, a dramatic improvement in several metrics of confinement.

O 22.5 Mon 13:30 P

Elucidation of Disordered Mesopore Constructs: A Kernel-Based Approach — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University

Detailed characterisation of the structure of mesoporous solids presents key insights into the accurate design of various industrial applications such as catalysis, molecular separations and adsorption, among others. Routine characterisation tools, such as gas sorption, typically utilise the general adsorption isotherm (GAI) equation derived for ordered pore systems. For disordered porous solids, the complex morphology with its resulting cooperativity effects in thermodynamic phase transitions renders characterisation more complex than what the GAI supports.

Herein, we present a kernel-based approach with the serially connected pore model (SCPM); an extension of the GAI which incorporates cooperativity effects in phase transitions arising from pore complexity. Modelled as a statistical linear chain of pores, the SCPM is validated with data from solid-liquid phase transitions of water in synthesized porous silica material of similar pore construct, MCM-41. To show its robustness, we employ the SCPM to reveal disorder in SBA-15 mesoporous solid.

O 22.6 Mon 13:30 P

Single-Hemisphere Photoelectron Momentum Microscope with Time-of-Flight Recording — •Gerd Schönhense, Sergey Babenkov, Dmitry Vasilyev, Hans-Joachim Elmers, and Katerina Medjanik — Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany

Photoelectron momentum microscopy is an emerging powerful method for angle-resolved photoelectron spectroscopy (ARPES). These instruments record k_x - k_y images, typically exceeding a full Brillouin zone. As energy filters double-hemispherical [1] or time-of-flight (ToF) [2] devices are in use. Here we present a new approach for momentum mapping of the full half-space, based on a large single hemispherical analyzer [3]. Excitation by an unfocused He lamp yielded an energy resolution of 7.7 meV. The method circumvents the preconditions of previous theoretical work on the resolution limitation due to the alpha-square term and the transit-time spread (detrimental for time-resolved experiments). Data recording in the Fourier plane allows for large range of entrance angles in the analyzer (up to ±7°, opposed to typically ±2° in conventional analyzers). A dispersive-plus-ToF hybrid mode with ToF analyzer behind the exit slit yields a gain up to N^2 in recording efficiency (N number of resolved time slices). A key application will be ARPES at sources with high pulse rates like synchrotrons with 500 MHz time structure; the prototype will be installed at Diamond, UK. [1] C. Tusche et al., Ultramicrosc. **159**, 520 (2015); [2] K. Medjanik et al., Nature Mat. **16**, 615 (2017); [3] G. Schönhense et al., Rev. Sci. Instrum. **91**, 123110 (2020).

O 23: Poster Session II: Topology and symmetry-protected materials

Time: Monday 13:30–15:30 Location: P

O 23.1 Mon 13:30 P

Discovery of chiral topological semimetals with multifold fermions and long surface Fermi-arcs — •Niels B. M. Schröter — Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Chiral topological semimetals (which possess neither mirror nor inversion symmetries) are a new family of topological materials that are expected host numerous novel phenomena, such as multifold fermions with large topological charge, long Fermi-arc surface states, and a quantized response to circularly polarized light. However, until recently, all known topological semimetals crystallized in space groups that contain mirror operations, which means that the aforementioned phenomena must vanish.

Here, I will present evidence from angle-resolved photoelectron spectroscopy that a family of chiral intermetallic catalysts, including PtAl and PdGa, are chiral topological semimetals. We directly visualize the multifold fermions in these compounds and show that they carry the largest possible Chern number that can be realized in any solid by imaging their extremely long surface Fermi-arcs and resolving a spin-orbit coupling induced band splitting. We also show experimentally that there is a direct relationship between the handedness of the crystal structure and the electronic chirality (i.e. the Chern number sign) of the multifold fermions. This finding demonstrates that structural chirality can be used as a control parameter to manipulate phenomena that are sensitive to electronic chirality, such as the direction of topological photocurrents.

O 23.2 Mon 13:30 P

Spin and orbital texture of the Weyl semimetal MoTe$_2$ studied by spin-resolved momentum microscopy — •Kenta Hagiwara[1], Xin Liang Tan[1], Philipp Rüssmann[1], Ying-Jiun Chen[1,2], Koji Fukushima[3], Keiji Ueno[3], Vitaliy Feyer[1], Shigemasa Suga[1,4], Stefan Blügel[1], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg — [3]Saitama University, 338-8570, Saitama, Japan — [4]Osaka University, 567-0047, Osaka, Japan

Weyl semimetals host chiral fermions in solids as a pair of non-degenerate linear dispersions with band crossing points in bulk. These Weyl points are protected by topology, forming a Fermi arc, which is a connection between a pair of Weyl points with opposite chirality at the surface. Momentum microscopy provides two dimensional photonelectron maps of the in-plane crystal momentum over the whole Brillouin zone, simultaneously. Together with an imaging spin filter, we have revealed the spin-resolved electronic structure of the type-II Weyl semimetal 1T$_d$ MoTe$_2$ in the full Brillouin zone. Combined with the use of differently polarized light, we have revealed the spin texture and the orbital texture of the Weyl cones in comparison with first-principles calculations. We give evidence that a pair of Weyl cones exhibits a strong circular dichroism with reversed sign, indicating the different charge of the respective Weyl points in the Fermi surface.

O 23.3 Mon 13:30 P

Observation of backscattering induced by magnetism in a topological edge state — •Berthold Jaeck[1,2], Yonglong Xie[1,3], Bogdan Andrei Bernevig[1], and Ali Yazdani[1] — [1]Princeton University, Joseph Henry Laboratories and Department of Physics, Princeton, USA — [2]Present Address: The Hong Kong University of Science and Technology, Department of Physics, Clearwater Bay, Kowloon, Hong Kong — [3]Present Address: Harvard University, Department of Physics, Cambridge, USA

We have investigated the effects of time-reversal symmetry breaking on the topological edge state of bismuth. Using spectroscopic imaging and spin-polarized measurements with the STM, we have compared quasiparticle interference (QPI), occurring in the edge state of a pristine bismuth bilayer with that occurring in the edge state of a bilayer, which is terminated by ferromagnetic iron clusters. Our experiments on the decorated bilayer edge reveal an additional QPI branch that can be associated with spin-flip scattering across the Brioullin zone center between time-reversal band partners. The observed QPI characteristics exactly match with theoretical expectations for a topological edge state, having one Kramer's pair of bands. Our results provide further evidence for the non-trivial nature of bismuth and, in particular, demonstrate backscattering inside a helical topological edge state induced by broken TRS through local magnetism (1).

This work is supported by the ONR, the Moore foundation, NSF-DMR, NSF-MRSEC and the Humboldt foundation.

(1) B. Jäck *et al.*, PNAS 117 (28), 16214-16218 (2020)

O 23.4 Mon 13:30 P

Unveiling the complex band structure of the potential non-symmorphic topological insulator TaNiTe$_2$ — •Tim Figgemeier[1], Jennifer Neu[2], Simon Moser[3], David J. Singh[4], Theo M. Siegrist[2,5], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg — [2]National High Magnetic Field Laboratory, Tallahassee, Florida — [3]Experimentelle Physik IV, Universität Würzburg — [4]University of Missouri, Columbia, Missouri — [5]College of Engineering, FAMU-FSU, Tallahassee, Florida

NbNiTe$_2$ and TaNiTe$_2$ are layered van-der-Waals systems. While NbNiTe$_2$ was discussed as a Weyl-semimetal candidate lately [1,2], TaNiTe$_2$ (space group #53, *Pmna*) is predicted to be a topological insulator with non-symmorphic crystal structure, characterized by a topological inavriant of $Z_4 = 1$, that have rarely been studied experimentally up to now [3]. In this study we investigated the electronic structure of TaNiTe$_2$ by means of angle-resolved photoemission (ARPES) experiments and first-principles calculations. Systematic photon-energy- and polarization-dependent measurements allow us to disentangle the highly complex band structure. Furthermore, we discuss indications for the presence of a topological surface state.

[1] Wang et al., PRB 95, 165114 (2017)
[2] Neu et al., PRB 100, 144102 (2019)
[3] Vergniory et al, Nature 544, 480-450 (2019)

O 23.5 Mon 13:30 P

Molecular beam epitaxy and spectroscopy on the antiferromagnetic topological insulator (MnBi$_2$Te$_4$)(Bi$_2$Te$_3$) — •Philipp Kagerer[1,2], Celso Fornari[1,2], Sebastian Buchberger[1,2], Sergio Luiz Morelhao[3], Raphael Crespo Vidal[1,2], Abdul Tcakaev[4,2], Volodymyr Zabolotnyy[4,2], Eugen Weschke[5], Vladimir Hinkov[4,2], Martin Kamp[6], Bernd Büchner[2,7,8], Anna Isaeva[2,7,8], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Exp. Physik VII, Uni Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Inst. de Fisica, Univ. de Sao Paulo — [4]Exp. Physik IV, Uni Würzburg — [5]HZB Berlin — [6]Phys. Inst. and RCCM, Uni Würzburg — [7]Leibnitz IFW Dresden — [8]Inst. für Festk.- und Materialphysik, TU Dresden

With the discovery of $MnBi_2Te_4$ as the first antiferromagnetic topological insulator, the material systems has emerged as a candidate for applications in quantum technologies [1]. Presently, the interplay between magnetism and topology in this compound is not fully understood. We have established the MBE-growth of $(MnBi_2Te_4)(Bi_2Te_3)$ heterostructures on BaF$_2$ as a basis for further research into the magnetic and electronic properties of these compounds [2]. MBE allows us to access and tailor various structural as well as electronic material properties and may give access to the underlying physics. We will present a study on the growth of the compound including an analysis of XRD patterns, as well as photoemission and XMCD/XLD results. [1] M.M. Otrokov et al., Nature 576, 416 (2019) [2] P. Kagerer et al., JAP 128, 135303 (2020)

O 24: Poster Session II: Plasmonics and nanooptics II

Time: Monday 13:30–15:30 Location: P

O 24.1 Mon 13:30 P

Direct observation of Surface Plasmon Polaritons on permalloy nanostructures with femtosecond photoemission electron microscopy — •Maximilian Paleschke and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

Due to remarkable progress in nanofabrication on the one hand and magneto optical methods on the other, the vivid field of magnetoplasmonics has become more and more accessible by a variety of excitation and investigation techniques.

Although it is well established that surface plasmon polaritons (SPP) can be imaged by photoemission electron microscopy (PEEM) in silver nanostructures[1], similar observations have not been reported for ordinary ferromagnetic materials like iron or nickel. Here, we report on dichroism images in threshold photoemission facilitating a tuneable femtosecond laser setup. The dichroism images show clear edge-induced standing waves with sub-micrometer wavelength. Analyzing the observed beating pattern as well as the coupling of the photon's spin-angular momentum to the direction of the fringe fields hint to propagation characteristics exclusive to evanescent waves, such as SPPs.[2, 3] This implies the possibility that many materials with a high plasma frequency allow for excitation and experimental observation of SPPs via this method.

[1] M. Dabrowski *et al.*, Chem. Rev. **120**, 6247 (2020)
[2] A. Y. Bekshaev *et al.*, Nature Com. **5**, 8 (2014)
[3] Y. Dai *et al.*, ACS Photonics **6**, 2005 (2019)

O 24.2 Mon 13:30 P

Particle Plasmon Induced Electronic Excitations on Silicon and Tetracene Crystals — •Katharina Engster[1,2], Kevin Oldenburg[2], Chris Rehhagen[1,2], Stefan Lochbrunner[1,2], Karl-Heinz Meiwes-Broer[1,2], Sylvia Speller[1,2], and Ingo Barke[1,2] — [1]Institut für Physik, Universität Rostock, Germany — [2]Department Leben-Licht-Materie, Universität Rostock, Germany

Utilizing plasmonics of metal nanoparticles to locally excite organic semiconductors is promising with respect to transfer energy from a defined starting point over longer distances. Two-photon photoemission electron microscopy (2P-PEEM) enables observation of near-fields with high lateral resolution due to the increased photoemission yield. With excitation spectroscopy we show that the particles can be addressed individually by their distinct plasmonic properties [1]. This results in an enhanced excitation of both, the substrate and nearby organic structures. The coupling to the substrate was studied by analyzing the occurring surface photovoltage (SPV) on Si(100)-(2x1). The distance dependence from the particles reveals an enhanced plasmon induced charge carrier density in the vicinity of the nanoparticles. For tetracene nanostructures we observe a plasmonically assisted local triplet exciton density. We do not observe clear migration in these small structures, which we attribute to inhomogeneities of the molecule aggregate [2]. Therefore, we present first measurements on larger, solution grown tetracene microcrystals.

[1] K. Oldenburg et al., J. Phys. Chem. C 123 (2019).
[2] G. M. Akselrod et al., Nat. Commun. 5 (2014).

O 24.3 Mon 13:30 P

Combining GW-BSE and PCM approaches for the description of real time electronic dynamics of molecules close to a plasmonic nanoparticle: application to LiCN and p-nitro-aniline (PNA) molecules. — •Margherita Marsili and Stefano Corni — Dipartimento di Scienze Chimiche, Università di Padova, via Marzolo 1, Padova, Italy

In the presence of a plasmonic nanoparticle (NP) the optical response of molecules is strongly modified. The theoretical modeling of this phenomenon is especially challenging due to the inherent multiscale nature of the system. Recently, the simulation of the simultaneous electronic dynamics of molecule and NP was achieved by combining a time-dependent configuration interaction approach for the molecule, and a description of the NP as a continuous dielectric. The model takes into account the reciprocal effect of the molecule and NP time-dependent polarization, and the coupling with an external electromagnetic field. We combine this approach with the description of the molecule at the GW-BSE level, which is suited to treat extended and charge-transfer systems. We apply this methodology to study Rabi oscillations of the ground and excited states population of a LiCN molecule, an ideal test system for the study of optical dipole switching. The molecule is set at increasing distances with respect to a plasmonic NP probing the local field enhancement and the strength of the mutual interaction. Moreover, the population and dipole dynamics of the prototypical push–pull PNA molecule in proximity of a tip-shaped NP is studied with the tip scanning the molecule at different positions.

O 24.4 Mon 13:30 P

Mechano-optical switching of a single molecule with doublet emission — Jiří Doležal[1], Pingo Mutombo[1], Dana Nachtigallová[2], Pavel Jelínek[1], •Pablo Merino[3], and Martin Švec[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Praha, Czech Republic — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz 3, E28049, Madrid, Spain

Phthalocyanine and derived metal complexes on thin insulating layers studied by scanning tunneling microscope-induced luminescence (STML) offers an excellent playground for tuning their excitonic and electronic states by Coulomb interaction and to showcase their high environmental sensitivity.[1] Copper phthalocyanine (CuPc) has an open-shell electronic structure and its lowest-energy exciton is a doublet which brings interesting prospects in its application for optospintronic devices. Here, we demonstrate that the excitonic state of a single CuPc molecule can be reproducibly switched by atomic scale manipulations permitting precise positioning of the molecule on the NaCl ionic crystal lattice.[2] Using a combination of STML, AFM and ab-initio calculations, we show the modulation of electronic and optical bandgaps, and the exciton binding energy in CuPc by tens of meV. We explain this effect by spatially-dependent Coulomb interaction occurring at the molecule-insulator interface, which tunes the local dielectric environment of the emitter.

[1] J. Doležal et al., Nano Letters, 19 8606 (2019).
[2] J. Doležal et al., ACS Nano, 14, 8931 (2020).

O 24.5 Mon 13:30 P

Vibrational Heating of a Single C60 Molecule in a Current-Carrying Plasmonic Picocavity — •Borja Cirera[1], Chenfang Lin[1], Shuyi Liu[1], Yair Litman[2], Alaa Akkoush[2], Martin Wolf[1], Mariana Rossi[2], and Takashi Kumagai[1,3] — [1]PC Department Fritz Haber Institute, Berlin, Germany — [2]MPI for Structure and Dynamics of Matter, Hamburg, Germany — [3]IMS, Okazaki, Japan

Vibrational heating in single-molecule junctions under non-equilibrium conditions is of fundamental importance in molecular electronics. Here we report on single-molecule thermometry of fullerene (C60) in a current-carrying plasmonic picocavity by combining tip-enhanced Raman spectroscopy (TERS) with low-temperature scanning tunneling microscopy (STM). Thanks to the exceptional sensitivity of TERS, intense Stokes and anti-Stokes Raman bands can be observed from single C60, enabling direct access to heating of individual vibrational modes. The precise gap-distance control in STM allows performing single-molecule thermometry in two distinct regimes, where the molecule is in contact with one or two electrodes (tip/surface), respectively. In both cases, optically induced heating is dominant for low bias voltages. At high bias voltages, the vibrational population is increased by injecting electrons into the LUMO of C60 in tunneling conditions. Upon contacting with both electrodes, the molecule strongly hybridizes with metallic states and vibrational pumping is dominated by inelastic electron scattering due to a much larger current density.

O 24.6 Mon 13:30 P

Plasmon-excited near-field luminescence of semiconductor quantum dots — •Vlastimil Křápek, Petr Dvořák, Lukáš Kejík, Michal Kvapil, Petr Liška, Jan Krpenský, and Tomáš Šikola — Brno University of Technology, Brno, Czech Republic

On-chip integration of light sources would benefit from near-field handling of the emission with a subwavelength spatial resolution. Here we present a fully near-field photoluminescence study of semiconductor quantum dots, with a surface plasmon interference device (SPID) used for the excitation and an aperture-type scanning near-field optical microscope (SNOM) combined with a spetrometer for the collection.

The SPID consists of an opaque metallic layer with thin subwavelength slits fabricated using focused-ion-beam milling. When illuminated from bottom, a near-field standing wave forms at the top interface [1,2,3] where it excites quantum dots deposited directly at the top interface.

We demonstrate the plasmon-excited near-field luminescence of CdSe/ZnS quantum dots with rather a weak effect of the excitation mechanism on the spectral profile of the emitted light. This makes the plasmon-excited luminescence a suitable tool for the on-chip integration of semiconductor light sources, as well as a characterization technique with the subwavelength spatial resolution.

[1] P. Dvořák et al., Nano Lett. **13**, 2558 (2013).
[2] P. Dvořák et al., Opt. Express **25**, 16560 (2017).
[3] P. Dvořák et al., Nanoscale **45**, 21363 (2018).

O 24.7 Mon 13:30 P

Hot electrons masquerading as plexcitons in J-aggregate/ plasmonic nanoparticle systems — •Victoria C. A. Taylor[1], Sara Núñez-Sánchez[2], and Thomas A. A. Oliver[3] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Universidade de Vigo, Departamento de Química Física, Campus Universitario As Lagoas, Marcosende, 36310 Vigo, Spain — [3]School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

Surface plasmon polaritons (SPPs) can produce localised high electric field strengths. Through strong coupling with quantum emitters, they can create hybrid states with novel and promising properties. Excitons in J-aggregates, coupled with SPPs on metallic nanoparticles, are ideal systems for studying these effects. The hybrid quasiparticles that form in these systems under strong coupling are sometimes referred to as plexcitons (plasmon/exciton). Several studies have investigated the dynamics of these plexcitons and report lifetimes on the order of picoseconds, which is in strong contrast to the tens of femtoseconds lifetimes that are typically associated with SPPs.

In this work, we investigate the ultrafast transient absorption response of a TDBC J-aggregate/hollow gold nanoshells (HGNs) hybrid system. Through our excitation wavelength dependence measurements, and comparison with the response of the uncoupled HGNs, we show that the observed picosecond signal does not result from long-lived plexcitons; rather, it is caused by the hot electron population that remains after the plexciton has dephased.

O 25: Poster Session II: Surface magnetism II

Time: Monday 13:30–15:30 Location: P

O 25.1 Mon 13:30 P

Real-time MOKE measurements of CoTMPP on magnetic Ni/Cu(110)-(2x1)O — •Gizem Mendirek[1], Aleksander Brozyniak[2], Michael Hohage[1], Andrea Navarro-Quezeda[1,3], and Peter Zeppenfeld[1] — [1]Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich — [2]CD-Labor für Nanoskalige Phasenumwandlungen, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich — [3]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität Linz, Altenberger Str. 69, 4040 Linz, Österreich

In this work, we report real-time investigations of an organic/ferromagnetic interface by employing a sinusoidal modulation of the magnetic field with the synchronous detection of the Reflectance Difference Magneto-Optical Kerr Effect (RDMOKE) signal. Besides improving the detection limit to variations of the Kerr rotation angle below 1 μrad/mT, the present setup allows recording hysteresis loops continuously as a function of coverage, time or temperature. We illustrate the capabilities of the setup for Ni thin films grown on a Cu(110)-(2x1)O surface and the subsequent deposition of cobalt tetramethoxyphenylporphyrin (CoTMPP) thin layers. The adsorption of the molecules induces characteristic changes in the magnetic properties (magnetization amplitude, remanence and coercive field) that are monitored as a function of the coverage with submonolayer resolution and as a function of temperature, revealing the decrease of the Curie temperature upon CoTMPP deposition on Ni films with different thicknesses.

O 25.2 Mon 13:30 P

Domain Walls in the Row-Wise Antiferromagnet Mn/Re(0001) — •Martin Grünebohm, Jonas Spethmann, Roland Wiesendanger, Kirsten von Bergmannv, and André Kubetzka — Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Typical domain walls (DWs) in antiferromgnetic (AFM) systems can be described by a coherent rotation, which allows a mapping onto ferromagnetic DWs. Experiments show, that in fcc-stacked monolayers of manganese on Re(0001), competing nearest and next-nearest neighbor Heisenberg exchange in combination with higher order interactions lead to a row-wise antiferromagnetic state (or 1*Q* state) [1]. We find that DWs, that separate the rotational domains, cannot be described by a coherent spin rotation. Instead, the low symmetry of the row-wise AFM state facilitates a new type of DW, which connects rotational domains by an opposite rotation of adjacent spin pairs across the wall. Interestingly, the non-collinear spin texture in the center of the DW has an angle of 90° between neighboring spins, characteristic of a so-called 2Q state. We propose an analytical description and test it using spin dynamics simulations based on DFT calculations in comparison to spin-polarized STM measurements [2].

[1] J. Spethmann *et al.*, Phys. Rev. Lett. **124,** 227203 (2020).
[2] J. Spethmann *et al.*, arXiv:2011.05678 (2020).

O 25.3 Mon 13:30 P

Magnetic force microscopy on a cobalt thin film deposited on a trampoline-type free hanging silicon nitride membrane — •Denis Goman[1], Dhavalkumar Mungpara[1], Federico Maspero[2], Simone Cuccurullo[3], Riccardo Bertacco[2,3], and Alexander Schwarz[1] — [1]Institute of Nanostructure and Solid State Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — [2]CNR Istituto di Fotonica e Nanotecnologie, Piazza Leonardo da Vinci 32, 20133, Milano, Italy — [3]CNR Istituto di Fotonica e Nanotecnologie, Piazza Leonardo da Vinci 32, 20133, Milano, Italy

We apply magnetic force microscopy (MFM) in ambient conditions employing the lift mode to study the magnetic domain structure of a 130 nm thick cobalt film deposited on a 1000 nm thick silicon nitride trampoline-type membrane attached to a 0.2 mm thick silicon frame. The cobalt is deposited only onto the central rectangular part of the trampoline membrane. The four strings attached to the corners of the the 0.15 mm × 0.15 mm window are uncoated.

MFM images show that the cobalt thin film exhibit out-of-plane stripe domains predominantly aligned along the sides of the rectangular shaped film. We find a periodicity of 230 nm in the central part where the film thickness is constant. At the edges, where the film thickness decreases linearly, the domain width decreases as well. We also studied the effect of an external magnetic field on the genuine domain structure.

The authors gratefully acknowledge funding from the ERC H2020 research and innovation program grant agreement No 828784.

O 25.4 Mon 13:30 P

Chimera-type skyrmion collapse revealed by sub-nm maps of the transition rate — •Stephan von Malottki[1], Florian Muckel[2], Christian Holl[2], Benjamin Pestka[2], Marco Pratzer[2], Pavel F. Bessarab[3,4], Stefan Heinze[1], and Markus Morgenstern[2] — [1]ITAP, University of Kiel — [2]Institute of Physics B and JARA-FIT, RTWH Aachen University — [3]University of Iceland, Reykjavík — [4]ITMO University, St. Petersburg

In addition to the conventional radial symmetric collapse of magnetic skyrmions, recent studies predicted the occurrence of skyrmion annihilation processes via the chimera skyrmion state [1-3]. Here, we demonstrate the realization of both the radial symmetric and the chimera transition mechanism in the ultra-thin film system fcc-Pd/Fe/Ir(111) [4]. Scanning tunneling microscopy is used to create transition rate maps of magnetic switching events induced by single electron events. In combination with energy density maps of the transition states obtained by atomistic spin simulations parametrized from first principles, they allow for the identification of both annihilation mechanisms. It is further shown, that a transition between both mechanisms can be achieved by the application of external in- and out-of-plane magnetic fields, yielding a sound agreement between experiment and theory.

[1] Meyer et al., Nat. Commun. 10, 3823 (2019)
[2] Heil et al., Phys. Rev. B 100, 134424 (2019)
[3] Desplat et al., Phys. Rev. B 99, 174409 (2019)
[4] Muckel et al., Nat. Phys. (2021)
https://doi.org/10.1038/s41567-020-01101-2

O 25.5 Mon 13:30 P

Probing the magnetism of single atoms with orbital sensitivity — Aparajita Singha[1,2], •Daria Sostina[1,2], Christoph Wolf[1,2], Safa Ahmed[1,3], Denis Krylov[1,2], Luciano Colazzo[1,2], Pierluigi Gargiani[4], Stefano Agrestini[4], Woo-Suk Noh[5], Jae-Hoon Park[5,6], Marina Pivetta[7], Stefano Rusponi[7], Harald Brune[7], Andreas Heinrich[1,3], Alessandro Barla[8], and Fabio Donati[1,3] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [4]ALBA Synchrotron Light Source, Cerdanyola del Vallès, Catalonia, Spain — [5]MPPC-CPM, Max Planck POSTECH/Korea Research Initiative, Pohang, Korea — [6]Department of Physics, Pohang University of Science and Technology (POSTECH), Pohang, Korea — [7]Institute of Physics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [8]Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR), Trieste, Italy

Lanthanide atoms are promising candidates for atomic data storage and quantum logic due to the long magnetic lifetime.[Science 352, 318 (2016)]. Here, we use the orbital sensitivity of x-ray absorption spectroscopy to investigate the valence magnetism of rare earth atoms and clusters on MgO/Ag(100). We find both Gd and Ho atoms in a monovalent state, with one electron transferred to the underneath substrate. Combining our experiments with multiplet calculations and density functional theory we clarify the controversy on the ground state of Ho single atom magnets [Phys. Rev. Lett. 121, 027201 (2018)].

O 25.6 Mon 13:30 P

Electrical and thermal transport in antiferromagnet-superconductor junctions — •Martin Fonnum Jakobsen[1], Kristian Naess[1], Paramita Dutta[2], Arne Brataas[1], and Alireza Qaiumzadeh[1] — [1]Norwegian University of Technology — [2]Uppsala University

We demonstrate that antiferromagnet–superconductor (AF–S) junctions show qualitatively different transport properties than normal metal–superconductor (N–S) and ferromagnet–superconductor (F–S) junctions. We attribute these transport features to the presence of two new scattering processes in AF–S junctions, i.e., specular reflection of holes and retroreflection of electrons. Using the Blonder–Tinkham–Klapwijk formalism, we find that the electrical and thermal conductance depend nontrivially on antiferromagnetic exchange strength, voltage, and temperature bias. Furthermore, we show that the interplay between the Néel vector direction and the interfacial Rashba spin-orbit coupling leads to a large anisotropic magnetoresistance. The unusual transport properties make AF–S interfaces unique among the traditional condensed-matter-system-based superconducting junctions.

O 25.7 Mon 13:30 P

Spin-spiral state of a Mn monolayer on W(110) at variable temperatures as seen by x-ray absorption spectroscopy — •Ondrej Sipr[1], Kirsten von Bergmann[2], Hubert Ebert[3], Roland Wiesendanger[2], and Jan Honolka[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha — [2]University of Hamburg, Germany — [3]Ludwig-Maximilians-Universität München, Germany

The noncollinear magnetic state of epitaxial Mn monolayers on tungsten (110) crystal surfaces is investigated by means of soft x-ray absorption spectroscopy, to complement earlier spin-polarized STM experiments. X-ray absorption spectra (XAS), x-ray linear dichroism (XLD) and x-ray magnetic circular dichroism (XMCD) Mn $L_{2,3}$-edge spectra were measured in the temperature range from 8 to 300 K and compared to results of fully-relativistic *ab initio* calculations. We show that antiferromagnetic (AFM) helical and cycloidal spirals give rise to significantly different Mn $L_{2,3}$-edge XLD signals, enabling thus to distinguish between them.

It follows from our results that the magnetic ground state of a Mn monolayer on W(110) is an AFM cycloidal spin spiral. Based on temperature-dependent XAS, XLD and field-induced XMCD spectra we deduce that magnetic properties of the Mn monolayer on W(110) vary with temperature, but this variation lacks a clear indication of a phase transition in the investigated temperature range up to 300 K — even though a crossover exists around 170 K in the temperature dependence of XAS branching ratios and in XLD profiles.

O 25.8 Mon 13:30 P

Lifetimes of skyrmions and antiskyrmions in exchange frustrated systems — •Moritz A. Goerzen[1], Stephan v. Malottki[1], Sebastian Meyer[1], Pavel F. Bessarab[2,3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel — [2]University of Iceland, Reykjavík, Iceland — [3]ITMO University, St. Petersburg, Russia

A recent study [1] on a Rh/Co bilayer on Ir(111) shows an interesting energy landscape for noncollinear magnetic states due to a high degree of exchange frustration. In particular we find, that both skyrmions and antiskyrmions co-exist in this system, which is beneficial for future spintronic technologies. Based on an atomistic spin model parameterized from density functional theory, we investigate the lifetime of co-existing states by long time scale spin dynamic simulations using the geodesic nudged elastic band method as well as transition state theory in harmonic approximation [2,3]. Due to a different number of internal degrees of freedom for skyrmions and antiskyrmions in systems without inversion symmetry, we find large differences between lifetimes of these states.

[1] Meyer, Perini *et al.*, Nature Comm. **10**, 3823 (2019)
[2] Bessarab *et al.*, Sci. Rep. **8**, 3433 (2018)
[3] von Malottki *et al.*, Phys. Rev. B **99**, 060409 (2019)

O 26: Poster Session II: Nanostructures at surfaces II

Time: Monday 13:30–15:30 Location: P

O 26.1 Mon 13:30 P

Single-crystal graphene on Ir(110): a uniaxial template — •Stefan Kraus[1], Felix Huttmann[1], Timo Knispel[1], Jeison Fischer[1], Ken Bischof[1], Alexander Herman[2], Marco Bianchi[3], Raluca-Maria Stan[3], Ann Julie Holt[3], Vasile Caciuc[4], Shigeru Tsukamoto[4], Heiko Wende[2], Philip Hofmann[3], Nicolae Atodiresei[4], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Universität Duisburg-Essen, Germany — [3]Aarhus university, Denmark — [4]Forschungszentrum Jülich, Germany

A single-crystal sheet of graphene is grown on the low-symmetry substrate Ir(110) by thermal decomposition of ethylene at 1500 K. While the bare Ir(110) is heavily reconstructed at room temperature due to the formation of nanofacets, scanning tunneling microscopy reveals that the adsorbed graphene suppresses this reconstruction entirely and large atomically flat areas are observed. The superposition of the graphene with the Ir(110) lattice gives rise to a wave pattern with clear crests and troughs along the [001] direction while the atomic lattice of the graphene is under very weak lateral strain ($<$ 0.2% compared to graphite). Density functional theory calculations confirm the observed wave pattern and show a strong variation from weak (crests) to strong chemical binding (troughs). Angle-resolved photo emission spectroscopy shows no sign of a Dirac cone, which is in agreement with the large variety of binding motifs and partial sp^3 hybridization. We showcase the use of this uniaxial template by the global alignment of sandwich-molecular wires — one-dimensional organometallic structures — parallel to the crests and troughs.

O 26.2 Mon 13:30 P

Selective Area Growth of III-V Nanowires on High-Index GaAs Substrates — •Gunjan Nagda[1,2], Daria Beznasiuk[1,2], Tobias Saerkjaer[1,2], Martin Espineira[1,2], Sara Martí-Sanchez[3], Jordi Arbiol[3], and Peter Krogstrup[1,2] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — [2]Microsoft Quantum Materials Lab, 2800 Lyngby, Denmark — [3]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, 08193 Bellaterra, Barcelona, Catalonia, Spain

Using a patterned SiO$_2$ mask we report on selective area growth of III-V materials on high-index GaAs substrates using molecular beam epitaxy (MBE). This platform is used to define 1D semiconductor nanowire (NW) networks with excellent surface selectivity for quantum transport studies. Due to the dependence of NW faceting on the substrate orientation and the trench direction within the oxide mask, non-standard substrate orientations such as (211)A and (211)B, and (311)A and (311)B open the pathway to obtain a multitude of geometries. The NW faceting observed using atomic force microscopy (AFM) and cross-sectional transmission electron microscopy (TEM) is in good agreement with the facets predicted on the basis of the stereographic projections of the substrate orientations. The equilibrium shapes are determined using Wulff construction along with constraints imposed by the oxide mask. Comparison with experimental findings is used to determine whether a particular growth is driven by thermodynamically determined surface energy minimization or by kinetic parameters.

O 26.3 Mon 13:30 P

2D covalent organic frameworks on monolayer MoS2 — •wenbo lu[1], davor čapeta[2], mihaela enache[1], and meike stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have received increasing attention as promising materials for different applications. One possibility to precisely tune the electronic and optical properties to the desired applications is based on adsorbing well-ordered organic assemblies TMDs. Here, a study of on-surface synthesis of 2D covalent organic frameworks (COFs) on monolayer molybdenum disulfide (MoS2) on highly oriented pyrolytic graphite (HOPG) will be presented. Monolayer MoS2 films were synthesized by chemical vapor deposition and transferred to HOPG. The transferred MoS2 was characterized by atomic force microscopy and scanning tunneling microscopy (STM), from which we conclude that the transferred MoS2 is of high-quality with micrometer sized domains. For COF formation, 1,4-benzenediboronic acid (BDBA) was deposited onto the MoS2/HOPG. The structure of the formed 2D COFs was studied with STM. The dehydration of BDBA results in the formation of a long-range ordered honeycomb molecular network on MoS2. Our results show the possibility of using 2D COFs to build up ordered organic/2D TMDs interfaces, which is promising for the fabrication of hybrid organic-inorganic devices possessing tailored structures and properties.

O 26.4 Mon 13:30 P

Theoretical analysis of chemical transformation of π-conjugated polymers steered by internal vibrational modes — •Adam Matěj[1,2], Michal Otyepka[1], Miroslav Medveď[1], and Pavel Jelínek[1,2] — [1]Regional Centre of Advanced Technologies and Materials, Palacký University, Šlechtitelů 27, 783 71 Olomouc, Czech Republic — [2]Institute of Physics, The Czech Academy of Sciences, Cukrovarnická 10, 162 00, Prague 6, Czech Republic

The rational design of increasingly complex electronic materials for molecular electronics and quantum technologies has been an active field of research in organic electronics. Recent developments of on-surface synthesis open novel strategies to tailor one-dimensional π-conjugated polymers. In this work, we employ quantum-mechanical calculations for the description of structural and electronic properties of π-conjugated ethynylene bridged polymers. Additionally, we introduce novel synthetic strategy forming π-conjugated ladder polymers with non benzenoid pentalene bridges by exploiting the relation between π-conjugation, topological phase and vibrational modes of the polymer. Selected vibrational mode of ethynylene bridged bisanthene polymer is shown to be the key feature allowing the cyclization of ethynylene into pentalene linker, which is not observed in topologically trivial anthracene polymer. Finally, we present reaction mechanism highlights differentiating anthracene and bisanthene π-conjugated ethynylene bridged polymers, leading to successful cyclization in bisanthene but prevent the reaction on anthracene polymer completely, which is in direct agreement with experiments.

O 26.5 Mon 13:30 P

Coupling of YSR states in 1D chains of Fe atoms on Nb(110) — •Felix Friedrich, Robin Boshuis, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The pair-breaking potential of magnetic impurities in a superconducting host material gives rise to in-gap peaks, so called Yu-Shiba-Rusinov (YSR) states. Coupling of these states leads to the formation of molecular-like bonding and antibonding modes in impurity dimers [1], YSR bands in many impurity systems [2], and constitutes a platform for the formation of Majorana fermions at the ends of one-dimensional chains [3]. To obtain a more detailed understanding of the interaction of multiple magnetic impurities, we investigate the coupling of YSR states in short one-dimensional Fe chains on clean Nb(110). By functionalizing STM tips with a CO molecule we are able to resolve single atoms in nearest neighbor lattice positions of self-assembled Fe chains. Spectroscopic measurements reveal that the splitting of the single atom YSR states becomes more complex with increasing chain length. Furthermore, differential conductivity maps uncover an intriguing dependence of the odd or even spatial symmetry of the individual states on the chain length. The experimental results will be compared to theoretical models.

[1] S.-H. Ji *et al.*, Phys. Rev. Lett. **100**, 226801 (2008)
[2] M. Ruby *et al.*, Phys. Rev. Lett. **115**, 197204 (2015)
[3] S. Nadj-Perge *et al.*, Science **346**, 602 (2014)

O 26.6 Mon 13:30 P

Tailoring vortex core polarity and vortex chirality by in-plane and out-of-plane magnetic fields — •Andrea Ehrmann[1] and Tomasz Blachowicz[2] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, Bielefeld, Germany — [2]Silesian University of Technology, Institute of Physics - Centre for Science and Education, Gliwice, Poland

Vortex states in magnetic nanodots can be used to store data, defined by the core polarity and/or the vortex chirality. Preparing nanodots with dimensions leading to magnetization reversal by vortex states is technologically not problematic if material and dimensions are chosen carefully [1,2]. Defining core polarity and vortex chirality reliably, however, needs more sophisticated approaches [3]. Here we give an overview of the influence of different out-of-plane and in-plane bias fields on these values, showing that in clusters of circular nanodots, out-of-plane fields can be applied to define and to switch the vortex core polarity without influencing the vortex chirality simultaneously. This enables defining both properties independently and thus preparing quaternary vortex-based memory devices.

[1] A. Ehrmann, T. Blachowicz, J. Magn. Magn Mater. 475, 727-733 (2019)
[2] A. Ehrmann, T. Blachowicz, Hyperfine Interactions 239, 8 (2018)
[3] A. Ehrmann, T. Blachowicz, Proc. of 2018 IEEE 8th International Conference on ”Nanomaterials: Applications & Properties” 1, 01NMM08 (2020)

O 26.7 Mon 13:30 P

A differential equation for plowing-induced structuring of polymer films — •Enrico Gnecco[1], Jana Hennig[1], Pedro J. Martinez[2], and Juan J. Mazo[2] — [1]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Germany — [2]Department of Condensed Matter Physics, University of Zaragoza, Spain

The formation of ripple structures out of plowing wear is a well-known but scarcely understood phenomenon in polymer physics. Here we discuss this process on the example of polystyrene thin film scratched by silicon nanotips. The physical interpretation relies on the stick-slip motion of the tip, which is simultaneously indented and elastically pulled along the surface. The dependence of the ripple orientation on the geometry of the scanned area is numerically reproduced with an original equation for the tip motion in an energy landscape mirroring the surface evolution. Eye-catching examples will include square, circle, star and heart shaped geometries, but potential applications of our model will be also mentioned.

[1] J.J. Mazo et al., Plowing-induced structuring of compliant surfaces, PRL 122 (2019) 256101 [2] P.J. Martinez et al., Numerical study of pattern formation in compliant surfaces scraped by a rigid tip, PRE, accepted (2021)

O 26.8 Mon 13:30 P

Comparing the Nanomechanics and the Chemical Properties of NC-AFM Tips — •Damla Yesilpinar[1,2], Bertram Schulze Lammers[1,2], Alexander Timmer[2], Zhixin Hu[3], Wei Ji[4], Saeed Amirjalayer[1,2,5], Harald Fuchs[1,2], and Harry Mönig[1,2] — [1]Physikalisches Institut, Westfalische Wilhelms-Universitat, Muenster, Germany. — [2]Center for Nanotechnology, Muenster, Germany. — [3]Center for Quantum Joint Studies and Department of Physics, Tianjin University, Tianjin, China — [4]Department of Physics and Beijing Key Laboratory of Optoelectronic Functional Materials & Micro-Nano Devices, Renmin University of China, Beijing, China — [5]Center for Multiscale Theory and Computation, Muenster, Germany

Controlling the identity of the tip-terminating species in AFM constitutes a milestone for investigations of surfaces and adsorbates. Highlighting the importance of the mechanical tip properties, we consolidate the interpretation of such studies by comparing the performance of four atomically defined tips, namely Cu-, Xe-, CO-, and CuOx-tips. Using a nano-structured copper oxide surface, we investigated their imaging performances and capabilities in force mapping during the lateral manipulation of single adsorbed atoms. Cu-tips easily reacts with surface oxygen or the adsorbate, while chemically inert Xe- and CO-tips allow entering the repulsive force regime enabling increased resolution. But their high flexibility leads to tip-deflection and related artefacts. The combination of chemical passivation and mechanical rigidity for the CuOx-tip turns out decisive for chemical-specific imaging and for a superior performance in manipulation experiments.

O 27: Poster Session II: Poster to Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces I

Time: Monday 13:30–15:30 Location: P

O 27.1 Mon 13:30 P

Temperature-dependent trapping probability measurements of *n*-butane on ionic liquid surfaces using molecular beam techniques — •Leonhard Winter, Radha G. Bhuin, Matthias Lexow, Florian Maier, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Ionic Liquids (ILs) are room temperature liquids consisting only of cations and anions. IL thin films are the key components in the catalytic concepts Supported Ionic Liquid Phase (SILP) and Solid Catalyst with Ionic Liquid Layer (SCILL), for which the transfer of hydrocarbons through the ionic liquid/gas interface plays a crucial role.

We have built a new ultra-high vacuum apparatus dedicated for the investigations of ILs with molecular beam techniques. It was used to study the first step of the interaction dynamics of *n*-butane on a series of alkylimidazolium ionic liquids with varying chain lengths and anions ($[C_nC_1Im][X]$). Based on the temperature-dependent behavior of the initial trapping probability at low temperatures, measured by the direct method of King and Wells, we found that the binding energy is dominated by the interaction with the alkyl chain of the cation, whereas the ionic headgroups contribute only weakly.

L.W., R.G.B, M.L. and H.-P.S. thank the European Research Council (ERC) for financial support of this research in the context of an Advanced Investigator Grant to H.-P.S (No. 693398-ILID).

Bhuin *et al.*, Angew. Chem. Int. Ed., **2020**, 59, 14429-14433.

Winter *et al.*, J. Chem. Phys., **2020**, 153, 214706.

O 27.2 Mon 13:30 P

Surface tension measurement of pure water in vacuum. — •Jiri Pavelec, Paul Ryan, Jan Balajka, Michael Schmid, and Ulrike Diebold — IAP, Vienna University of Technology, Austria

Very little is known about the surface tension of pure liquids in contact with their pure gaseous phases, i.e. without the presence of other gases or liquid phase contaminants. This is surprising given that contaminants are known to greatly affect surface tension values [1].

Recently we have developed a method to dose liquid water onto pristine surfaces in UHV using a small cryostat [2,3]. We combine this approach with the pedant drop method [4] to measure the surface tension of ultra-clean liquids in contact with their pure gaseous phases. The upgraded version of the small cryostat, replaces the syringe typically used in the pendant-drop method. The ultra-clean liquid is condensed onto a small cryostat placed in a vacuum chamber. A pendant drop is formed, photograph and analyzed allowing the surface tension of the liquid to be directly determined.

The design of the apparatus will be discussed and preliminary measurements of ultra-clean water will be presented.

[1] Uematsu, Bonthuis, Netz, Current Opinion in El., Vol. 13, (2019)

[2] Balajka, Pavelec, Komora, Schmid, and Diebold, Review of Scientific Instruments 89, (2018)

[3] Balajka, Hines, DeBenedetti, Komora, Pavelec, M Schmid, U Diebold, Science, 361, (2018)

[4] Berry, Neeson, Dagastine, Chan, Tabor, J. Coll. Interface Sci. 454, 226, (2015)

O 27.3 Mon 13:30 P

pH-dependence of the surface enrichment of inorganic ions mediated by amino acids — •Isaak Unger[1], Geethanjali Gopakumar[1], Olle Björneholm[1], Carl Caleman[1,6], Christophe Nicolas[2], Gunnar Öhrwall[3], Tulio Costa Rizuti da Rocha[4], and Arnaldo Naves de Brito[5] — [1]Uppsala university — [2]Synchrotron SOLEIL — [3]MAX IV Laboratory — [4]Brazilian Synchrotron Light Laboratory — [5]University of Campinas — [6]Center for Free-Electron Laser Science, DESY

Sea spray is one of the most prominent sources for non-anthropogenic aerosol, thus understanding sea spray aerosol plays a pivotal role in understanding the Earth*s atmosphere. Aqueous sea spray aerosol is a complex mixture of organic surfactants and inorganic ions and is also the subject to changes over time as the particles are suspended in the atmosphere and engage in chemical reactions. One of the dynamic parameters in the particles is the pH, as sea spray aerosol is generated from slightly basic sea water but quickly assumes acidic pH. How changes in the pH affect the surface composition of such particles has only recently become the subject for in-depth research. Our results attempt to fill the knowledge gap by investigating the pH-dependent surface propensity of K^+ and Cl^- in a mixed KCl-amino acid solution. We used X-ray photoelectron spectroscopy on liquid jets to explore the impact of a variety of amino acids with different side chains on the ratio of K^+ and Cl^- close to the liquid surface.

O 27.4 Mon 13:30 P

Probing the Gold/Water Interface with Surface Specific Spectroscopy — •Stefan Piontek, Stephanie Sanders, Dennis Naujoks, Alfred Ludwig, and Poul Petersen — Ruhr Universität, Bochum, DE

Water is integral in electrochemistry, in the generation of the electric double layer, and propagating the interfacial electric fields; yet our molecular-level understanding of interfacial water near functioning electrode surfaces is limited.

Sum-frequency-generation (SFG) spectroscopy offers an opportunity to investigate the structure and dynamics of the solvent near working electrochemical interfaces, as the method is inherently surface-specific. Previous attempts which propagated IR beams through the solvent have suffered due to the IR absorption of water. Furthermore, sending visible and IR beams through standard electrode films obscures the SFG spectra, due to the large nonlinear response of conduction band electrons.

To overcome this limitation, we have investigated thin yet conductive gradient sputtered Au films on CaF2 using SFG, FTIR, AFM, and UV-Vis spectroscopies to explore the ideal thickness of an Au electrode layer. SFG spectra of dry and wet 8.0-0.4 nm thick Au films suggest that unobscured interfacial water spectra can be obtained using Au films with a thickness of ~2 nm or less. With the newfound ability to probe interfacial solvent structure at electrode/aqueous interfaces we hope to provide insights into more efficient electrolyte composition and electrode design.

O 28: Key Note II

Time: Monday 15:30–16:00 Location: R1

Plenary Talk O 28.1 Mon 15:30 R1

Physical chemistry and chemical physics of environmental interfaces — •Vicki Grassian — University of California San Diego, La Jolla CA 92093

The focus of this talk is on environmental interfaces which are defined as any surface in equilibrium with its surrounding environment. From this broad definition, there are a myriad of different types of environmental interfaces that include atmospheric aerosols, nanomaterials and indoor surfaces. The physical chemistry and chemical physics of environmental interfaces puts an emphasis on molecular and nanoscale level interactions that occur in these inherently complex systems. Examples of the complexity of these interfaces and how a deeper understanding can be obtained through molecular-based approaches are highlighted.

O 29: Key Note III

Time: Tuesday 10:00–10:30 Location: R1

Plenary Talk O 29.1 Tue 10:00 R1

Electrochemistry of platinum: new views on an old problem — •Marc Koper — Leiden University, Leiden, The Netherlands

Platinum is the most used electrocatalyst in electrochemical energy conversion devices such as fuel cells and electrolysers. In this talk I will highlight the recent work of my group on understanding the surface chemistry of platinum in an aqueous electrolyte, by combining single-crystal electrochemistry, density functional theory calculations, ultra-high-vacuum modeling, in situ spectroscopy and in situ electrochemical scanning tunneling microscopy. I will challenge some existing explanations and interpretations of platinum electrochemistry, and show the sometimes surprising surface disordering of platinum that happens at both positive (anodic) and negative (cathodic) potentials.

O 30: Mini-Symposium: Electrified solid-liquid interfaces I

Time: Tuesday 10:30–12:30 Location: R1

Introduction by Symposium Organizers

Invited Talk O 30.1 Tue 10:35 R1

A Theoretical Framework for Investigating Electrochemical Reactions — •Wolfgang Schmickler — Institut für Theoretische Chemie, Universität Ulm, Deutschland

Electrochemical reactions take place at the interface between an electronic and an ionic conductor. Here we consider the most important case, a metal in contact with an electrolyte solution. The challenge is to treat electrocatalytic reaction, in which either the initial of the final state of the reaction is adsorbed on the electrode surface.

Consider the deposition of a silver ion on a silver electrode as an example. In the initial state, the 4s orbital is empty and the ion has a solvation energy of -5.1 eV. To get deposited, the ion has to approach the electrode, losing a part of its solvation energy. A thermal fluctuation takes the valence orbital, which is broadened by the interaction with the electrode, to the Fermi level. The ion takes up an electron, loses the solvation energy, and gains the energy of ionization, and the sublimation energy of silver; the potential drop between the solution and the electrode surface enters into the energy required to approach the electrode. Obviously, a good theory must treat all components of the interface, metal and solution, with the same atomic detail.

For this purpose we have developed a framework based on a model Hamiltonian, which combines ideas from Marcus theory, Anderson-Newns theory, Green's function techniques with our own ideas. The detailed form of the Hamiltonian depends on the reaction under consideration. We consider a few examples, and will how to obtain the parameters from DFT and molecular dynamics.

Invited Talk O 30.2 Tue 11:10 R1

Dynamic Evolution of CO_2 Electroreduction Catalysts — •Beatriz Roldan Cuenya — Department of Interface Science, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Tailoring the chemical reactivity of nanomaterials at the atomic level is one of the most important challenges in catalysis research. In order to achieve this elusive goal, we must first obtain a fundamental understanding of the structural and chemical properties of these complex systems. In addition, the dynamic nature of the nanostructured films and nanoparticle (NP) catalysts and their response to the environment must be taken into consideration. To address the complexity of real-world electrocatalysts, a synergistic approach taking advantage of a variety of cutting-edge experimental methods (EC-AFM, LC-TEM, XPS, XAFS, Raman Spect., GC) has been undertaken.

This talk will provide insight into the electrocatalytic reduction of CO_2 and will feature the parameters that determine the reaction's selectivity. Important aspects that will be discussed are: (i) the design of size- and shape-controlled catalytically active nanoparticles (Cu, Zn, Cu-Zn, Cu-Ag) (ii) the role of the NP size and shape on the catalytic activity and selectivity, (iii) the evolution of the structure and composition of the electrocatalysts under operando reaction conditions and their influence on the catalytic performance, (iv) the possibility of using pulsed-electrolysis to tune the reaction selectivity. These findings are expected to open up new routes for the reutilization of CO_2 through its direct conversion into valuable chemicals and fuels such as ethylene and ethanol.

O 30.3 Tue 11:45 R1

Tuning the Stability of Platinum by means of Scan Rate — •Jon Bjarke Valbaek Mygind[1], Francesc Valls Mascaro[1], Marc T.M. Koper[1], and Marcel J. Rost[2] — [1]Leiden Institute of Chemistry, Leiden University — [2]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University

Platinum is widely used as an electrocatalyst in several applications like fuel cells and electrolysers, due to its high catalytic activity. However, platinum is scarce and its industrial feasibility is limited by its degradation under oxidizing conditions. Repeated oxidation and reduction of a platinum electrode leads to the roughening of the surface, caused by the nucleation and growth of nano-islands, which first grow laterally (2D) and then in height (3D) [1]. The nucleation and growth of these islands is promoted by the creation of adatom vacancy pairs [2,3]. Unfortunately, the precise mechanism responsible for this process is still not fully understood. Here, we examine the growth rate of the roughness on a Pt(111) surface by analysing cyclic voltammograms at different sweep rates. From our understanding of surface growth, we have indications that the mechanism responsible for the creation of adatom-vacancy pairs is kinetically (surface diffusion) limited. At faster sweep rate, less roughening is observed, which could be explained by fewer adatoms and vacancies being created on the surface, supporting our hypothesis.

[1] Jacobse L. et al., ACS Cent. Sci. 5 (12), 1920 (2019)
[2] Rost, M.J. et al., M.T.M., Nat. Commun. 10, 5233 (2019)
[3] Ruge, M. et al., J. Am. Chem. Soc., 139, 4532-4539 (2017)

O 30.4 Tue 12:00 R1

Observing the oxidation of platinum under operando electrochemical conditions — •Leon Jacobse[1], Ralf Schuster[2], Xin Deng[1], Silvan Dolling[1], Tim Weber[3], Herbert Over[3], Jörg Libuda[2], Vedran Vonk[1], and Andreas Stierle[1] — [1]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [2]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen — [3]Physikalisch-Chemisches Institut and Zentrum für Materialforschung, Justus Liebig University, Giessen

Platinum electrocatalyst degradation forms a large barrier for the wide-spread application of electrolysers and fuel cells, which are crucial for a sustainable energy society. A detailed understanding of the catalyst surface structure during the chemical reaction is required to design more stable catalysts. We have developed a Rotating Disk Electrode (RDE) setup that enables a structural characterization by synchrotron High-Energy Surface X-Ray Diffraction (HE-SXRD) experiments while maintaining well-defined diffusion conditions and high catalytic reaction rates (current densities). With this setup we followed the oxidation of Pt(111) and Pt(100) model electrodes; starting from the Place-Exchange surface oxidation occurring around 1.1V until the formation of a (bulk) oxide at potentials relevant for the oxygen evolution reaction. In contrast with heterogenous oxidation experiments, no ordered oxide structures are observed.

O 30.5 Tue 12:15 R1

Electrochemical interfaces: applications to batteries — •Jean-sebastien Filhol[1], Arthur Hagopian[1], and Anja Kopac-Lautar[2] — [1]Institut Charles Gerhardt Montpellier/ENSCM/CNRS/Université de Montpellier — [2]National Institute of Chemistry, Ljubljana, Slovenia

Electrochemical interfaces are fundamental to understand electrochemical reactions either for energy storage in devices such as Li-ion batteries. Nevertheless, these interfaces are extremely complex to model not only because of the occurring electrochemical effects, but also because of the complexity of the electrode-solvent interactions.

We will present an approach allowing the modeling of realistic electrochemical interfaces at a limited cost and demonstrate the predictive capabilities of these calculations. We will first discuss electrochemical effects on interface using implicit solvent approach in order to investigate how interfaces morphology is changed with the applied potential in particular to investigate dendritic growth Then, we will use a mixed implicit/explicit solvent approach (exemplified by Li/Ethylene carbonate (EC) and Mg/Dimethoxyéthane (DME) interfaces) that allows investigating electrochemical reactivity at a limited cost. We will show that the interfacial species can be very different from the ones of the electrolyte given some new insights the specific double layer rectivity. To rationalize this reactivity, specific tools within conceptual DFT framework were developed. This allows obtaining quantitative and predictive index of the interfacial electrochemical reactivity in order to improve the electrochemical devices development, in particular in link with batteries.

O 31: Mini-Symposium: Manipulation and control of spins on functional surfaces I

Time: Tuesday 10:30–12:30 Location: R2

Invited Talk O 31.1 Tue 10:30 R2

What can we learn from atoms? — •Alexander Khajetoorians — SPM department, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

Based on scanning tunneling microscopy, magnetic atoms and films on surfaces have become a model playground to understand and design magnetic order, bottom-up. However, magnetic order in these model systems have been confined to the limits dominated by bistability. In this talk, based on the recently discovered concept of orbital memory and the anisotropic behavior of black phosphorus, I will illustrate new model atomic platforms to realize multi-modal landscapes and their resultant dynamics. I will first review the concept of energy-based neural networks and how they are linked to the physics of spin glasses in atomic systems. I will then highlight new examples based on the recent discovery of the so-called spin Q glass and the atomic Boltzmann machine. I will illustrate the creation of atomic-scale neurons and synapses, in addition to new learning concepts based on the separation of time scales and self-adaptive behavior. I will also discuss recent cutting-edge developments that enable magnetic characterization in new extreme limits, for example ESR-STM at the lowest temperatures available today, and the application of this platform. This work was performed with funding from NWO, with project number 680-47-534, and from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (SPINAPSE: grant agreement No 8183).

O 31.2 Tue 11:00 R2

Quantum Stochastic Resonance in Fe atoms and Nanostructures — •Gregory McMurtrie[1], Max Hänze[1,2], Susanne Baumann[1], Luigi Malavolti[2], Susan N. Coppersmith[3], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]School of Physics, University of New South Wales, Sydney, Australia

Stochastic resonance [1], where noise synchronizes a system's response to an external modulation, is a widespread phenomenon found in systems ranging from the dynamic behavior of neurons [2] to the periodicity of glaciation [3]. Here we apply stochastic resonance to open quantum systems, namely atoms and nanostructures strongly coupled to a dissipative bath, which unlocks a path to resonant interaction that does not require coherence. In particular, applying modulation via a scanning tunneling microscope's tip gives control of the spin state evolution in this resonant regime of spin dynamics in both real-time and real-space on the atomic scale. This phenomenon has never been observed previously in atomic systems, and gives unprecedented insight into the interaction of quantum spins and their noise sources, even allowing transduction of picosecond-speed dynamics. [1] R. Benzi, J. Phys. A: Math. Gen 14, L453 (1981) [2] A. J. Bulsara et al. Theor. Biol. 152, 531-555 (1991) [3] P. N. Pearson et al. Paleontological Society Papers 18, 1-38 (2012)

Invited Talk O 31.3 Tue 11:15 R2

Artificial spin chains on superconductor surfaces — •Jens Wiebe — Department of Physics, Hamburg University, Germany

A magnetic chain on an s-wave superconductor hosting a spin spiral or strong spin-orbit coupling can potentially realize a one-dimensional topological superconductor with Majorana bound states on its edges [1-5]. Here, we investigate artificial spin chains, which have been built atom-by-atom, with respect to the emergence of such topologically nontrivial electron phases. By this approach we not only vary the substrate and adatom species [6,7,8], but also tailor the interactions between the Yu-Shiba-Rusinov states induced by the adatoms [8] which eventually results in the formation of multi-orbital in-gap bands for the chain. We correlate the electronic properties of these bands with the spin structures of the chains as revealed by spin-resolved scanning tunneling spectroscopy [9].

We acknowledge funding by the ERC via the Advanced Grant ADMIRE (No. 786020), and by the DFG via the Cluster of Excellence 'Advanced Imaging of Matter' (EXC 2056-project ID 390715994) and the SFB-925-project 170620586.

[1] Klinovaja et al., PRL 111, 186805 (2013). [2] J. Li et al. PRB 90, 235433 (2014). [3] S. Nadj-Perge et al., Science 346, 6209 (2014). [4] M. Ruby et al., Nano Letters 17, 4473, (2017). [5] H. Kim et al., Science Advances 4, eaar5251 (2018). [6] L. Schneider et al., npj Quantum Materials 4, 42 (2019). [7] L. Schneider et al., Nature Commun. 11, 4707 (2020). [8] Ph. Beck et al., arXiv:2010.04031 [cond-mat.supr-con] (2020). [9] L. Schneider et al., Science Advances 7, eabd7302 (2021).

O 31.4 Tue 11:45 R2

Coupling of Yu-Shiba-Rusinov states on $2H$-NbSe$_2$ — •Eva Liebhaber[1], Lisa Rütten[1], Gaël Reecht[1], Kai Rossnagel[2,3], Felix von Oppen[1,4], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany. — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany. — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. — [4]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany.

A magnetic impurity adsorbed on a superconducting substrate leads to the formation of Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap. YSR wave functions of two adjacent magnetic adatoms can hybridize and form symmetric and antisymmetric linear combinations. Increasing the number of adatoms leads to the formation of Shiba bands.

We investigate magnetic Fe atoms on the superconductor $2H$-NbSe$_2$ which is a layered van der Waals material. Its strong 2D electronic character leads to a large spatial extent of the YSR wave functions facilitating the coupling between them [1]. We assemble adatom chains using a superconducting tip and track the evolution of the YSR states. As the YSR states have been shown to be sensitive to the CDW [2] that coexists with superconductivity in NbSe$_2$ at low temperatures we further investigate the role of the CDW for the hybridization along extended chains.

[1] S. Kezilebieke *et al.*, *Nano Lett.* **18**, 2311 (2018)
[2] E. Liebhaber *et al.*, *Nano Lett.* **20**, 339 (2020)

O 31.5 Tue 12:00 R2

Hyperfine fields of magnetic adatoms on ultrathin insulating films — •SUFYAN SHEHADA[1,2], Manuel dos Santos Dias[1], Filipe Souza Mendes Guimarães[1], Muayad Abusaa[3], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Department of Physics, Arab American University, Jenin, Palestine — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Individual nuclear spin states can have very long lifetimes and could be useful as qubits. Promising steps in this direction were realized on MgO/Ag(001) via STM detection of the hyperfine interaction (HFI) of Fe and Ti adatoms [1] and the electrical control of the nuclear polarization of Cu adatoms [2]. Here, we report on systematic first-principles calculations of the HFI for $3d$ adatoms (Sc–Cu) atop ultra-thin insulators (MgO, NaF, NaCl, h–BN and Cu$_2$N) [3]. We analyze the trends and the dependence of the computed HFI on the filling of the magnetic s and d-orbitals of the adatoms and on bonding type and strength with the substrate. Finally, we identify promising candidates for future experimental investigations with scanning probe techniques.

–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] Willke *et al.*, Science **362**, 336 (2018); [2] Yang *et al.*, Nat. Nanotechnol. **13**, 1120 (2018); [3] Shehada et al. ArXiv:2012.11639.

"Meet our speakers". Open discussion with all speakers of the session

O 32: Mini-Symposium: Frontiers of electronic-structure theory: Focus on electron-phonon interactions II

Time: Tuesday 10:30–12:30 Location: R3

Open panel discussion led by Prof. Claudia Draxl (HU Berlin), Prof. Feliciano Giustino (U Texas at Austin) and Prof. Matthias Scheffler (Fritz-Haber-Institut der MPG)

O 33: Poster Session III: Semiconductor substrates I

Time: Tuesday 10:30–12:30 Location: P

O 33.1 Tue 10:30 P

Engineering the surface of homoepitaxially MBE grown InAs(111)A — •Steffen Zelzer[1,2], Rajib Batabyal[1,2], Mohana Rajpalke[2], and Peter Krogstrup[1,2] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — [2]Microsoft Quantum Materials Lab Copenhagen, 2800 Lyngby, Denmark

The surface morphology in the μm and (sub) nm range of homoepitaxially molecular beam epitaxy (MBE) grown planar InAs(111)A buffer layer has been studied by scanning tunneling microscopy (STM) and reflection high energy electron diffraction (RHEED). We show how an optimized cool-down procedure can lead to atomically clean surfaces and present an approach to map the growth parameter space for the two relevant stages of nucleation (step flow and 2D nucleation) on this surface which determines the macroscopical surface morphology. Transition state kinetics are used in combination with critical growth conditions extracted from RHEED intensity measurements to explain the transition from step flow to 2D nucleation.

O 33.2 Tue 10:30 P

Virtual III-V-on-Si substrates grown by MOVPE - reduction of stacking faults — •Manali Nandy[1], Agnieszka Paszuk[1], Markus Feifel[2], Christian Koppka[1], Peter Kleinschmidt[1], Frank Dimroth[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Ilmenau, Germany — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany

The performance of III-V-on-Si multijunction solar cells is still limited by their density of defects at the GaP/Si(100) heterointerface and in the GaP buffer layers. In order to improve the crystal quality of the GaP buffer layer, we modified the GaP pulse nucleation by substituting the first five TEGa pulses with TMAl. Influence of Al on the defect density in the GaP buffer layers are investigated by electron channeling contrast imaging. 60 nm thick GaP(100) buffer layers grown on GaP nucleation exhibit short misfit dislocations (MDs) and therefore, a high density of threading dislocations (TDs). In contrast, GaP(100) buffer layers grown on AlGaP nucleation exhibit less, but longer MDs, which result in a lower density of TDs. In addition, the density of stacking faults and stacking faults pyramids in the GaP layer grown on the AlGaP nucleation is significantly reduced. The surface morphology at the initial growth stage of GaP buffer layers grown on AlGaP nucleation, is smoother compared to the buffer layer grown on the GaP nucleation. The application of TMAl in the GaP nucleation process provides a two-dimensional, smooth layer, on which subsequent, high-quality GaP films could be grown, and therefore, shows a promising pathway for improving the performance of III-V-on-Si devices.

O 33.3 Tue 10:30 P

Atomic and electronic structure of the GaP/Si(001) heterointerface studied by HAXPES — •Agnieszka Paszuk[1], Oleksandr Romanyuk[2], Igor Bartoš[2], Regan G. Wilks[3], Manali Nandy[1], Jakob Bombsch[3], Claudia Hartmann[3], Raül Garcia-Diez[3], Shigenori Ueda[4], Ivan Gordeev[2], Jana Houdkova[2], Peter Kleinschmidt[1], Marcus Bär[3], Peter Jiříček[2], and Thomas Hannappel[1] — [1]Institute of Physics, University of Technology, Ilmenau, Germany — [2]Institute of Physics, Prague, Czech Republic — [3]Department Interface Design, Helmholtz-Zentrum Berlin, Germany — [4]SPring-8, National Institute for Materials Science, Japan

For highly efficient III-V-on-Si optoelectronic devices it is crucial to prepare defect-free heterointerfaces with defined electronic properties. Commonly a thin, pseudomorphic GaP epilayer is deposited on Si prior to further III-V buffer growth, due to its close lattice matching to Si. Here, the atomic and electronic structure of buried GaP/Si(001) heterointerfaces prepared by MOCVD were investigated by hard X-ray photoelectron spectroscopy combined with theoretical modelling. 4 - 50 nm thick GaP films with a different density of antiphase domain boundaries were grown on Si(001) H-terminated surfaces, as controlled by optical *in situ* spectroscopy. We found that the core-level positions and width changes with GaP film thickness and Si substrate type. These observations were related to charge displacements and band bending effects at the interface. In consequence, an inter-diffused layer interface structure model based on the formation of Si-P bonds at the heterointerface and P-doping of the Si substrate was suggested.

O 33.4 Tue 10:30 P

Structural LEED analysis of the reconstructed Si(001) surface — •Jascha Bahlmann[1], Kris Holtgrewe[2], Simone Sanna[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Germany — [2]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Previous attempts to solve the atomic geometry of the Si(001)-(2x1) reconstructed surface by means of LEED yielded so far only ambiguous results. We present a geometrical model with asymmetric and buckled dimers with an excellent agreement between the experimental and calculated spectra by dynamic LEED theory. Furthermore, we reveal which parts of the analysis were particularly crucial for obtaining this conclusive IV-LEED result.

Additionally, a comparison between our model, the models of DFT calculations and X-ray diffraction is presented. Moreover, we go a step further and examine also the transition to the higher order reconstruction c(4x2).

O 33.5 Tue 10:30 P

Temperature dependent adsorption of Trimethylamine (TMA) on water-functionalized Si(001)-(2x1) surfaces — •Niklas Fornefeld[1], Lucia Pérez Ramírez[2], François Rochet[2], Stefan Kubsky[3], and Ulrich Köhler[1] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, Bochum, Germany — [2]Laboratoire de Chimie Physique matière et Rayonnement, Univ. P. et M. Curie, Paris, France — [3]Synchrotron Soleil, St. Aubin (Paris), France

Concerning functionalization of Si(001)-(2x1) with organic molecules, an intermediate water layer enables better control of the adsorption processes due to the reduction of possible adsorption sites. To investigate the binding properties on surface silanols (SiOH) and to examine the chemical reactivity we studied the vibrational modes of TMA in the temperature range between 100 K and 300 K during adsorption on a H_2O/D_2O reacted Si(001)-(2x1) surface using HREELS in comparison to XPS results. Both complementary techniques indicate that TMA adsorbs non-dissociatively to surface silanols forming acceptor H-bonds at $T < 120$ K and at $T < 135$ K under constant TMA flux. Self-limited TMA adsorption was found to occur already for $T < 175$ K affecting 80 % of the SiOH without the appearance of the characteristic ν(SiO-H) redshift for H-bonding seen at lower temperature. Both adsorption reactions are reversible processes involving TMA N lone pair electrons thus ruling out TMA protonation by either SiH or SiOH. Analyzation of the $\nu(CH_3)$ Bohlmann band allows us to estimate the bond strength of adsorbed TMA to be in between dative and intermolecular bonding found in TMA mono-/multilayers on pristine Si(100).

O 33.6 Tue 10:30 P

Enhancing structural order by random Au adsorption on the Si(553)-Au system — •Christa Fink[1], Kris Holtgrewe[1], Simone Sanna[1], Zamin Mamiyev[2], and Herbert Pfnür[2] — [1]Justus-Liebig-Universität, Gießen, Germany — [2]Leibniz Universität, Hannover, Germany

Nanowires on semiconductor surfaces have drawn the attention from a broad research community as they are promising systems for realizing and studying quasi 1D physics. We investigate the adsorption of additional Au adatoms on the Au double chain system supported by the silicon (553) surface by means of density functional theory and slab models. One adatom per (5×2) unit cell strongly enhances the Au chain dimerization, although the favored adsorption site is at the Si step edge far away from the chains. This non-local structure manipulation is related to the two-dimensional coupling between the wire and the substrate. The electronic band structure proves that the hybridization between the Au adatom and the Si step edge transfers charge to the surface. Because of the strong electronic correlation, a band gap opens within the Au related states which is accompanied by an increased dimerization of the Au chains. The Au adsorption has a similar impact on the surface morphology as a pure electron injection. As the enhanced dimerization puts a penalty on the formation energy of defects, the not necessarily ordered adsorption of Au adatoms reduces the number of defects and leads to more order in the wires. This counter-intuitive order-by-disorder mechanism is confirmed by experimental results and transferable to other quasi 1D nanowire systems.

O 34: Poster Session III: Organic molecules on inorganic substrates: Adsorption and growth III

Time: Tuesday 10:30–12:30 Location: P

O 34.1 Tue 10:30 P

Elucidating the bonding of 2-mercaptobenzimidazole on Cu(111) by STM and DFT — •Marion A. van Midden, Matic Lozinšek, Tone Kokalj, and Erik Zupanič — Jožef Stefan Institute, Ljubljana, Slovenia

While organic corrosion inhibitors such as 2-mercaptobenzimidazole are widely used to protect the surface of copper, their bonding mechanism on the atomic scale remains elusive. DFT calculations have shown that different bonding configurations have comparable energies when considering the binding of a single molecule to the surface. In the case of larger coverages, which are common in real-life applications, various inter-molecular interactions have to be considered as well, further complicating calculations. To determine which interactions are most significant for the bonding and self-assembly of 2-mercaptobenzimidazole on the surface of Cu(111) we prepared samples in ultra high vacuum and imaged them using STM. Varying the evaporation rate and time as well as the substrate temperature allowed us to control the coverage and limit the energy the molecules have available to self assemble. Surprisingly the molecules formed ordered self-assembled structures even when depositing on samples cooled to approximately 50 K. These structures reassembled at temperatures below 100 K. Similarly, most of the observed structures rearranged when slightly heated. This opposes the idea that strong binding to specific sites on the surface is crucial for corrosion prevention. The large variety of obtained self-assembled structures at different deposition parameters suggests, that the energy scales of competing interactions must be similar.

O 34.2 Tue 10:30 P

Comparison of the adsorptions of ethanol and azobenzene molecules on single-layer hexagonal boron nitride on Rh(111) — •Krisztián Palotás[1,2], Arnold Farkas[2,3], Ádám Szitás[2], Dániel Jurdi[2], Richárd Gubó[2,3], Tibor Pásztor[2], Tibor Ajtai[2,3], László Óvári[2,3], János Kiss[2], András Berkó[2], and Zoltán Kónya[2] — [1]Wigner Research Center for Physics, Budapest, Hungary — [2]University of Szeged, Szeged, Hungary — [3]ELI-ALPS, Szeged, Hungary

The nanomesh structure of single-layer hexagonal boron nitride (hBN) on various metal surfaces can be used as a nanotemplate for molecular adsorption. Possible applications can be molecular electronics, heterogeneous catalysis, sensing, or light harvesting. We investigate the adsorption properties of ethanol [1] and azobenzene [2] molecules on the hBN/Rh(111) surface by density functional theory calculations and experimental methods. We find high selectivity of the nanomesh structure for the azobenzene adsorption [2], but no selectivity for the ethanol adsorption [1]. The latter finding is in line with experimental observations of a very weak interaction between ethanol and the hBN/Rh(111) substrate [1]. Finally, we analyze the trans- and cis-azobenzene adsorption and azobenzene-azobenzene interactions in great details by using theoretical means [2]. These latter results contribute to the understanding of the behavior of photoswitching molecules on nanotemplated surfaces.

[1] A. P. Farkas et al. Appl. Catal. A: Gen. 592, 117440 (2020).

[2] Á. Szitás et al. J. Phys. Chem. C 124, 14182 (2020).

O 34.3 Tue 10:30 P

Investigating kinetics of organic molecules on inorganic substrates — •Anna Werkovits and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Growth processes of organic thin films are strongly influenced by the interplay of thermodynamics and kinetics. Following Ostwald's rule of stages, metastable structures often form first during the deposition process. Transitions to more stable structures may be prevented by fast aggregation and growth of the thermodynamically less stable seed, leading to a kinetically trapped polymorph. The selective growth of specific polymorphs, therefore, requires balancing growth and phase transitions via appropriately chosen deposition conditions.

The poster introduces a roadmap for achieving selective growth of organic-inorganic systems and gives an overview of the corresponding challenges and limitations. While thermodynamics can be sufficiently treated by now, kinetics are still an issue as reliable transition state searches devour computational resources. This is primarily caused by the lack of suitable force fields and the high dimensionality of the potential energy surface. We provide first insights about the kinetics for the model system tetracyanoethylene (TCNE) on Cu(111). Energies are obtained using density functional theory (PBE+TS$^{\text{surf}}$) and transition states mainly with the Nudged Elastic Band method.

O 34.4 Tue 10:30 P

Computational Structure Prediction for Interfaces: What is Currently Possible? — •Lukas Hörmann, Andreas Jeindl, Fabio Calcinelli, Johannes Cartus, and Oliver Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Studying the electronic structure of organic monolayers on inorganic substrates requires knowledge about their atomistic structure. Such monolayers often display rich polymorphism arising from diverse molecular arrangements in different unit cells. The large number of arrangements poses a big challenge for determining the different polymorphs from first principles. To meet this challenge, we developed SAMPLE[1], which employs coarse-grained modeling and machine learning to efficiently map the minima of the potential energy surface of commensurate organic adlayers. With only a few hundred DFT calculations as input, we use Bayesian linear regression to determine the parameters of a physically motivated energy model. These parameters yield meaningful physical insight and allow predicting adsorption energies for millions of possible polymorphs with high accuracy. Beyond that, we continuously push the boundaries of surface structure search, with three noteworthy developments: i) predicting the second adlayer pursuing the goal of studying thin film properties; ii) generalizing SAMPLE to investigate incommensurate adlayers; iii) employing feature recognition to reveal hidden relationships between the interface properties. [1] Hörmann et al., Comput. Phys. Commun. 244, 143*155, 2019

O 34.5 Tue 10:30 P

On-surface synthesis of BN-doped carbon nanostructures — •Tobias Weiss[1], Aleksandr Baklanov[1], Knud Seufert[1], Johannes Küchle[1], Marc Gonzalez Cuxart[1], Francesco Allegretti[1], Jacopo Dosso[2], Davide Bonifazi[2,4], Nicolas Bachellier[3], Matthias Muntwiler[3], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]School of Chemistry, Cardiff University, Cardiff, UK — [3]Paul Scherrer Institute, Villigen, Switzerland — [4]Institute of Organic Chemistry, Faculty of Chemistry, University of Vienna, Austria

Hybrid hexagonal boron nitride - carbon (BNC) layers provide promising properties for potential applications in electronics and gas adsorption [1]. Recently, BNC-based tectons were introduced to assemble covalent networks and supramolecular arrays on metal surfaces [1-3].

Here, we report the formation of BNC nanostructures on Ag(111) and Au(111) via bottom-up synthesis from borazine derivatives in UHV. We employed both a dehydrogenation approach using a BN-doped coronene derivative and an Ullmann-type coupling approach using a chlorine- and bromine-functionalized hexaphenylborazine. The resulting 2D structures, the sequential dehalogenation steps, and the Ullmann coupling are investigated with (fast) XPS and STM. Additionally, we probed the CO, CO$_2$, and borazine adsorption on the BNC structures, revealing the inertness of the borazine core.

[1] M. M. Lorenzo-García et al., Chimia, 2017 **71**, 9, 550-557.

[2] C. Sánchez-Sánchez et al., ACS Nano, 2015 **9**, 9, 922.

[3] M. Schwarz et al., Chem. Eur. J., 2018 **24**, 9565.

O 34.6 Tue 10:30 P

Self–assembly and metalation of a novel macrocyclic biquinazoline compound on Ag(111) — •Felix Haag[1], Peter S. Deimel[1], Peter Knecht[1], Raphael Lauenstein[2], Manuel Kaspar[2], Knud Seufert[1], Yang Bao[1], Marc Gonzalez Cuxart[1], Anthoula C. Papageorgiou[1], Corinna Hess[2], Willi Auwärter[1], Johannes V. Barth[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University Munich, Germany — [2]Chemistry Deparment, Technical University Munich, Germany

We report the first experimental study of the adsorption of the macrocyclic biquinazoline (H-Mabiq) compound on a model solid surface. Its two potential coordination sites for metal ions, combined with multi–electron transfer capacity ensure higher sophistication beyond the well–studied metallo–porphyrins and –phthalocyanines. As the coordination sites can be occupied by different metal atoms, adsorbed Mabiq complexes are promising candidates for photocatalytic applications and epoxidation reactions. Here, we present the self–assembly, on–surface binding and chemical state of H-Mabiq on Ag(111) by employing a toolbox of surface science techniques including XPS, NEXAFS, LEED, STM and TPD. We establish protocols for the preparation of well–ordered single layers and the controlled metalation with Co atoms. The ordering and packing of the pristine H-Mabiq single layer depend critically on the substrate temperature, evidenced through distinct changes in the LEED pattern and STM topography upon annealing. Moreover, the effect of Co deposition on the self–assembly and chemical state of the molecules is discussed.

O 34.7 Tue 10:30 P

Asymmetric cyclotrimerization of terminal alkenes on Au(111) — •Mirunalini Devarajulu[1], Kevin Dhamo[2], Konstantin Amsharov[3], Bernd Meyer[2], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Interdisciplinary Center for Molecular Materials (ICMM) and Computer-Chemistry-Center (CCC), Friedrich-Alexander-Universität Erlangen-Nürnberg — [3]Institute for Chemistry, Martin Luther University of Halle-Wittenberg

Most branched, crosslinked, and networked polyphenylene polymers that have been assembled on metal surfaces *via* on-surface synthesis are non-conjugated because they contain metaphenylene units. In contrast, the on-surface synthesis of conjugated orthophenylene units remained so far elusive as rare by-products.

Here, we demonstrate the on-surface synthesis of conjugated 1,2,4-triphenylbenzenes *via* selective asymmetric cyclotrimerization of terminal alkenes on Au(111). We provide a detailed analysis of the reaction intermediates and final products *via* dehydrogenative homocoupling of terminal alkenes of linear 4-vinyl-1,1'-terphenyl molecules on Au(111) using low-temperature scanning tunneling microscopy in combination with density functional theory.

O 34.8 Tue 10:30 P

Selective on-surface synthesis of oxygen heterocycles on metals — •Andreas Dörr[1], Nemanja Kocić[1], Konstantin Amsharov[2], and Sabine Maier[1] — [1]Department for Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute for Chemistry, Martin-Luther-Universität Halle-Wittenberg

Heterocycles with nitrogen, oxygen, or sulfur atoms are the basic units to incorporate chemical functionalization into carbon scaffolds. For oxygen-doped nanographenes, furan and pyran - having five- and six-membered rings, respectively - are the most common ones. However, their on-surface synthesis *via* cyclomerization reactions remains elusive so far. Here we present a low-temperature scanning tunneling microscopy study to understand the on-surface synthesis of furan and pyran derivatives from ketone-functionalized precursors on metal surfaces. We use thermally induced CH-activation reactions to fuse two ketone-derivatives in either *cis*- and *trans*-configuration selectively. Finally, cyclomerization reactions towards furan and pyran moieties are observed after further annealing. These results are highly unexpected because ketone derivatives are mostly known to convert to cyclic trimers or tetramers in solution-based chemistry. On the surface, however, the strong interaction of the ketones with the metal surface and adatoms opens up new reaction pathways.

O 34.9 Tue 10:30 P

[n]Phenacene: Growth, Electronic Properties and On-Surface-Synthesis — •Akash Gupta[1], Paul Yu-Hsiang Yen[1], Hsuan Ting Lin[1], Wun Chang Pan[1], Yong-He Pan[1], Germar Hoffman[1], and Hideki Okamoto[2] — [1]Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — [2]Department of Chemistry, Okayama University, Japan

Chemical functionalization of solid surfaces and the study of respectively formed organic-metal interfaces from self-assembled molecular films to stacked layers attain a lot of attention. By means of an atomically precise design through a chemical approach, new materials and interfaces for organic electronics can be engineered. This offers a path to low cost, mechanically flexible, low weight components for organic electronics, such as OLEDs and OFETs through a chemistry driven bottom-up approach.

Pentacene, with a linear arrangement of five benzene rings, is intensively studied for prototype transistors but degrades under the presence of Oxygen. The chemically more robust [n]Phenacene, with n in a repeating W-shaped pattern fused benzene rings, was recently introduced as a promising alternative. Thereby, the electron mobility increases with n, the number of benzene rings.

Here, we study the growth and electronic properties of [10]Phenacenes on Au(111) and Ag(111) by Scanning Tunneling Microscopy/Spectroscopy at 77K and compare it to [5], [7], [9]Phenacene. The possibility of On-Surface-Synthesis of functionalized Phenacenes is discussed.

O 35: Poster Session III: Surface dynamics I: Phase transitions and elementary processes

Time: Tuesday 10:30–12:30 Location: P

O 35.1 Tue 10:30 P

Interphase Formation in Solid Oxide Electrolysis Cells - A Close-up on the YSZ/LSM Grain Boundary — •Hanna Tuerk, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institute of the Max-Planck-Society

Solid oxide electrolysis cells (SOECs) are among the most efficient technologies for water splitting from fluctuating renewable electricity sources. While SOECs are in principle well adapted to intermittent operation, cell performance and lifetime is severely limited by degradation of the anode. This degradation goes hand in hand with the oxygen evolution reaction taking place at the triple-phase boundary (TPB) between the anode, the solid electrolyte and the gas phase. Up to now, the atomistic structure of this active catalyst region is essentially unknown though, which prevents a detailed analysis of the actual degradation mechanisms.

Here, we take a first step to elucidate the TPB structure by performing molecular simulations of the underlying interface between the oxygen-ion conducting electrolyte yttria-stabilized zirconia (YSZ) and the typical electrode material strontium-doped lanthanum manganite (LSM). Parallel-tempering Monte Carlo with a cumulatively growing swapping region centered at the interface yields an efficient simulation approach capable of addressing the structural complexity of this grain boundary region. Our experimentally validated results clearly evidence the formation of an extended interphase region with partial loss of crystalline order and distinct segregation profiles.

O 35.2 Tue 10:30 P

Time-Resolved 2D IR Pump-Probe Spectroscopy — Michael Lackner, •Marvin Hille, Tim Lämmerzahl, Nelli Kremer, and Eckart Hasselbrink — University of Duisburg-Essen, Essen, Germany

Internal vibrational energy distribution (IVR) in molecules is fundamental for understanding their chemical reactivity and research in this field has gained a lot of popularity in the past. It is, however, still fair to say that predictive power over the energy flow in vibrationally excited molecules has yet to be obtained. We will present newest findings regarding the energy flow dynamic of a fatty acid Langmuir-Blodgett film on a picosecond scale. Vibrational sum frequency generation (vSFG) spectroscopy allows precise monitoring of resonant vibrations of an adsorbate monolayer. In our setup we use a resonant ps narrowband IR laser pulse for pumping and a fs broadband IR-visible pulse pair for vSFG probing of the monolayer. Using this pump-probe setup we observed a very fast (< 2ps) energy transfer to the other modes when pumping the anti-symmetric methyl or methylene stretch, followed by a longer decay (~85 ps) into presumably bending and internal rotational modes.

O 35.3 Tue 10:30 P

Atomic Diffusion in O(2x2) on Ru(0001) - Spiral High Speed STM — •Leonard Gura[1], Joachim Paier[2], Zechao Yang[1], Florian Kalass[1], Matthias Brinker[1], Heinz Junkes[1], Markus Heyde[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany

The diffusion of atomic oxygen on Ru(0001) has been studied over the last decades. Conventional Scanning Tunneling Microscopy (STM) gave hopping rates for oxygen vacancies in an O(2x2) adlayer in the order of 1/100 s [1].

Here we present new results on the dynamics in the O(2x2) layer on Ru(0001) at room temperature. We used a novel STM spiral scan pattern to avoid internal resonance frequencies of the microscope body. With this approach we increased the frame rate to 40 Hz.

Thanks to the high frame rate we were able to observe frequent jumps in the O(2x2) adlayer with hopping rates in the order of 1/1 s. In addition, we resolved intermediate states during single jump events. Based on Density Functional Theory (DFT) calculations, we provide a plausible O migration pathway.

Ideas for future studies include oxygen coverage and temperature dependent measurements. With refined spiral geometries and tip velocities we hope to further increase the scan speed to then monitor more dynamic processes at the atomic scale.

[1] Wintterlin, J. et al. (1997). Surface science, 394(1-3), 159-169 and references therein.

O 35.4 Tue 10:30 P

Free energy QM/MM simulations of on-surface reaction pathways — •Aurelio Gallardo[1,2], Jesus Mendieta[1], and Pavel Jelínek[1,2] — [1]FZU of the CAS, Prague, Czech Republic — [2]RCPTM, Palacký University, Olomouc, Czech Republic

On-surface chemistry represents a fast-growing field allowing to synthetize molecular structures not available by traditional wet chemistry. In combination with high-resolution scanning probe technique providing the unprecedented spatial resolution, individual products of reactions can be precisely identified. Nevertheless, a deep understanding of the reaction mechanism under the conditions imposed by the substrate remains unknown. Widely adopted energy reaction path techniques will only describe the potential energy landscape at zero Kelvin, while the free energy landscape at given temperature enables a more appropriate description of the reaction. Such simulations including temperature effect include the effect of entropy, vibrations modes, concerted motion, etc. Consequently, such simulations avoid local minima and allows to explore different states, revealing lower energy pathways. We will present QM/MM simulations of strain-induced isomerization in one-dimensional metal-organic chains on Cu(111) surface [1]. The simulation demonstrates the importance of the temperature effect on proper description of the reaction mechanism.

[1] M. Telychko, J. Su, A. Gallardo, Y. Gu, J. I. Mendieta-Moreno, D. Qi, A. Tadich, S. Song, P. Lyu, Z. Qiu, H. Fang, M. Joo Koh, J. Wu, P. Jelínek J. Lu, Strain-Induced Isomerization in One-Dimensional Metal-Organic Chains, Angew. Chem 58, 8591-18597 (2019).

O 35.5 Tue 10:30 P

Nonadiabatic quantum dynamics of diffusion and scattering at metal surfaces — •James J Gardner, Svenja M Janke, and Reinhard J Maurer — University of Warwick, Coventry, United Kingdom

Dynamics at molecule-metal interfaces involve a close coupling between the electronic and nuclear degrees of freedom, violating the Born-Oppenheimer approximation. The Anderson-Holstein Hamiltonian provides a standard model for describing the nonadiabatic dynamics encountered at the metal surface. We present two forms of this Hamiltonian that encompass surface diffusion and scattering, both having an explicit structure for the electronic bath depending on only two parameters. With these models, we identify and analyse different parameter regimes in which quantum tunnelling and nonadiabatic effects are important. We further calculate quantum rates and scattering probabilities at different levels of theory. Our results provide a benchmark for the performance of existing and future simulation methods to describe accurate quantum reaction rates at metal surfaces.

O 36: Poster Session III: Electronic structure of surfaces: Spectroscopy, surface states I

Time: Tuesday 10:30–12:30 Location: P

O 36.1 Tue 10:30 P

Phonon mediated tunneling into a 2D electron gas on the Be(0001) surface — •Hermann Osterhage, Karoline Oetker, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Beryllium is a very unique element among the metals. Whereas the bulk behaves almost like a semiconductor, the (0001) surface is much more metallic, originating from electronic surface states. In our experiments, the clean Be(0001) surface was investigated using scanning tunneling spectroscopy at low temperatures [1]. A pronounced surface state is identified, additionally manifested by the observation of bias-dependent standing wave patterns. Fourier analysis reveals a parabolic dispersion, being characteristic for Friedel oscillations. In contrast to previous studies [2], no indications for the formation of a charge density wave were observed.

Our spectroscopy data reveal symmetric steps in the tunneling conductance around the Fermi level, which we assign to the opening of inelastic tunneling channels via coupling to phonon modes. The Be(0001) surface is found to represent an almost ideal model system to shed light on the details of fundamental electron-electron and electron-phonon interactions in low dimensions.

[1] H. Osterhage *et al.* (submitted).

[2] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).

O 36.2 Tue 10:30 P

The polar KTaO$_3$ (001) surface: Electronic structure and CO adsorption — •Martin Setvin[1,2], Michele Reticcioli[3], Zhichang Wang[2,4], Zdenek Jakub[2], Michael Schmid[2], Cesare Franchini[3], and Ulrike Diebold[2] — [1]Cherles University, Prague, Czech Republic — [2]TU Wien, Vienna, Austria — [3]University of Vienna, Vienna, Austria — [4]Xiamen University, Xiamen, China

Polar surfaces offer intriguing physical and chemical properties applicable in electronics or catalysis. Cleaving the KTaO$_3$ perovskite along its polar (001) plane provides a well-defined, bulk-terminated surface with KO and TaO$_2$ terminations [1]. As-cleaved surfaces exhibit a high concentration of in-gap states; these electrons predominantly reside at the TaO$_2$-terminated parts of the surface. These electrons can affect surface chemistry, as is demonstrated for CO molecules. CO has two adsorption configurations on the TaO$_2$ termination, and the CO differs in how it couples to the excess electrons. DFT calculations indicate that CO preferentially couples to electron bipolarons.

The work was supported by FWF project P32148-N36, by GACR 20-21727X and GAUK Primus/20/SCI/009.

O 36.3 Tue 10:30 P

Lifetime-measurements of surface electrons enclosured in a circular CO-Quantum Corral on Cu(111) — •Marco Weiss, Jakob Fuchs, Fabian Stilp, and Franz Josef Giessibl — University of Regensburg, 93040 Regensburg, Germany

Adsorbates scatter surface state electrons exhibited by a Cu(111) surface [1]. Artificial manipulation of these microscopic scatterers opens the path to a variety of manmade surface-potential landscapes. In 1993 Crommie et al. [2] assembled 48 Fe adatoms in a ring form shape with a diameter of about 15 nm. This so called Quantum Corral confines the surface electrons within a circular symmetric potential well. These past investigations revealed discrete, Bessel-type eigenstates of the enclosured electrons by using scanning tunneling microscopy and tunneling spectroscopy. But these studies on the Fe-Quantum-Corral showed a disadvantageous movement of the Corral-walls during spectroscopic measurements. [2]

Our solution approach for this problem is to use CO-molecules for upgrading the Quantum Corral with more stable walls. This permits a more reliable access for the spectroscopic analysis of this artificially built atomic feature. This poster presents the results of our spectroscopic investigations on the CO-Corral. The main focus is on determining the lifetime of such enclosuered surface state electrons.

[1] Crommie et al. Nature 363, 524 (1993)

[2] Crommie et al. Science 262, 218 (1993)

O 36.4 Tue 10:30 P

Importance of surface oxygen vacancies for ultrafast hot carrier relaxation and transport in Cu$_2$O: Insight from hybrid DFT — •Chiara Ricca[1], Lisa Grad[2], Matthias Hengsberger[2], Jürg Osterwalder[2], and Ulrich Aschauer[1] — [1]Department of Chemistry and Biochemistry and National Centre for Computational Design and Discovery of Novel Materials MARVEL, University of Bern, CH-3012 Bern, Switzerland — [2]Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

Efficient Cu$_2$O-based electrodes for photochemical water splitting can be engineered through a deeper understanding of the surface defects and of the mechanisms responsible for the capture of the excited carriers that limit the generated photovoltage in Cu2O heterostructures. Using hybrid DFT calculations, we confirmed that the ($\sqrt{3} \times \sqrt{3}$)-R30 reconstruction at the Cu$_2$O-(111) surface is associated with a 1/3 monolayer of charged surface oxygen vacancies forming ordered structures due to mutual repulsion. Comparison with experimental data obtained by two-photon photoemission spectroscopy indicates that the defect states associated with these vacancies can strongly suppress electron transport, while bulk defect states cannot act as electron traps. In particular, the excited electronic state of the singly charged oxygen vacancy plays a crucial role in the non-radiative electron capture process, with capture coefficients of about 10-9 cm^3/s and lifetimes of 0.04 ps, allowing to explain the experimentally observed ultrafast carrier relaxation.

O 36.5 Tue 10:30 P

Fermi Surface Tomography of Palladium via Momentum Microscopy — •Xin Liang Tan[1], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Jakub Schusser[3], Iulia Cojocariu[1], Vitaliy Feyer[1], Jan Minar[3], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic

The Fermi surfaces, which describe all thermodynamical and transport quantities of solids, of transition metals are often failed to be modeled by one-electron mean-field theory due to strong correlations among the valence electrons. Moreover, relativistic spin-orbit coupling pronounced in heavier elements lifts the degeneracy of the energy bands and modifies the Fermi surface. Palladium, a 4d metal attributed to both significant spin-orbit coupling and electron correlations, is ideal for a systematic and fundamental study on the two fundamental physical phenomena and their interplay in electronic structure. We will explore the experimentally determined electronic structure of palladium in four-dimensional energy-momentum space ($E_{Binding}$,k_x,k_y,k_z) obtained via momentum microscopy. The complete 3D-Fermi surface of palladium and corresponding isoenergy surfaces at higher binding energies were tomographically mapped with an energy- and polarization-variable light source. Spin-orbit coupling and electron correlations in palladium will be presented in the context of energy-momentum relations across the Fermi surface and isoenergy surfaces.

O 36.6 Tue 10:30 P

Emergence of unusually high Na2IrO3 surface conductivity prepared in UHV — •Máté Stark[1], Thomas Dziuba[1], Ina Pietsch[2], Philip Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, Germany

Na2IrO3 is a prototypical material in the honeycomb iridate family, where both a spin liquid ground state and topologically insulating behaviour are theoretically predicted [1]. In this work, we perform transport measurements of freshly cleaved Na2IrO3 crystals in ultra-high vacuum. Making use of the insulating nature of bulk Na2IrO3 allows us to separate surface-related conductivity of freshly cleaved crystals from bulk transport. We compare the electrical conductivity of the uncleaved and cleaved surface as well as of the surface after degradation in air as a function of temperature between 150 K and 300 K. We find a severe deviation from the usual variable-range-hopping transport [2] and complete domination of the surface conductivity for low temperatures. The freshly cleaved crystal showed a saturation of the sheet resistance at about 2,9 kΩ at low temperatures. After the degradation of the surface in air, the conductivity of the surface decreased, and we measured a general change in the temperature dependence compared to the freshly cleaved surface. Work supported by DFG through SPP 1666 and TRR80. Ref.: [1] Phys. Rev. 108, 106401 (2012), [2] Phys. Rev. B82, 064412 (2010)

O 36.7 Tue 10:30 P

Photoexcitation of Bulk Polarons in Rutile TiO2 — •Alex Tanner[1,2], Bo Wen[3], Yu Zhang[1,2], Li-min Liu[4], Helen Fielding[1], Annabella Selloni[3], and Geoff Thornton[1,2] — [1]Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom — [2]London Centre for Nanotechnology, University College London, 17-19 Gordon Street, London WC1H 0AH, United Kingdom — [3]Department of Chemistry, Princeton University, Princeton NJ 08540, United States — [4]School of Physics, Beihang University, Beijing, 100083, China

In recent years there has been considerable interest in the physics of polarons at reduced TiO2 surfaces. This includes two photon photoemission spectroscopy (2PPE) studies, which have proposed that polaron excitation may represent an alternative vector to band gap excitation in photocatalysis. These studies show that surface-localized polarons in rutile TiO2(110) couple with excited electronic states ca. 2.6 eV above the conduction band minimum. However, readily oxidised surface polarons likely have a minimal contribution in catalytic applications. In contrast, polarons in bulk TiO2 remain protected and therefore offer intriguing potential.

With 2PPE and hybrid density functional theory, we find bulk polarons are less bound by 0.2 eV compared with polarons at the surface. Because the excited state is also shifted to higher energy, bulk polarons have the same resonance energy as at the surface with a threshold at 3.1 eV. This is degenerate with the band gap, suggesting that bulk polarons could also provide an additional contribution to the photoyield.

O 37: Poster Session III: Surface magnetism III

Time: Tuesday 10:30–12:30 Location: P

O 37.1 Tue 10:30 P

Exchange bias in Co/CoO(110) bilayers — •Tomasz Blachowicz[1] and Andrea Ehrmann[2] — [1]Silesian University of Technology, Institute of Physics - Centre for Science and Education, Gliwice, Poland — [2]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, Bielefeld, Germany

Co/CoO is a ferromagnet/antiferromagnet system in which the exchange bias, a unidirectional anisotropy, was discovered [1]. The exchange bias can be accompanied by another anisotropy, the so-called 90° coupling, resulting in a rotation of hard and easy axes of the ferromagnet (FM) due to coupling to the antiferromagnet (AFM) at low temperatures [2]. Here we report on exchange bias and 90° coupling in Co/CoO(110) thin film systems, resulting not only in a rotation of the easy axes of the FM below the blocking temperature, but also in a significant increase of the coercive fields near the blocking temperature for one sample orientation. Combining Brillouin light scattering (BLS) and superconducting quantum interference device (SQUID) measurements, we show the temperature-dependent effect of the different superposed anisotropies.

[1] T. Blachowicz, A. Ehrmann: Exchange bias in thin films - an update, Coatings 11, 122 (2021)

[2] T. Błachowicz, A. Tillmanns, M. Fraune, B. Beschoten, and G. Güntherodt: Exchange-bias in (110)-oriented CoO/Co bilayers with different magnetocrystalline anisotropies, Phys. Rev. B 75, 054425 (2007)

O 37.2 Tue 10:30 P

Wavelength-dependent magnetization dynamics in Ni|Au bilayers — •Christopher Seibel, Marius Weber, Sebastian T. Weber, Hans Christian Schneider, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany

Existing experimental and theoretical studies of ultrafast demagnetization in ferromagnets rely mostly on only one fixed wavelength to excite the sample. However, recent experiments indicate that the dynamics of the demagnetization and remagnetization process depend on the wavelength of the exciting laser pulse [1, 2].

In this contribution, we apply the temperature-based μT-model to investigate the magnetization dynamics of a thin nickel layer on a gold substrate. Our model relies on realistic densities of states of both materials and includes energy and spin transfer at the interface. Additionally, we focus on the absorption of the exciting laser by calculating a spatially resolved absorption profile of the sample. We show the influence of wavelength-dependent excitation on the magnetization dynamics based on the energy deposition and energy transfer in the layers.

[1] V. Cardin *et al.*, Phys. Rev. B 101, 054430 (2020)

[2] U. Bierbrauer *et al.*, JOP: Cond. Mat. 29, 244002 (2017)

O 37.3 Tue 10:30 P

Ultrafast demagnetization dynamics including spin resolved charge and heat transport. — •Sanjay Ashok, Sebastian T. Weber, Christopher Seibel, Johan Briones, and Bärbel Rethfeld — Fachbereich Physik and OPTIMAS Research Center, TU Kaiserslautern, Kaiserslautern, Germany

Ultrafast Demagnetization of metallic ferromagnets due to excitation with a femtosecond laser pulse was discovered by Beaurepaire et al. in 1996 [1]. In case of metallic magnets with thickness lesser than pene- tration depth of the laser, the film is heated homogeneously. Therefore, due to absence of temperature and density gradients within the material there would be no heat- or charge-currents. For thicker magnetic metals, the heating is not uniform and therefore one needs to distinguish the resulting role of heat and spin-resolved charge transport in ultrafast de- and re- magnetization [2]. This is a pivotal issue owing to rich possibilities in its applications.

Here we study the role of spin-resolved charge and heat transport in ultrafast demagnetization of thick magnetic metal using Thermodynamic μT-model [3] and obtain spatial and temporal evolution of magnetization. We also present the role of applied fluence and trans- port channels.

[1] E. Beaurepaire, J.-C. Merle, A. Daunois and J.-Y. Bigot, Phys. Lett. 76, 4250 (1996).

[2] Y. Liu et al. JMMM 502, 166477 (2020).

[3] B. Y. Mueller and B. Rethfeld, Phys. Rev. B 90, 144420 (2014).

O 37.4 Tue 10:30 P

The role of magnon-phonon hybridization in the lifetime broadening of surface states in rare-earth metals — •Bo Liu, Huijuan Xiao, and Martin Weinelt — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Magnons and phonons are fundamental quasiparticle excitations in magnetic materials. Here we show that magnon-phonon hybridization plays an important role in the lifetime broadening of the surface state of ferromagnetic terbium due to large spin-lattice coupling in this material. This is evidenced by a comparison with Gd that has almost the same electronic structure as Tb but negligible 4f spin-orbit coupling. For the Gd surface state we show that magnon emission determines the photo-hole relaxation at low temperatures where the minority spin component exhibits clearly larger linewidth broadening than the majority component. With increasing temperature electron-phonon scattering becomes dominant evidenced by a larger coupling parameter λ in the majority spin channel. In contrast in Tb, majority and minority spin components of the surface state show very similar linewidths and the fitted electron-phonon coupling is twice as large as in Gd. The negligible spin dependence suggests the formation of magnon-polarons in line with our findings of ultrafast magnon emission in Tb [1].

[1] B. Frietsch et al., Science Advances 6, eabb1601 (2020).

O 37.5 Tue 10:30 P

Néel vector induced manipulation of valence states in the collinear antiferromagnet Mn2Au — •Hans-Joachim Elmers[1], S. V. Chernov[1], S. P. Bommanaboyena[1], S. Yu. Bodnar[1], K. Medjanik[1], S. Babenkov[1], O. Fedchenko[1], D. Vasilyev[1], S. Y. Agustsson[1], C. Schlueter[2], A. Gloskovskii[2], Y. Matveyev[2], V. N. Strocov[5], Y. Skourski[3], S. Dsouza[4], J. Minar[4], L. Šmejkal[1], J. Sinova[1], M. Klaeui[1], G. Schoenhense[1], and M. Jourdan[1] — [1]Institut für Physik, Universität Mainz, Germany — [2]DESY, Hamburg, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]University of West Bohemia, Czech Republic — [5]Paul Scherrer Institut, Switzerland

Manipulation of the electronic valence states of the collinear metallic antiferromagnet Mn$_2$Au was achieved by reorienting the direction of the staggered magnetisation (Néel vector). Pulsed magnetic fields of 50 T were used to direct the sublattice magnetisations of capped epitaxial Mn$_2$Au (001) thin films perpendicular to the applied field direction by a spin-flop transition. The electronic structure was investigated by hard X-ray angular-resolved photoemission spectroscopy. Our results confirm that the magnetic order parameter in real space provokes considerable changes of electronic states in reciprocal space near the Fermi Level and close to the X points. [1] ACS Nano 14, 17554 (2020).

O 37.6 Tue 10:30 P

Internal magnetic field increase at surface and interface of palladium thin films — •Gesa Welker[1], Martin de Wit[1], Tjerk H. Oosterkamp[1], John A. Mydosh[1], Thomas Prokscha[2], and Lucia Bossoni[1,3] — [1]Leiden Institute of Physics, Leiden University, The Netherlands — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villingen, Switzerland — [3]C.J. Gorter Center for High Field MRI, Department of Radiology, Leiden University Medical Center, The Netherlands

We experimentally investigated three undoped and iron-doped palladium (Pd) 100 nm thin films and found an increased internal magnetic field at the surface and interface compared to the bulk-like middle of the film. Pd surfaces have recently become of interest in the field of spin-orbitronics. Furthermore Pd nanomaterial shows many applications where surface properties play a role, such as for example catalysis, magnetoresistance spin valves and phase coherence superconducting junctions. Understanding the magnetic surface properties of Pd is therefore relevant for various fields of research.

In our low-energy muon spin spectroscopy (MuSR) study, we implanted muons in Pd samples at varying depths to probe the local magnetic field in the implantation region. The field increase at the surface/interface is temperature-independent, stronger for iron-doped samples, accompanied by an increased field inhomogeneity and extending over a few nanometers. We discuss potential origins for this magnetic surface state. Orbital moments induced by the surface/interface and localized spins/charges are the most likely explanation.

O 37.7 Tue 10:30 P

Local pairwise exchange interactions for noncollinear states in itinerant-electron magnets — •Ksenia Vodenkova[1] and Pavel Bessarab[1,2] — [1]ITMO University, St. Petersburg, Russia — [2]University of Icelad, Reykjavik, Iceland

The microscopic origin of the exchange interactions for noncollinear ordering of atomic magnetic moments in itinerant-electron systems is a subject of ongoing scientific discussions. In this work, we derive by means of the multiple-scattering theory a general expression for pairwise magnetic exchange interaction parameters for an arbitrary noncollinear, nonstationary magnetic state. In contrast to previous approaches, our formalism takes into account the variation of the fast degrees of freedom such as charge density and magnetic moment length. Application of the formalism to a tight-binding model reveals a range of magnetic systems that can be described by a classical Heisenberg Hamiltonian reasonably well. For other systems, our approach makes it possible to systematically derive atomistic spin Hamiltonians beyond the Heisenberg model. Moreover, the expression for the pairwise interaction tensor describes a local curvature of the energy surface of the system as a function of the orientation of magnetic vectors. This can be used in various contexts including description of thermal stability of magnetic states within the harmonic transition state theory and efficient identification of stable magnetic configurations using the Newton-Raphson method.

This work was funded by the Russian Science Foundation (Grant No.19-72-10138).

O 38: Poster Session III: Tribology: Surfaces and nanostructures I

Time: Tuesday 10:30–12:30 Location: P

O 38.1 Tue 10:30 P

Thermal Activation of Nanoscale Wear — Wen Wang[1,2], •Dirk Dietzel[1], and Andre Schirmeisen[1] — [1]Institute of Applied Physic, University of Giessen, 35392 Giessen, Germany — [2]School of Mechanical Engineering, Southwest Jiaotong University, 610031 Chengdu, China

Atomic force microscopy under ultrahigh vacuum conditions was used to study the temperature dependence of nanoscale wear occurring on freshly cleaved NaCl (001) and KBr (001) single crystals during continuous line scanning. Independent of the material, we observe non-monotonous wear-rates as a function of temperature, where a distinct transition between two regimes can be correlated to the onset of quasi-periodic ripple formation at higher temperatures. We find that a thermally activated bond breaking model quantitatively fully describes the wear rates in the low temperature regime and can also be applied to the high temperature regime once the alternating structure of mounds and troughs is accurately considered. Based on this agreement with Arrhenius kinetics over the whole temperature range, also the velocity dependence of the wear rate can be explained, where the amount of wear only depends on the overall scan length but is independent of sliding velocity.

O 38.2 Tue 10:30 P

Temperature dependence of friction anisotropy on crystalline materials — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, University of Giessen, 35392 Giessen, Germany

On the nanoscale, the dependence of the friction force on the sliding direction is a well-known phenomenon. This anisotropy occurs as a consequence of the surface structure and is related to different energy barrier heights along different directions of the sample surface. If the sample temperature is varied, the friction force as deduced from the thermally activated Prandtl Tomlinson model is expected to change, with direct influence on the stability of the different sliding directions. In this work, the directional friction force is now analyzed under UHV conditions as a function of temperature on different crystalline materials. Our results show that the both the absolute friction and the anisotropy are not only influenced by temperature itself but also reflect temperature dependent wear effects which ultimately eliminate any frictional anisotropy.

O 38.3 Tue 10:30 P

Frictional Behavior of Antimony Nanoparticles on HOPG at Elevated Temperatures — •Ebru Cihan, Dirk Dietzel, and Andre Schirmeisen — Justus-Liebig University Giessen Institute of Applied Physics 35392 Giessen, Germany

Structural Lubricity describes an effect leading to almost vanishing friction for the case of incommensurate interfaces. But although very low, friction still depends on the exact interface conditions, where especially relaxations between substrate and slider can lead to a dynamic enhancement of the effective energy barrier for lateral motion. Here, we present a tribological study of antimony nanoparticles sliding on highly oriented pyrolytic graphite (HOPG) at elevated temperatures. The high temperatures of up to several 100°C are used to drive the structural relaxation of nanoparticles on the substrate and the corresponding effects of contact aging are analyzed by both static and sliding friction and their respective contact area dependence. In addition, our experimental set-up should even allow to approach temperatures where sublimation of the antimony sets in and fundamentally changed interface conditions can be expected.

O 38.4 Tue 10:30 P

On-surface synthesis and mechanical stabilization of class 1 atropoisomers — •Philipp D'Astolfo[1], Guilherme de Vilhena[1], Carl Drechsel[1], Jung-Ching Liu[1], Xunshan Liu[2], Silvio Decurtins[2], Shi-Xia Liu[2], Rémy Pawlak[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

The torsion and rotation about single carbon-carbon bonds is a natural process that is ever-present in Chemistry- and Surface-Sciences. Due to their small magnitude, measurements of force-induced rotational changes between units of a long polymeric chain have proven difficult until now. To shed light on these processes, we synthesized sterically frustrated asymmetric cyclopentaaceanthrylene-polymers on a gold surface and performed lifting- and redeposition experiments using atomic force microscopy (AFM) at 4.8K. We detected repeating jumps in the frequency shift signal related to successive unit detachments of the poly-aceanthrylene units vertically lifted from the Au(111) surface. After performing a lifting experiment, we also redeposited the polymer on the surface while preserving the distinct bond-motif. Molecular dynamic (MD) simulations of the lifting- and redeposition experiments with different tethering of one end, ranging from hard anchored to slightly bonded and free ends, provide an atomistic understanding of the experimentally observed molecular anchoring on the peeling process and shed further light on the stabilization mechanism of sterically frustrated polymers.

O 39: Poster Session III: Poster to Mini-Symposium: Free-standing functional molecular 2D materials I

Time: Tuesday 10:30–12:30 Location: P

O 39.1 Tue 10:30 P

Electronic and Optical Properties of Protonated Triazine Derivatives — Michele Guerrini[1,2], •Enrique Delgado Aznar[2], and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

The peculiar electronic and optical properties of covalent organic frameworks (COFs) are largely determined by protonation, a ubiquitous phenomenon in solution environments. Resulting effects are non-trivial and yet crucial for the intriguing functionalities of these materials. We investigate from first principles the impact of protonation of triazine and amino groups in molecular building blocks of COFs in water solution. We find that proton uptake leads to bandgap reduction and to a reorganization of the electronic structure. The interplay between bandgap renormalization and exciton binding strength determines whether the absorption onsets is red or blue shifted with respect to the pristine species. Structural distortions induced by protonation are found to play only a minor role.Our results [1] offer a quantitative and microscopic insight into the role of protonation in the electronic and optical response of triazine derivatives as building blocks of COFs and to the rationalization of the relationship between structure, property, and functionality in these materials.

[1] M. Guerrini, E. D. Aznar, C. Cocchi J. Phys. Chem. C 2020 DOI: 10.1021/acs.jpcc.0c08812

O 39.2 Tue 10:30 P

Controlled Electron-Induced Fabrication of Metallic Nanostructures on 1 nm Thick Membranes — Christian Preischl[1], •Linh Hoang Le[2], Elif Bilgilisoy[1], Florian Vollnhals[1], Armin Gölzhäuser[2], and Hubertus Marbach[1] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Functional metallic nanostructures precisely deposited on insulating 2D materials are desired in many applications in optics, electronics, and magnetics. Such miniaturized details can be realized by using focused electron beam induced deposition (FEBID). With this technique, we directly deposit iron structures from Fe(CO)5 precursors onto terphenylthiol self-assembled monolayers (SAMs). We then apply electron irradiation to crosslink the functionalized SAMs into porous carbon nanomembranes (CNMs) while the iron structures remain on their surfaces. The resulting ultrathin, flexible and mechanically stable CNMs preserves the written iron patterns. They can be transferred onto either solid substrates or onto grids to obtain free-standing metal/CNM hybrids. In this way, we can achieve clean iron nanostructures of arbitrary size and shape on top of the 1 nm thick CNMs. Combining the ease and versatility of CNMs with the flexibility of FEBID leads to a promising route for the fabrication of functional hybrid nanostructures.

O 39.3 Tue 10:30 P

Ru(II) polypyridine nanomembranes by low-energy electron irradiation of SAMs — •Maria Küllmer[1], Felix Herrmann-Westendorf[1,3], Stefan Götz[2], Christof Neumann[1], Patrick Endres[2], Rebecka Glässner[1], Andreas Winter[2], Ulrich Sigmar Schubert[2,4], Benjamin Dietzek[1,3,4], and Andrey Turchanin[1,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Organic Chemistry and Makromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Germany — [3]Leibniz Institute of Photonic Technology e. V., Jena, Germany — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Germany

Artificial photosynthesis is of great importance for the development of sustainable energy sources. Due to their unique chemical and physical properties molecular 2D materials are highly promising building blocks to this end. Here we present two different concepts for the introduction of the Ru(II) polypyridine photosensitizers into Carbon Nanomembranes (CNMs) - a molecular nanosheet generated by electron irradiation induced cross-linking of self-assembled monolayers (SAMs). The photoactive units are either incorporated into the SAMs before or covalently attached after the crosslinking. We characterize the developed molecular nanosheets using high-resolution X-ray photoelectron spectroscopy and surface-enhanced Raman scattering. The combination of atomic force and scanning electron microscopy shows the formation of 2D nanomembranes. Photothermal deflection spectroscopy (PDS) is employed to characterize the absorption properties.

O 39.4 Tue 10:30 P

Gas permeation through a series of chemically inert carbon nanomembranes — •Vladislav Stroganov[1], Daniel Hüger[1], Monika Kruk[2], Christof Neumann[1], Krzysztof Kozieł[3], Piotr Cyganik[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow — [3]Faculty of Chemistry, Jagiellonian University, 30-387 Krakow

Due to their unique physical and chemical properties, atomically or molecularly thin sheets are promising nanomaterials for future energy conversion and separation technologies. In this study, we investigate carbon nanomembranes (CNMs) synthesized by low energy electron beam irradiation cross-linking of self-assembled monolayers based on a homologue series of biphenyl substituted carboxylic acids (C_6H_5-C_6H_4-$(CH_2)_n$-COO/Ag, n=2-6). Their permeation properties for various gases (He, Ar, D_2, D_2O, O_2) were studied by highly sensitive mass spectrometry measurements. The results demonstrate that the permeation of CNMs can be intimately tuned by structure of the molecular precursors. A difference of only one aliphatic carbon unit can significantly modify the permeation of gases with various kinetic diameters. Based on the conducted measurements, we evaluate the size and the density of nanopores in CNMs. Both quantities are otherwise hardly accessible for the studied molecular nanosheets by conventional microscopy techniques.

O 39.5 Tue 10:30 P

Preparation of Carbon Nanomembranes without Chemically Active Groups — Christof Neumann[1], Monika Szwed[2], •Martha Frey[1], Zian Tang[1], Krzysztof Kozieł[3], Piotr Cyganik[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow — [3]Faculty of Chemistry, Jagiellonian University, 30-387 Krakow

The electron-irradiation-induced synthesis of carbon nanomembranes (CNMs) from aromatic thiol-based self-assembled monolayers (SAMs) on gold substrate is a well-established method to form molecular thin nanosheets. These molecular two-dimensional materials can be prepared with tunable properties; therefore, they find a variety of applications in nanotechnology ranging from ultrafiltration to nanobiosensors. However, having advantages for some applications, chemically inert CNM cannot be prepared from thiol-based SAMs, as the reactive thiol group is present on the membrane surface even after transferring it to other substrates. Here, we study the electron irradiation of carboxylic acid-based SAMs on a silver substrate as an alternative route for CNM formation. Our analysis, based on a combination of X-ray photoelectron spectroscopy and scanning electron microscopy demonstrates that for this type of SAMs, purely carbonaceous CNMs with tunable porosity can be obtained. Neumann et al. ACS Appl. Mater. Interfaces 11 (2019) 31176.

O 39.6 Tue 10:30 P

Optically triggered control of carrier density in hybrid graphene-carbon nanomembranes field effect transistors — •Antony George[1], Zian Tang[1], Andreas Winter[1], David Kaiser[1], Christof Neumann[1], Thomas Weimann[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany

Field effect transistors (FETs) based on 2D materials are of great interest for applications in ultrathin electronic and sensing devices. Here we demonstrate the possibility to add optical switchability to graphene FETs (GFET) by functionalizing the graphene channel with optically active azobenzene molecules. The azobenzene molecules have been incorporated to the GFET channel by building a van der Waals heterostructure with carbon nanomembrane (CNM) which is used as a molecular interposer to attach the azobenzene molecules. Under exposure with 365 nm and 455 nm light, azobenzene molecules undergo cis- and trans- molecular conformations respectively, resulting in a switching of the molecular dipole moment. Thus the effective molecular field acting on the GFET channel is switched by optical stimulation and the carrier density is modulated.

O 40: Poster Session III: Poster to Mini-Symposium: Infrared nano-optics I

Time: Tuesday 10:30–12:30 Location: P

O 40.1 Tue 10:30 P

Broad spectral tuning of ultra-low-loss polaritons in a van der Waals crystal by intercalation — •Pablo Alonso-González — University of Oviedo

Phonon polaritons (PhPs) -light coupled to lattice vibrations- hold great promises for an unprecedented control of the flow of energy at the nanoscale because of their strong field confinement and long propagation. Moreover, recent experiments in polar van der Waals (vdW) crystals such as h-BN and *-MoO31*3, have demonstrated PhPs with anisotropic propagation, and ultra-long lifetime in the picosecond range. However, a main drawback of these PhPs is the lack of tunability of the narrow and material-specific spectral range where they exist * the so-called Reststrahlen Band (RB) *, which severely limits their implementation in nanophotonics technologies. Here, we demonstrate that intercalation allows for a broad spectral shift of RBs in a vdW crystal, and that the PhPs excited within them show ultra-low losses (lifetime of 5 ps) similar to PhPs in the non-intercalated crystal (lifetime of 8 ps). As a difference to previous attempts, which fail in keeping the polaritonic activity of the intercalated compound, our results are possible by employing an intercalation method based on single crystal growth, that we carried out in the vdW semiconductor *-V2O5, thereby also adding a new member to the library of vdW materials supporting PhPs. We expect this intercalation method to be applied in other vdW materials, opening the door for the use of PhPs in broad spectral bands that eventually cover the whole mid-IR range, which seems to be elusive with currently known polaritonic materials.

O 40.2 Tue 10:30 P

In_3SbTe_2 as a Programmable Nanophotonics Material Platform for the Infrared — •Andreas Hessler[1], Sophia Wahl[1], Till Leuteritz[2], Matthias Wuttig[1], Stefan Linden[2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen University — [2]Physikalisches Institut, University of Bonn

The high dielectric optical contrast between the amorphous and crystalline phases of non-volatile phase-change materials (PCMs) provides a promising route towards tuneable nanophotonic devices [1]. Here [2], we employ the next-generation PCM In_3SbTe_2 (IST) whose optical properties change from dielectric to metallic upon crystallization in the whole infrared spectral range. We demonstrate how resonant metallic nanostructures can be directly written, modified and erased on and below the meta-atom level in an IST thin film by a pulsed switching laser. With this technology, we demonstrate large resonance shifts of nanoantennas of more than 4 μm, a tuneable mid-infrared absorber with nearly 90% absorptance as well as screening and nanoscale "soldering" of metallic nanoantennas. Our novel concepts can empower new and improved designs of programmable nanophotonic devices for telecommunications, (bio)sensing and infrared optics, e.g. programmable infrared detectors, emitters and reconfigurable holograms.

[1] M. Wuttig, H. Bhaskaran and T. Taubner. Nature Photonics 11, 465-476 (2017)

[2] A. Heßler, S. Wahl, T. Leuteritz et al.. in submission at Nature Communications (2020)

O 40.3 Tue 10:30 P

Reconfiguring magnetic resonances with the plasmonic phase-change material In_3SbTe_2 — Andreas Hessler, •Lukas Conrads, Konstantin Wirth, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen University

Phase-change materials (PCMs) have been established as promising materials for tunable nanophotonic devices [1]. Normally, they feature a large optical contrast between their dielectric amorphous and crystalline phases. However, the recently introduced plasmonic PCM In_3SbTe_2 (IST) changes from dielectric to metallic in the infrared upon crystallization which enables novel resonance tuning mechanisms and direct laser writing of plasmonic nanostructures [2]. Here, directly optically written metallic, crystalline IST antennas with electric dipole (ED) resonances are first reconfigured into split-ring resonators (SRRs) with ED and magnetic dipole (MD) resonances by local optical switching. By selectively decreasing the arm lengths of the SRRs with reamorphizing laser pulses, we demonstrate tuning of the MD resonances by more than 2.4 μm, while the ED resonances for the same polarization are unchanged. Our work may pave the way towards engineering ultrathin, tunable, plasmonic devices for infrared nanophotonics which rely on separate tuning and superposition of ED and MD resonances.

[1] M. Wuttig, H. Bhaskaran and T. Taubner. Nature Photonics 11, 465-476 (2017)

[2] A. Heßler, S. Wahl, T. Leuteritz et al.. in submission at Nature Communications (2020)

O 40.4 Tue 10:30 P

Infrared-to-THz near-field nanoscopy with the free-electron laser FELBE — •Lukas Wehmeier[1,3], Tobias Nörenberg[1,3], Thales V.A.G. de Oliveira[1,2], J. Michael Klopf[2], Lukas M. Eng[1,3], and Susanne C. Kehr[1] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]ct.qmat, Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

Infrared nanoscopy of 2D materials, metamaterials, and optical nano-structures is often limited by the wavelength range provided by table-top laser sources. Radiation from the tunable narrow-band free-electron laser FELBE (Dresden, Germany) uniquely enables near-field nanoscopy over the broad spectral range from 5 to 250 μm (i.e. 1.2 - 60 THz), particularly covering also the *so-called* THz gap [1-7]. I will present intriguing applications of FELBE in IR-optical nanoscopy by demonstrating extreme field confinement, anisotropic dispersion tracking, and resonant phenomena of THz polaritons in van der Waals crystals [1], nano-structures [2,3] and functional perovskite oxides [4-8].

[1] T.V.A.G. de Oliveira et al., Advanced Materials 33, 2005777 (2021).
[2] D. Lang et al., Nanotechnology 30, 084003 (2018).
[3] F.H. Feres et al., submitted.
[4] J. Döring et al., Nanoscale 10, 18074 (2018).
[5] L. Wehmeier et al., Phys. Rev. B 100, 035444 (2019).
[6] L. Wehmeier et al., Appl. Phys. Lett. 116, 071103 (2020).
[7] S.C. Kehr et al., Nat. Commun. 2, 249 (2011).
[8] H. Aminpour et al., Opt. Express 28, 32316 (2020).

O 40.5 Tue 10:30 P

SNOM-examination of THz polaritons in the van der Waals crystal α-MoO_3 — •Maximilian Obst[1], Thales V. A. G. de Oliveira[1,2], Tobias Nörenberg[1,3], Susanne C. Kehr[1], and Lukas M. Eng[1,3] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Universität Dresden, Germany

The confinement of electromagnetic fields to the nanometer length scale is of great importance for advancing nanophotonic technologies, since allowing for enhanced light-matter interaction. For terahertz (THz) radiation, extreme field confinement can be achieved via the excitation of low-loss phonon-polaritons e.g. in van der Waals (vdW) crystals.

Nevertheless, experimentally proving such highly-confined phonon-polaritons at THz frequencies is very challenging. In the present work, we combine scattering-type scanning near-field optical microscopy (s-SNOM) with an IR-2-THz free-electron laser, in order to enable nanometer-scale optical resolution at narrow-band and tunable THz excitation. This poster presents measurements of low-loss polaritonic excitations at frequencies between 8 to 12 THz in the vdW semiconductor α-MoO_3 [1].

[1] T.V.A.G. de Oliveira et al., Advanced Materials 2005777 (2020)

O 40.6 Tue 10:30 P

Near-field optical investigations of the switching behavior of Ta_2O_5-based ReRAMs — •Christoph M. Bauerschmidt[1], Konstantin G. Wirth[1], Thomas Heisig[2], Sophia Wahl[1], Andreas Hessler[1], Regina Dittmann[2], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]Peter Grünberg Institute, Research Center Jülich

Tantalum oxide (Ta_2O_5) shows promising properties for applications as non-volatile Resistive Random Access Memories (ReRAMs). Local resistive switching through a valence change mechanism[1] leads to the formation of reduced Ta_2O_x-filaments of ≈10-100nm in size, accompanied by a difference in conductivity to pristine Ta_2O_5 by seven orders of magnitude[2]. The different stoichiometry and the increase in charge carrier density of Ta_2O_x cause changes of the dielectric function. Our calculations suggest that this change in the dielectric function of the switched Ta_2O_x will lead to a strong near-field contrast in the infrared region. Therefore, scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is performed during this work to investigate these local optical properties with nm-sized spatial resolution. s-SNOM allows us to characterise single switched Ta_2O_x-filaments in Ta_2O_5-films. Furthermore, s-SNOM yields promising opportunities for in-situ investigations of switched filaments through transparent graphene electrodes.

[1] Waser et al., *Adv. Mat.*, 21, 2632-2663 (2009)
[2] Dittmann et al., *Adv. Func. Mat.*, 25, 7154-7162 (2015)

O 41: Poster Session III: Poster to Mini-Symposium: Ultrafast surface dynamics at the space-time limit I

Time: Tuesday 10:30–12:30 Location: P

O 41.1 Tue 10:30 P

Microscopic theory for the real-time magnetization dynamics in bilayer-surfaces driven by ultrafast laser pulses — •Hanan Hamamera[1], Filipe Souza Mendes Guimaraes[2], Manuel dos Santos Dias[1], and Samir Lounis[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [3]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

We study the ultrafast magnetic reversal of spin moments by a single laser pulse [1] from a microscopic point of view. This is done by employing a realistic tight-binding Hamiltonian parameterized from density functional theory calculations to describe the real-time evolution of the electronic states. We map the parameter space characterizing the magnetic reversal of bulk Ni by the applied laser pulse, explaining the underlying physics and dissecting various intertwined spin-dynamics regimes. The knowledge gained on Ni is then utilized to explore the case of bilayer surfaces such as Co/Pt(001), where the non-magnetic heavy-metal substrate provides additional channels for angular momentum dissipation via spin and orbital pumping mechanisms, as well as stronger spin-orbital conversion.

Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] J. Gorchon *et al.*, Appl. Phys. Lett. **111**, 042401 (2017)

O 41.2 Tue 10:30 P

Exchange-striction driven ultrafast nonthermal lattice dynamics in NiO — •Yoav William Windsor[1], Daniela Zahn[1], Robin Kamrla[2], Johannes Feldl[3], Helene Seiler[1], Cheng-Tien Chiang[2], Manfred Rammsteiner[3], Wolf Widdra[2], Ralph Ernstorfer[1], and Laurenz Rettig[1] — [1]Fritz Haber Institute def MPG, Berlin — [2]Martin-Luther-Universität Halle-Wittenberg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

We use femtosecond electron diffraction to study ultrafast lattice dynamics in the highly correlated antiferromagnetic (AF) semiconductor NiO. Using the scattering vector (Q) dependence of Bragg diffraction, we introduce a Q-resolved ensemble of temperatures describing the lattice, and identify a nonthermal lattice state with preferential displacement of O compared to Ni ions, which occurs within ~0.3 ps and persists for 25 ps. We associate this with transient changes to the AF exchange striction-induced lattice distortion, supported by the observation of a transient Q-asymmetry of Friedel pairs. Our observation highlights the role of spin-lattice coupling in routes towards ultrafast control of spin order.

O 41.3 Tue 10:30 P

Heavy fermion dynamics in semimetallic and insulating phases — •Chulhee Min[1], Michael Heber[2], Simon Müller[3], Lukas Wenthaus[2], Steffen Palutke[2], Dmytro Kutnyakhov[2], Federico Pressacco[2], Lenart Dudy[4], Matthieu Silly[4], Hendrik Bentmann[3], Kiana Baumgärtner[3], Woojae Choi[5], Yong Seung Kwon[5], Markus Scholz[6], Friedrich Reinert[3], and Kai Rossnagel[1,2] — [1]IEAP, CAU Kiel, Germany — [2]DESY, Hamburg, Germany — [3]EP7 and ct.qmat, University of Würzburg, Germany — [4]Synchrotron-SOLEIL, Saint-Aubin, France — [5]Dep. of EMS, DGIST, South Korea — [6]EuXFEL, Schenefeld, Germany

Due to time–energy correlation, heavy fermion systems with hard-to-detect meV energy scales are expected to show relatively slow dynamics on ps time scales, which are relatively easy to measure. Using the free-electron laser FLASH, we have performed time-resolved pump-probe photoemission spectroscopy (PES) of mixed valent TmSe$_{1-x}$Te$_x$ at a probe photon energy where the photoionization cross-section of the localized $4f$ states is two orders of magnitude higher than the ones of the other states. The system consists of two magnetic $4f^{12}$ and $4f^{13}$ configurations in the ground state and can be tuned from a semimetallic to an insulating phase via x without destroying the periodicity of the Tm ions. Here, we present and discuss the transient dynamics of the $4f$ states near E_F showing a remarkably strong dependence on x. Particularly, we identify a renormalized $4f$ peak whose time-domain signature is distinct from all other $4f$ multiplet peaks.

O 41.4 Tue 10:30 P

Direct Access to Auger Recombination in Graphene — •Marius Keunecke[1], David Schmitt[1], Marcel Reutzel[1], Marius Weber[2], Christina Möller[1], G. S. Matthijs Jansen[1], Tridev A. Mishra[3], Alexander Osterkorn[3], Wiebke Bennecke[1], Klaus Pierz[4], Hans Werner Schumacher[4], Davood Momeni Pakdehi[4], Daniel Steil[1], Salvatore R. Manmana[1], Sabine Steil[3], Stefan Kehrein[2], Hans Christian Schneider[1], and Stefan Mathias[1] — [1]1. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [2]TU Kaiserslautern, Kaiserslautern, Germany — [3]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

The Auger scattering channels are of fundamental importance in the non-thermal charge-carrier dynamics of graphene and govern processes of technological relevance like carrier-multiplication and population inversion. These band-crossing scattering events can be separated into impact excitation (IE) and Auger recombination (AR) events which increase (IE) or decrease (AR) the charge-carriers in the conduction band. In this contribution, we apply time-resolved momentum-microscopy to study the non-thermal charge carrier dynamics in n-doped graphene with energy and full in-plane momentum resolution. We report on direct experimental evidence and quantification of AR in graphene and support our conclusions by model calculations.

O 42: Poster Session III: Poster to Mini-Symposium: Machine learning applications in surface science I

Time: Tuesday 10:30–12:30 Location: P

O 42.1 Tue 10:30 P

Learning electron densities in condensed phase space — •Alan Lewis[1], Andrea Grisafi[2], Michele Cerrioti[2], and Mariana Rossi[1] — [1]MPI for Structure and Dynamics of Materials, Hamburg, Germany — [2]École Polytéchnique Fédèrale de Lausanne, Lausanne, Switzerland

The electron density is a fundamental quantity for modelling and understanding physical phenomena in materials. Not only is it central to theories like density-functional theory, but it also allows the calculation of a wide range of observables that are either directly or indirectly connected to it, like total energies, dipole moments, the electrostatic potential, work functions, and others. In this work, we present a model that is able to learn and predict the electronic density of diverse materials, ranging from liquids to solid semiconductors and metals. This is achieved by extending the framework presented by Grisafi et al [1] to work with periodic boundary conditions and when using a resolution of the identity on a numeric atom-centered orbital basis [2] to obtain coefficients for the expansion of the periodic density. This density is learned through a Gaussian process regression model that makes use of local symmetry-adapted representations of the atomic structure, which makes our method both data-efficient and highly transferable. We discuss the applicability of this model for large-scale periodic systems and its transferability across the periodic table.

[1] Grisafi et al, ACS Cent. Sci. 5, 57-64, 2019

[2] Blum et al, Comput. Phys. Commun. 180, 2175-2196, 2009

O 42.2 Tue 10:30 P

A fourth-generation high-dimensional neural network potential — •tsz wai ko[1], jonas a. finkler[2], stefan goedecker[2], and jörg behler[1] — [1]Theoretische Chemie, Institut für Physikalische Chemie, Georg-August-Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany — [2]Department of Physics, Universität Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Machine learning potentials (MLPs) have become an important tool for performing reliable atomistic simulations in surface science due to their nearly ab-initio accuracy and efficiency comparable to empirical force field. The majority of MLPs relies on the representation of energies and sometimes charges as a function of the local atomic environments. They are thus unable to describe non-local changes in the electronic structure due to long-range charge transfer or different global charges of a system.

Here we proposed a fourth-generation high-dimensional neural network potential (4G-HDNNP) for capturing the global charge distributions and corresponding non-local effects. We demonstrate the performance of 4G-HDNNPs for different benchmark systems showing that 4G-HDNNPs are in excellent agreement with electronic structure calculations.

O 42.3 Tue 10:30 P

Neural Network Analysis of Neutron and X-Ray Reflectivity Data: Pathological Cases, Performance and Perspectives — •Alessandro Greco[1], Vladimir Starostin[1], Alexander Hinderhofer[1], Alexander Gerlach[1], Maximilian Skoda[2], Stefan Kowarik[3], and Frank Schreiber[1] — [1]Institute of Applied Physics, University of Tübingen, Germany — [2]Rutherford Appleton Lab, ISIS Neutron and Muon Source, UK — [3]Department of Physical Chemistry, University of Graz, Austria

Neutron and X-ray reflectometry (NR and XRR) are powerful techniques to investigate the structural, morphological and even magnetic properties of solid and liquid thin films. Having demonstrated the general applicability of neural networks to analyze XRR and NR data before [1], this work discusses challenges arising from certain pathological cases as well as performance issues and perspectives. These cases include a low signal to noise ratio, a high background signal (e.g. from incoherent scattering), as well as a potential lack of a total reflection edge (TRE). We show that noise and background intensity pose no significant problem as long as they do not affect the TRE. However, for curves without strong features the prediction accuracy is diminished. Furthermore, we discuss the effect of different scattering length density combinations on the prediction accuracy. The results are demonstrated using simulated data of a single-layer system.

[1] Greco et al., *J. Appl. Cryst.*, **52**, 1342 (2019)

O 42.4 Tue 10:30 P

Analysis of grazing-incidence wide-angle X-ray scattering by neural networks — •Vladimir Starostin, Alessandro Greco, Alina Pleli, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Germany

Grazing-incidence wide-angle x-ray scattering (GIWAXS) is an indispensable tool for studying nanostructure surfaces and thin films. It is widely used in real-time studies of thin film growth. However, high acquisition rates of real-time experiments lead to enormous amounts of data to be analysed. For instance, a modern 2D X-ray detector has around 4.5 million of pixels and produces up to 6 Gb of data per second at the maximum frame rate of 750 Hz. In the future, these numbers will only increase and it may become unfeasible to analyze or even save unprocessed data. To address these problems, some automated tools need to be developed [1].

In this work, we present a machine learning approach that provides feature detection of GIWAXS images in an automated fashion. This simplifies the experimental data analysis and might enable on-the-fly preprocessing of GIWAXS data.

[1] Greco et al., *J. Appl. Cryst.*, **52**, 1342 (2019)

O 42.5 Tue 10:30 P

Symmetry-Equivariant Representations of Ab Initio Hamiltonians for Machine Learning Purposes — •Michael Luya[1] and Reinhard Maurer[2] — [1]Department of Mathematics, University of Warwick — [2]Department of Chemistry, University of Warwick

High-dimensional machine learning is consistently improving the quality of condensed matter simulations. These simulations provide us with the Hamiltonian matrix, useful for calculating a wide variety of material properties. Predicting these matrices requires a deep understanding of covariance properties and directional coordinate dependence.

In an attempt to capture rotation invariance we introduce methods involving crystal field theory and bijective minimal basis transformations, in order to extract symmetry invariant parameters that can describe high-order contributions to the Hamiltonian, with application towards modelling a variety of molecules, metallic clusters, and eventually metal-organic interfaces. We also investigate the physical significance of these parameters and present a scheme as to how they should be best extracted from data, for the purposes of providing significant training data for neural network models.

O 42.6 Tue 10:30 P

Active Discovery of Organic Semiconductors — •Christian Kunkel[1,2], Johannes T. Margraf[1], Ke Chen[1], Harald Oberhofer[1], and Karsten Reuter[1,2] — [1]Chair for Theoretical Chemistry and Catalysis Research Center — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft

Improving charge-transport of organic semiconductors (OSCs) for electronic applications is usually tackled by empirical structural tuning of promising compounds. Howver, the versatility of organic molecules generates a rich design space whose vastness dictates efficient search strategies. We thus here present an active machine learning (AML) approach that explores this virtually unlimited design space iteratively. Judging suitability of OSC candidates by charge injection and mobility-related descriptors, the AML approach iteratively queries first-principle evaluation on well-selected molecules. We first optimize the approach in a fully characterized, but truncated molecular test space, gaining deep methodological insight about its exploratory behavior. Outperforming a conventional computational funnel, the devised algorithm can thereby successfully leverage its gradually improving knowledge and focus on promising regions of the design space. When subsequently lifting the artificial truncation, high-performance candidates are constantly found while the algorithm meanders ever more deeply through the endless OSC design space. The demonstrated high efficiency in the detection of candidate compounds with superior charge conduction properties highlights the usefulness of autonomously operating systems for a targeted OSC design.

O 42.7 Tue 10:30 P

Ab initio structure search of flexible molecules at interfaces — •Dmitrii Maksimov[1,2] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

We investigate how the accessible conformational space of two flexible amino acids, Arg and Arg-H$^+$, changes upon adsorption, by building and analyzing a database of thousands of structures optimized at Cu(111), Ag(111) and Au(111) surfaces with the PBE functional including screened pairwise (vdW) interactions. We employ an unsupervised dimensionality reduction procedure that enables us to understand the alteration of the high-dimensional conformational space [1]. The creation of this database, which is paramount to train further diverse machine-learning models, suffers from well-known bottleneck related to the efficiency of the geometry optimizer. We introduce a flexible way of preconditioning approximate Hessian matrices in the BFGS algorithm that is tailored to accelerate the relaxation of vdW bonded structures that can handle large structural changes. An automated sampling of these systems is implemented within a random structure search package [2] that can take explicitly into account the flexibility of molecules, their position and orientation with respect to fixed surroundings and interfaces.

[1] Maksimov et. al., Int. J. Quantum Chem., e26369 (2020)

[2] https://github.com/sabia-group/gensec

O 42.8 Tue 10:30 P

IrO$_2$ surface complexions identified through machine-learned interatomic potentials — •Jakob Timmermann[1,2], Yonghyuk Lee[1,2], Carsten Staacke[1,2], Christoph Scheurer[1,2], and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der MPG — [2]Technische Universität München

IrO$_2$ is currently the preferred catalyst for the electrochemical oxygen evolution reaction in proton exchange membrane electrolyzers. Full *ab initio* molecular dynamics (MD) simulations of the reactive processes at the surface would be highly desirable for mechanistic catalyst improvement, but are computationally not tractable for a foreseeable time. To overcome the limitations regarding system size and propagation time, MDs based on machine-learned interatomic potentials are an appealing alternative. Here, we present a Gaussian Approximation Potential (GAP) approach for IrO$_2$ combining two-body and smooth overlap of atomic positions (SOAP) descriptors to capture the atomic environments. For maximum data efficiency, we pursue an iterative parametrization protocol, in which preliminary GAP potentials based on limited first-principles data are used to generate most meaningful additional structures for retraining. The final GAP potential enables a global geometry optimization of low-index rutile IrO$_2$ facets through simulated annealing. Consecutive *ab initio* thermodynamics and detailed surface science investigations fully confirm the identified novel (101) and (111) (1x1) terminations as competitive with the most studied (110) facet in reducing environments [1]. [1] J. Timmermann *et al.*, Phys. Rev. Lett. **125**, 206101 (2020).

O 42.9 Tue 10:30 P

The data-driven search of new catalysts for an OCM reaction based on the properties of surface carbonates — •Aliaksei Mazheika[1], Frank Rosowski[1,2], and Ralph Kraehnert[1] — [1]BasCat, Technische Universitaet Berlin, Berlin, DE — [2]BASF SE, Ludwigshafen, DE

The interest in oxidative coupling of methane (OCM) reaction is caused by the fact that this is a relatively simple way for conversion of methane to C2 products (ethane, ethylene). Despite quite many years spent for the search of an efficient catalyst, still a catalyst which would be commercially viable has not been found. Recently Wang et al. have experimentally observed the volcano-like dependence of OCM performance of oxide catalysts on decomposition of their carbonates [1]. In this study we develop a way for calculations of carbonates formation energies based on adsorption of CO$_2$ on the surfaces of corresponding oxides. This allows us to reformulate experimentally observed volcano-like dependence in terms of theoretically calculated quantities. Based on this, we develop the strategy for high-throughput screening using artificial intelligence methodology - subgroup discovery [2] and SISSO [3]. With that we have done the screening of more than 800k materials, and obtained new materials promising for OCM reaction.

[1] H. Wang, PhD thesis, TU Berlin (2018).

[2] M. Boley *et al.*, Data Min. Knowl. Disc. **31**, 1391 (2017).

[3] R. Ouyang *et al.*, Phys. Rev. M **2**, 083802 (2018).

O 43: Mini-Symposium: Electrified solid-liquid interfaces II

Time: Tuesday 13:30–15:30 Location: R1

Invited Talk O 43.1 Tue 13:30 R1
Electrocatalysis beyond surface reaction energetics — •Karen Chan — Fysikvej, Building 311, Room 4, Kongens Lyngby Denmark 2200
Beyond surface reaction energetics, the structure and composition of the electric double layer exerts an influence on the activity and selectivity of electrochemical reactions. In this talk, I first discuss the impact of pH and the electrolyte on electrocatalytic activity from the perspective of adsorbate-field interactions. I then discuss the impact of mass transport on activity and selectivity. I draw examples from hydrogen evolution and CO_2 electroreduction reduction.

Invited Talk O 43.2 Tue 14:05 R1
Design and application of an ab initio electrochemical cell — Sudarsan Surendralal, Florian Deissenbeck, Stefan Wippermann, Christoph Freysoldt, Mira Todorova, and •Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
Having accurate simulation techniques to explore and predict the structure and chemical reactions at the electrified electrode-water interface will be crucial to overcome major materials limitations related to energy-conversion, storage and sustainability. The last few years showed some exciting new developments that allow us a realistic description of electric fields at the interface and to (thermo)-potentiostat the electrode potential [1, 2]. These approaches are easy to implement in standard and well-established first principles codes and allow us thus to address and resolve pressing materials science questions in electrochemistry or corrosion sciences. The talk will give a brief overview over the key concepts of these new methodologies and show their application for two examples: The role of the hydrogen evolution reaction (HER) in the corrosion of Mg [1] and the role of water co-adsorption on the electrode potential and HER on Pt surfaces [3].

[1] S. Surendralal, M. Todorova, M. Finnis, J. Neugebauer, PRL 120, 246801 (2018).

[2] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, PRL (under review), arXiv:2003.08156 .

[3] S. Surendralal, M. Todorova, J. Neugebauer, PRL (under review).

O 43.3 Tue 14:40 R1
Dielectric properties of nano-confined water: a canonical thermopotentiostat approach — •Florian Deissenbeck, Christoph Freysoldt, Mira Todorova, Jörg Neugebauer, and Stefan Wippermann — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf
With the advent of robust techniques to apply electric fields in density-functional calculations, there has been continuous interest to use ab initio molecular dynamics (MD) simulations to study electrically triggered processes, such as electrochemical reactions. Here we introduce a novel approach to sample the canonical ensemble at constant temperature and applied electric potential [1]. Our thermopotentiostat approach can be straightforwardly implemented into any density-functional code. To demonstrate the power of our new approach, we compute the dielectric constant of nano-confined water without any assumptions for the dielectric volume. We show that the extremely low dielectric constant of nano-confined water is related to the existence of a dielectrically dead layer within interfacial water.

[1] F. Deißenbeck, C. Freysoldt, M. Todorova, J. Neugebauer, S. Wippermann, Phys. Rev. Lett. (submitted), arXiv:2003.08156

General discussion

O 44: Mini-Symposium: Manipulation and control of spins on functional surfaces II

Time: Tuesday 13:30–15:30 Location: R2

Invited Talk O 44.1 Tue 13:30 R2
Atomic-scale spin sensing with a single molecule at the apex of a STM — •Laurent Limot — Université de Strasbourg, CNRS, IPCMS, Strasbourg, France
The decoration of metal probe-tips by a molecule intentionally picked up from a surface has proven to be a powerful method to improve the measurement capabilities of a scanning tunneling microscope (STM). The degrees of freedom of the molecule introduce tip-surface interactions across the vacuum gap that are usually absent when using a metallic apex. These interactions can endow STM with an enhanced sub-molecular resolution and provide new chemical insight.

The success of this approach opens the prospect of introducing spin sensitivity through the tip functionalization by a magnetic molecule. We show here that it is possible to use metallocene-terminated tips to monitor surface magnetism through the inelastic component of the tunneling current, which provides an electrical access to the metallocene spin states. When the tip is 100 picometers away from point contact, the exchange interaction between the tip and a magnetic sample changes the metallocene spin states. This detection scheme can then be used to simultaneously probe the sample exchange field and spin polarization with atomic-scale resolution.

O 44.2 Tue 14:00 R2
Free coherent evolution of a coupled atomic spin system initialized by electron scattering — Lukas M. Veldman[1], •Laetitia Farinacci[1], Rasa Rejali[1], Rik Broekhoven[1], Jeremie Gobeil[1], David Coffey[1], Markus Ternes[2,3], and Alexander F. Otte[1] — [1]Delft University of Technology, The Netherlands — [2]RWTH Aachen University, Germany — [3]Peter-Grünberg-Institute, Jülich, Germany
Observing the free evolution of a coupled spin system is an essential step towards studying collective quantum spin dynamics, as well as gaining insight into the fundamental mechanisms leading to spin excitation. Here, we combine pump-probe and ESR techniques with STM to study the free evolution of a single atomic spin depending on its level of entanglement with a second one. We build TiH dimers on MgO/Ag(100) in which the two spins are inherently detuned. We then make use of the magnetic interaction with the STM tip to tune the level of entanglement between the two spins: using ESR, we characterize the energy diagram of the dimer and identify the tip height at which both spin precess at the same frequency. Subsequently, we use a pump-probe scheme to, first, initialize the system via an electron induced spin excitation and, second, study the free evolution of the spin under the tip. We show that only when the two spins entangle, the excitation is swapped back and forth at a frequency that is given by their coupling strength. These results provide insight into the locality of electron-spin scattering: only the spin directly underneath the tip is affected, irrespective of its global quantum state.

Invited Talk O 44.3 Tue 14:15 R2
Quantum sensing and operation of single molecules on the surface — •Xue Zhang — Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — Ewha Womans University, Seoul 03760, Republic of Korea
Scaling down information devices to atom-scale has brought the interest of using individual spins as basic unit for data storage. Scanning tunneling microscopy (STM) combined with fast electric pulse and electron spin resonance (ESR) technique has been proved a powerful tool to access and coherently control individual spins in atomic scale.

Here, we investigated the spin properties and dynamics of artificially built Fe-tetracyanoethylene (TCNE) complexes by using electronic spin pump-probe spectroscopy. Further, we spatially imaged the location of the spin center within the complex [J. Phys. Chem. Lett., 2020, 11, 14, 5618]. This work highlights that the combination of STM with electronic spin relaxometry can provide highly valuable clues for investigating magnetic metal-organic nanostructures. While current ESR-STM studies have focused on atom spins, we achieved driving ESR on single molecules (metal phthalocyanine) on a bilayer magnesium oxide (MgO) surface atop Ag(100) [under review]. We probed and differentiated the exchange and dipole interaction between molecular dimers. This work demonstrates the feasibility of employing single molecules in atom-scale quantum control studies and shed light on intriguing magnetic interactions between molecular spins, which is crucial for developing molecule-based spintronic devices.

Invited Talk O 44.4 Tue 14:45 R2
Longitudinal and transverse electron paramagnetic resonance in a scanning tunneling microscope — •Tom S. Seifert[1,2], Stepan Kovarik[2], Dominik Juraschek[3], Nicola A. Spaldin[2], Pietro Gambardella[2], and Sebastian Stepanow[2] — [1]Freie Universität Berlin — [2]Eidgenössische Technische Hochschule Zürich — [3]Harvard University
Combining the sub-atomic resolution of scanning tunneling microscopy (STM) with the spectral resolution of electron-paramagnetic resonance (EPR) allows for sensitively probing magnetic interactions of single atoms on a surface [1]. However, the experimental requirements for driving the EPR transitions are still under debate. In-depth understanding of the EPR-STM driving is mandatory to explore novel material systems and optimize the sensitivity of this technique.

Here, we acquire and model EPR spectra of single Fe and hydrogenated Ti atoms on bilayer MgO on Ag [2]. We investigate the impact of radiofrequency excitation strength and tunneling parameters on the EPR signal and find strong evidence for a piezoelectric coupling mechanism [3]. In this mechanism, the surface atom oscillates at radiofrequencies in the inhomogeneous tip magnetic field. Based on density functional theory and atomic-multiplet calculations, we reveal different driving mechanisms for single Fe and hydrogenated Ti atoms on the surface. Specifically, transverse magnetic field gradients drive the spin-1/2 hydrogenated Ti, whereas longitudinal magnetic field gradients drive the spin-2 Fe. [1] S. Baumann et al., Science 350 (2015); [2] T. S. Seifert et al., PRR 2 (2020); [3] T. S. Seifert et al., Sci. Adv. 6 (2020)

"Meet our speakers". Open discussion with all speakers of the session

O 45: Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces I

Time: Tuesday 13:30–15:30 Location: R3

Invited Talk O 45.1 Tue 13:30 R3
A Superficial Look At Water — •Olle Björneholm — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Water is of key importance for life itself and in numerous environmental and technical processes. Despite its importance and its simple molecular structure, the behavior of liquid water remains enigmatic. Molecules at interfaces have different environments compared to those in bulk water, resulting in various interface-specific phenomena. These are highly challenging to investigate, and our understanding of the water interfaces is therefore in many respects even more incomplete than for bulk water. In addition to their fundamental importance, water interfaces are also crucial in e.g. environmental sciences, biology and technology. In this talk, I will present some results on aqueous solutions obtained by x-ray photoelectron spectroscopy. I will exemplify how the aqueous surface differs from the bulk, including both fundamental properties, and examples relevant to atmospheric sciences.

O 45.2 Tue 14:00 R3
A Flow-Focused Droplet Train for Investigating Liquid Phase Processes with Ambient Pressure XPS — •Pip Clark, Michael Sear, Marco Favaro, Roel van de Krol, and David Starr — Institute for Solar Fuels Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-14109 Berlin, Germany

Here we present a newly commissioned droplet train designed for measuring the chemical and physical properties of liquids in pressures up to 30 mbar using ambient pressure XPS. Our droplet train generates thousands of uniform droplets a second, tunable in diameter between 100 to 500 microns.

We present results from commissioning experiments on aqueous solutions and colloidal systems, and describe the advantages of using flow focusing. We also discuss the capability of time-resolved XPS using the droplet train. By changing the height of the droplet generation point above the spectroscopic analysis position and introducing a suitable time-zero trigger, different delay times can be measured. Depending on the speed of the droplets chosen, we can access delay times between tens of μs and hundreds of ms. Examples of possible systems to study include (but are not limited to) gas uptake at the liquid/vapor interface, photoinduced physical and chemical reactions in solution, and nucleation and growth of salt crystallites or nanoparticles.

The droplet train module is a part of the SpAnTeX end station, which focuses on AP-XPS experiments in the tender X-ray regime (AP-HAXPES). Commissioning experiments were performed at the KMC-1 beamline, at BESSY II in Berlin.

O 45.3 Tue 14:20 R3
Chemical kinetics at the water-water interface of a liquid flat-jet — •Hanns Christian Schewe[1], Bruno Credidio[2], Aaron Ghrist[1,3], Sebastian Malerz[1], Christian Ozga[4], Henrik Haak[1], Gerard Meijer[1], Bernd Winter[1], and Andreas Osterwalder[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Molecular Physics, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Institute for Chemical Sciences and Engineering (ISIC), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland — [3]Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482, USA — [4]Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Two colliding cylindrical microjets from aqueous solutions are used to produce a planar leaf-shaped flowing sheet. Using jets from two different aqueous solutions, each containing a reactant for a fast chemiluminescence reaction, we image the emitted photons to spatially visualize the mixing of the solutions at any position of the leaf. Diffusion across the planar liquid-liquid interface leads to mixing of chemical species from the two solutions, allowing for chemical reactions and their detection. Such a micrometer-thin flowing two solution structure offers novel opportunities for spectroscopic and kinetic studies at liquid-liquid interfaces. We present a quantitative model that describes diffusion-limited reaction kinetics at the liquid-liquid interface, which can also be extended to account for interactions at the liquid-vapour interface.

Invited Talk O 45.4 Tue 14:40 R3
Exploring Collisions and Reactions at the Vacuum-Water Interface using Water Microjets — •Gilbert Nathanson — Department of Chemistry, University of Wisconsin, Madison, Wisconsin, USA

Gas-liquid scattering experiments provide molecular insights into collisions and reactions at the vacuum-liquid interface while minimizing interference from collisions in the vapor. Studies of liquid water in vacuum are especially challenging because of water's high vapor pressure. This tutorial will describe collisions of inert, organic, and atmospheric gases with a water microjet, a fast-flowing liquid stream no thicker than a strand of hair. The small surface area of the jet generates a thin vapor cloud that can be readily traversed by incoming and outgoing gas molecules with almost no gas-vapor collisions. Many other liquids can form microjets as well, including gasoline and jet fuel. I will illustrate the utility of these microjets by surveying experiments measuring the entry and longtime uptake of organic acids and bases into salty water and reactions of the atmospherically important gas N2O5 in water containing both salts and surfactants. These experiments help to unravel the mechanisms by which collisions lead to scattering, trapping, solvation, and interfacial acid-base and oxidation-reduction reactions.

O 45.5 Tue 15:10 R3
Imaging Gas-Liquid Scattering Processes in Real Space — •Maksymilian Roman, Robert Bianchini, Adam Knight, Daniel Moon, Kenneth McKendrick, and Matthew Costen — Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom

A novel technique for studying the dynamics of gas-liquid scattering was used to image the products of hydroxyl radical (OH) collisions with low-vapour-pressure liquids. A pulsed molecular beam of OH was aimed at layers of squalane, squalene and perfluoropolyether and probed by exciting laser-induced fluorescence (LIF) with pulsed laser light shaped into a sheet. The LIF signal emitted from pre- and post-collision packets of OH was intensified and captured by a camera. The images showed that OH scattered with broad angular distributions, but with superthermal speeds and rotational distributions, suggesting a predominantly impulsive mode of scattering from an atomically rough surface. The experiment has been recently modified to include a physically narrower ingoing packet of radicals and a better shaped laser probe sheet. Together with a custom-made Monte Carlo simulation of the scattering process, these are expected to provide even greater insight into the angular and speed distributions of the scattered products and hence the underlying scattering dynamics.

O 46: Poster Session IV: Semiconductor substrates II

Time: Tuesday 13:30–15:30 Location: P

O 46.1 Tue 13:30 P
Atomistic Modeling for the Vapor-Phase Growth of GaAs Nanowires: from DFT to Growth Kinetics — •In Won Yeu[1], Gyuseung Han[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[2] — [1]Electronic Materials Research Center, Korea Institute of Science and Technology, Seoul, Korea — [2]Department of Materials Science and Engineering, Seoul National University, Seoul, Korea

Based on density functional theory (DFT), this study introduces an ab initio approach tackling the vapor-phase growth kinetics of III-V nanowire (NW) depending on temperature (T) and pressure (P) conditions. By evaluating the vibrational entropy contribution to the surface energy through surface phonon calculations, the T-P dependent variation in surface reconstructions was successfully predicted by the authors. Considering the surface transitions, the change in Gibbs free energy is calculated as a function of T and P at each growth process on surfaces: adsorption and nucleation. The comparison of the free energy among different surfaces enables us to predict the relative rate of growth depending on crystallographic directions and stacking sequences. As a result, we identify the mechanism of extreme anisotropic growth of GaAs (spontaneous NW formation) along a certain polar direction, <111>B; the preferential adsorption of vapor sources on (111)B surface, allowed at narrow T-P range, induces the unidirectional growth. In addition, the asymmetric formation of stacking sequence during the growth along the two opposite directions of a polar direction, <111>A and <111>B, is elucidated, showing a perfect agreement with experimental observations.

O 46.2 Tue 13:30 P

3D Active Sites of Te in Hyperdoped Si by Hard X-ray Photoelectron Kikuchi-Diffraction — •Moritz Hoesch[1], Mao Wang[2], Shengqiang Zhou[2], Christoph Schlüter[1], Olena Fedchenko[3], Katerina Medjanik[3], Sergej Babenkov[3], Aimo Winkelmann[4], Hans-Joachim Elmers[3], and Gerd Schönhense[3] — [1]DESY Photon Science, Notkestraße 85, Hamburg, Germany — [2]Helmholt-Zentrum Dresden-Rossendorf, — [3]JGU, Institut für Physik, Mainz, Germany — [4]Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Krakow, Poland

n-type doping of Si by the deep chalcogen donor Te in excess of the solubility limit was recently demonstrated to lead to hyperdoped material [1]. These samples are made by ion im*plantation into an intrinsic Si substrate combined with pulsed laser melting. Our investigation by hard x-ray photoelectron spectroscopy (hXPS) reveals at least two different Te species with different binding energy and systematically varying concentrations as a function of increasing Te-content. At the highest doping concentration we study the photoelectron scattering patterns using hard x-ray photoelectron diffraction (hXPD) [2]. Substitutional site occupation of both Te monomers as well as dimers is identified with increasing binding energy leading to the main features in the XPS spectra. The sharp hXPD patterns allow the detailed analysis of the local surrounding of the dopant atoms [3]. — References: [1] M. Wang et al. Phys. Rev. Appl. 11 054039 (2019) and references therein. [2] O. Fedchenko et al NJP 21, 113031 (2019); [3] O. Fedchenko et al NJP 22, 103002 (2020).

O 46.3 Tue 13:30 P

GaInP(100) and InP(100) with different surface reconstructions for photoelectrochemical water splitting — •Olfa Dani[1], David Ostheimer[1], Mario Kurniawan[2], Agnieszka Paszuk[1], Andreas Bund[2], and Thomas Hannappel[1] — [1]Institute of Physics, Technische Universitaet Ilmenau, Germany — [2]Institute of Materials Science and Engineering, Technische Universitaet Ilmenau, Germany

To date, III-V semiconductor device structures enable the highest solar-to-hydrogen efficiencies, exceeding 19%. In this approach, a detailed understanding of the reactions at the semiconductor-electrolyte interface is essential to design the semiconductor surface for efficient charge transfer. In this present work, we study photoelectrochemical (PEC) performance of atomically well-ordered surfaces of GaInP(100)and InP(100) grown by MOVPE. p-type InP have been grown homoepitaxially on InP(100) substrates. GaInP buffer layers were grown lattice matched, on either GaAs or Ge (100) substrates. In order to avoid anti-phase boundaries in the III-V epilayers, the Ge(100) surface was prepared with double-atomic steps prior to growth. The surfaces involved were prepared with either P-rich (2x1) or III-rich (2x4) surface reconstructions via specific preparation routes controlled by optical in situ spectroscopy and identified in UHV by LEED. Selected samples were in system transferred in an inert nitrogen ambiance to a PEC cell, where they were exposed to an aqueous electrolyte. For comparison, the same measurements were performed on samples with a native oxide layer. We show that a precise surface preparation is crucial for efficient PEC processes.

O 46.4 Tue 13:30 P

Caesium deposition on GaN to obtain a photocathode for particle accelerators — •Jana Schaber[1,2], Rong Xiang[1], Jochen Teichert[1], and André Arnold[1] — [1]Department of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Physical Chemistry, Technical University Dresden, Dresden, Germany

Negative electron affinity (NEA) GaAs- and GaN-based photocathodes are used in modern night vison detectors and light emitting diodes. GaAs semiconductors are already used as electron sources in particle accelerators and well- studied. Like GaAs, GaN belongs to the III-V semiconductor group with similar properties. It is assumed that GaN, like GaAs, shows enormous potential as a novel electron source for particle accelerators.

P-type GaN on different substrate material (sapphire, silicon, copper or SiC) is activated by a thin layer of caesium and illuminated by ultra-violet (UV) light at the same time. As a consequence of negative electron affinity (NEA) and photoeffect, the generated photoelectrons enter into vacuum and are collected by a copper ring anode. The resulting photocurrent is detected during the whole activation process and stopped when a maximum photocurrent is reached. By a comparison of differences in substrate material, chemical pre-cleaning, thermal heat treatment and activation parameters (e.g. caesium-flux), the photocurrent, quantum efficiency and the re-activation of the photocathode is studied. Additionally the GaN samples are examined by AFM, SEM and EDX.

O 46.5 Tue 13:30 P

Au silicide nanowires on Si(110) — •Stephan Appelfeller — MAX IV Laboratory, Lund University, Sweden

The Au-Si phase diagram is of simple eutectic nature without any stable bulk Au silicide. Nevertheless, metastable Au silicide structures have been observed at Au-Si interfaces and on surfaces. Especially, Au atomic chains on planar and vicinal Si(111) surfaces were investigated in recent years since they showed very enticing properties, e.g., self-doping by adatoms, 1D metallic behavior, or spin chain formation.

Here, Au induced nanostructures on the Si(110) surface are studied using LEED, STM and STS, and core-level and valence band PES. Due to the symmetry of the substrate, single-domain Au reconstructions form, e.g., a 2×5 superstructure known to show a 1D metallic band structure, which show interesting adatom structures. However, the focus of this study is on Au silicide nanowires. Their diffraction data are not characterized by well-defined spots, but by streaky features. While the dimensions of the nanowires are directly obtainable in STM, they only show a structurless appearance for widely varying tunneling conditions. Nevertheless, structural information is available by tuning the surface sensitivity in PES indicating silicide formation. Both PES and STS experiments show a finite density of states at the Fermi level for the nanowires suggesting (semi-)metallic behaviour.

O 47: Poster Session IV: Organic molecules on inorganic substrates: networks and overlayers

Time: Tuesday 13:30–15:30 Location: P

O 47.1 Tue 13:30 P

Alkali Doping Leads to Charge-Transfer Salt Formation in a Two-Dimensional Metal Organic Framework — •Billal Sohail[1], Phil Blowey[1,3], Giovanni Costantini[1], Phil Woodruff[2], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, UK — [2]Department of Physics, University of Warwick, UK — [3]Department of Chemistry, University of Leeds, UK

A detailed characterisation of structure and electronic properties at metal-organic interfaces is crucial for the design of novel molecular electronic devices such as organic photovoltaics (OPVs). In such devices, strong donors such as alkali atoms and acceptor molecules, such as TCNQ (7,7,8,8,-tetracyanoquinodimethane), are added to organic electronics devices to tune the charge interjection properties at the metal-organic interfaces. We present a joint computational and experimental study to examine the intricate coupling of geometry and electronic structure of TCNQ coadsorbed with potassium atoms on Ag(111), which forms a strongly interacting organic salt. Conversely, pure TCNQ on Ag(111) forms strongly surface-bound adlayers containing silver adatoms. Quantitative agreement between theory and experiment required the rescaling of dispersion coefficients to account for strong charge transfer. We further identify the energetic driving force for organic salt formation and discuss the intricate competition between donor, acceptor and metal substrate.

O 47.2 Tue 13:30 P

Metalation of 2HTCNPP on Ag(111) with Zn - evidence for the sitting atop complex at room temperature — •Jan Kuliga[1], Rodrigo Cezar de Campos Ferreira[2], Rajan Adhikari[1], Stephen Massicot[1], Michael Lepper[1], Helen Hölzel[3], Norbert Jux[3], Hubertus Marbach[1], Abner de Siervo[2], and Hans-Peter Steinrück[1] — [1]Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, Campinas, 13083-859, SP, Brazil — [3]Organische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nikolaus-Fiebiger-Str. 10, 91058 Erlangen, Germany

Using STM at RT, we study the adsorption of the free base 2HTCNPP on Ag(111), and its metalation to ZnTCNPP by post-deposition of Zn atoms. The goal is to obtain further insights in the metalation reaction and the influence of the cyanogroups on this reaction. The interaction of 2HTCNPP with post-deposited Zn leads to the formation of three different 2D ordered island types that coexist on the surface. All contain a new species with a bright appearance, which increases with the amount of post-deposited Zn. We attribute this to metastable SAT (*sitting atop*) complexes formed by Zn and the macrocycle, that is, an intermediate in the metalation reaction to ZnTCNPP, which occurs upon heating to 500 K. Interestingly, the activation barrier for the successive reaction of the SAT complex to the metalated ZnTCNPP species can also be overcome by a voltage pulse applied to the STM tip.

O 47.3 Tue 13:30 P

Self-assembled 2D-coordination-Kagome, quadratic and closed-packed-hexagonal lattices formed from cyano-functionalized benzo-porphyrins on Cu(111) — •Rajan Adhikari[1], Jan Kuliga[1], Michael Ruppel[2], Norbert Jux[2], Hubertus Marbach[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Lehrstuhl für Organische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nikolaus-Fiebiger-Str. 10, 91058 Erlangen, Germany

We investigated the adsorption of 2H-TCNPTBP molecules on the Cu(111) surface by scanning tunneling microscopy in UHV at RT. Three types of network structures are observed to coexist at low coverages. The first two Kagome lattice and the quadratic pattern are stabilized by cyano-Cu-cyano interactions with Cu adatoms; the other is a close-packed hexagonal network, which is stabilized by H-bonds and dipole-dipole interactions of oppositely oriented cyano-end groups. The hexagonal network has a molecular density on the surface, which is a factor of 2.3 larger than that of the Kagome lattice and the quadratic structure, which is attributed to the energy gain upon adsorbing a higher number of molecules. This finding leads us to suggest a coverage dependent competition between strong metal-organic coordination bonds at low coverage and weak hydrogen bonds plus dipole-dipole interactions at high coverage. The results show that a subtle interplay between adsorbate-substrate and adsorbate-adsorbate interactions can steer on-surface metal-organic coordination.

O 47.4 Tue 13:30 P

Functional 1D template to drive the assembly and alignment of polycyclic molecules — Valeria Chesnyak[1,2], •Marc G Cuxart[1], Knud Seufert[1], and Willi Auwärter[1] — [1]Physics Department E20, Technical University of Munich, Garching, Germany — [2]IOM-CNR Laboratorio TASC, Trieste, Italy

Two-dimensional (2D) materials grown on metal substrates constitute excellent platforms to engineer the properties of organic molecules and molecular arrays [1,2]. Moiré superstructures emerging from the combination of distinct symmetries and periodicities of metal surface and 2D layer can guide the self-assembly of molecules, while the nature of the 2D layers and their interfacial properties determine the electronic (de)coupling between molecules and metal.

Here we present the formation of a one-dimensional (1D) template resulting from the growth of a 3-fold symmetric hexagonal boron nitride (*h*BN) layer on a 4-fold symmetric Ir(100) surface. Its functionality is probed by subsequent deposition of pentacene molecules and comprehensive characterization by STM, STS, LEED and XPS measurements. This reveals a linear alignment of individual molecules, shows that the templating functionality originates due to a 1D modulation of the work function, and indicates an electronic decoupling of the molecules from the metal. This system represents a suitable 1D template that provides prospect for the study of arrays of aligned molecules and other low-dimensional nanostructures.

[1] W. Auwärter, Surf. Sci. Rep. 74(1) (2019)

[2] A. Kumar *et al.*, Nanotechnology 28(8) (2017)

O 47.5 Tue 13:30 P

On-surface assembly of supramolecular graphyne-like 2D materials: from hydrogen- and halogen-bonded to organo-metallic networks — Zechao Yang[1], Lukas Fromm[2], Tim Sander[1], Julian Gebhardt[2], Tobias Schaub[3], Himadri Soni[2], Binbin Da[1], Andreas Görling[2], Milan Kivala[3], and •Sabine Maier[1] — [1]Department of Physics, FAU Erlangen-Nürnberg — [2]Chair of Theoretical Chemistry, FAU Erlangen-Nürnberg — [3]Organisch-Chemisches Institut, Universität Heidelberg

The on-surface assembly of graphyne-based 2D materials are directive for the synthesis of the elusive carbon allotrope graphyne. Here, we demonstrate a supramolecular approach to fabricate highly-ordered monolayered hydrogen- and halogen-bonded [1] as well as organometallic graphyne-like 2D materials [2] from functionalized triethynyltriazine derivatives on Au(111) and Ag(111). The supramolecular graphynes have been investigated by STM in combination with DFT. We found that the halogen-bondend networks with N...Br-C(*sp*)-bonds lead to significantly stronger bonded networks compared to the hydrogen-bonded networks with N...H-C(*sp*)-bonds. For the organometallic networks with Ag-bis-acetylide bonds, large-area networks of several hundred nanometers with topological defects at domain boundaries are obtained. The thermodynamically controlled growth mechanism is explained through the direct observation of intermediates, which differ on Ag(111) and Au(111).

[1] Z. Yang et al. Angew. Chem. Int. Ed., 59, 24, 9549-9555 (2020)

[2] Z. Yang et al. ACS Nano, 14, 12, 16887-16896 (2020)

O 48: Poster Session IV: Surface dynamics II: Phase transitions and elementary processes

Time: Tuesday 13:30–15:30 Location: P

O 48.1 Tue 13:30 P

Ultrafast microscopy of charge density wave phase transitions using pump-probe imaging ellipsometry — •Sebastian Rohrmoser, Tobias Heinrich, Julius B. Peters, Murat Sivis, and Claus Ropers — IV. Physical Institute, Georg-August-University Göttingen, Germany

Null Ellipsometry has a long history of being a powerful, surface sensitive tool for measuring small changes in the refractive index of a sample with a high lateral resolution. These changes may stem from molecular adsorption [1], thin film growth [2] or phase transitions [3]. However, electronic phase transitions between charge density wave (CDW) phases occur on a much shorter timescale and are therefore inaccessible by conventional ellipsometry. Here, we present an all-optical, ultrafast approach to analyzing the phase transition between the nearly commensurate and incommensurate CDW phase in the transition-metal dichalcogenide (TMDC) 1T-TaS2. By combining a null ellipsometer with a pump probe setup, we are able to study the optically driven phase transition with a femtosecond temporal and micrometer lateral resolution. Using heat transfer simulations, we can disentangle the phase transition from the temperature contributions to give better insight in the surface-near dynamics. These results open the pathway for analyzing phase transitions on microstructured surfaces to investigate possible applications of TMDC's as optoelectronic components.

[1] H. Elwing, Elsevier 19, Issues 4-5, 397-406 (1998)

[2] J. Lee et al., Rev. of Scientific Instr. 69, 1800-1810 (1998)

[3] S. Faiss et at., J. Phys. Chem. B, 111, 50, 13979-13986 (2007)

O 48.2 Tue 13:30 P

Local impedance of Li-ion dynamics through complex interfaces in solid-state electrolytes — •Sina Stegmaier[1], Roland Schierholz[2], Ivan Povstugar[3], Juri Barthel[4], Christoph Scheurer[5], and Karsten Reuter[5] — [1]Theoretische Chemie, TU München — [2]IEK-9, Forschungszentrum Jülich — [3]ZEA-3, Forschungszentrum Jülich — [4]ERC, Forschungszentrum Jülich — [5]Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft

All-solid-state batteries (ASSB) present a next-generation technology, promising increased operation safety and lifetime as compared to state-of-the-art Li-ion cells. The practical performance of solid-state electrolytes (SSE) in ASSBs, though, is severely limited by poorly understood interfacial processes. Atomistic insight into the structure and transport processes at working SSE grain boundaries [1] is required to enable insight-driven progress.

Molecular Dynamics simulations employing a first-principles derived force field allow for a precise localization of Li ion impedance in the grain boundaries of the LATP SSE material. An explicit, experimentally guided atomistic model of such buried interfaces is established to capture nanoscale complexions and investigate their role in the observed Li ion impedance. Following this novel approach, we leverage experimental insights from transmission electron microscopy and atom probe tomography for computational modeling of detailed ion dynamics across realistic functional solid-solid interfaces.

[1] A. Mertens *et al.*, Solid State Ionics **309**, 180 (2017).

O 48.3 Tue 13:30 P

Solid state dewetting of thin bismuth films: a quantitative analysis of crystal truncation rods — •Constantin Wansorra and Wolfgang Donner — TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany

The dewetting of a thin film in the solid state represents a prominent destruction mechanism of thin films at elevated temperatures and is therefore researched with increasing importance. The activation of surface diffusion by temperature results in the transition of a flat thin film into separated islands, caused by a reduction of surface and interface energies [1].

While the major part of research about this topic is covered by microscopy methods, we apply x-ray diffraction and analyze crystal truncation rods quantitatively. With additional support from electron backscatter diffraction (EBSD) experiments, we determine unit cell coverage, lattice spacings and gradients thereof to reveal the impeding influence of a strain gradient present in thin bismuth films on solid state dewetting [2]. Furthermore, models of the step edge diffusion of bismuth were developed and the possible influence of a strain gradient on this model is discussed.

[1] Thompson, *Rev. Mater. Res.* 42 (2012): 399-434.

[2] Wansorra, et al., *Acta Mater.* 200 (2020): 455-462.

O 48.4 Tue 13:30 P

Computational insights into the buried interface of silica-coated Pt electrocatalysts — •Alexander Urban — Department of Chemical Engineering, Columbia University, New York, NY 10027, USA

Semipermeable membranes are attractive as protective coatings for metal electrocatalysts in harsh environments, but their impact on the catalytic properties has not been fully understood. Experimentally probing buried membrane-catalyst interfaces *in situ* is challenging because standard surface-science techniques cannot be directly used.

Here, we discuss insights from first-principles modeling of silica-coated platinum electrocatalysts. We introduce the concept of *interface Pourbaix diagrams* to investigate the interaction of silica membranes with the surface of platinum metal electrocatalysts under different electrochemical conditions. The structure, composition, and adhesion energy of the buried SiO_2/Pt interface depend on the pH value of the aqueous electrolyte and the electrode potential. Membrane-coating also affects the electronic structure of the catalyst surface, which has direct implications for the catalytic reactivity

Our analysis indicates that semipermeable membrane coatings are not passive bystanders but affect the properties of electrocatalysts, thereby offering as yet unexplored tuning knobs for the design of corrosion-stable electrocatalysts.

O 48.5 Tue 13:30 P

Interfacial phase transition in multiphase systems of environmental relevance — •Thorsten Bartels-Rausch, Xiangrui Kong, Fabrizio Orlando, Luca Artiglia, Astrid Waldner, Thomas Huthwelker, and Markus Ammann — Paul Scherrer Institut, Villigen PSI, Switzerland

Laboratory experiments are presented on the phase change at the surface of sodium chloride - water mixtures at temperatures between 259 K and 240 K. A high selectivity to the upper few nanometres of the frozen solution - air interface is achieved by using electron yield near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. We find that sodium chloride at the interface of frozen solutions, which mimic sea-salt deposits in snow, remain as supercooled liquid down to 240 K. Below this temperature, hydrohalite exclusively precipitates, anhydrous sodium chloride is not detected. In this work, we present the first NEXAFS spectrum of hydrohalite.

Experiments were performed at the PHOENIX beam line of the Swiss Light Source (SLS) at the Paul Scherrer Institute using the Near Ambient Pressure Photoemission (NAPP) set-up. In this work, we focus on the sample environment an in particular the ability to accurately monitor and set temperature and partial pressure of water. The importance of precise knowledge the trajectories, or history of, relative humidity and temperature that the sample have been exposed to are discussed.

O 49: Poster Session IV: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Tuesday 13:30–15:30 Location: P

O 49.1 Tue 13:30 P

Intrinsic excess charge on polar surfaces: charge density waves, polarons and bipolarons. — •Michele Reticcioli[1], Zhichang Wang[2,3], Michael Schmid[2], Ulrike Diebold[2], Martin Setvin[2,4], and Cesare Franchini[1,5] — [1]University of Vienna (Austria) — [2]Technische Universitaet Wien, Vienna (Austria) — [3]Xiamen University (China) — [4]Charles University, Prague (Czech Republic) — [5]University of Bologna (Italy)

Surfaces of oxide materials hosting excess charge show electronic and chemical properties completely different than the corresponding bulk crystal. Due to uncompensated broken bonds, bulk-terminated polar surfaces are known to intrinsically host excess charge, conventionally assumed to form a metallic two-dimensional electron gas. Here, by investigating the $KTaO_3(001)$ polar surface by density functional theory calculations and surface sensitive experiments, we show that excess charge is accommodated more effectively by in-homogeneous distributions, with different degree of charge localization. Our data provide evidence for the coexistence of standing density waves with long periodicity, eventually combined with minor structural distortions, and strongly localized charge in form of small electron polarons and bipolarons (quasi particles originating from the electron-phonon coupling, associated to sharp in-gap states and local distortions). These novel solutions emerging spontaneously on polar surfaces, dominate the electronic and chemical properties of the material, with large impact on the device functionalities (*e.g.*, the effects of bipolarons on the CO adsorption are discussed in a separate session by M. Setvin).

O 49.2 Tue 13:30 P

Efficient orbital imaging using ToF momentum microscopy with a femtosecond HHG light source — •Wiebke Bennecke[1], G. S. Matthijs Jansen[1], David Schmitt[1], Marius Keunecke[1], Christina Möller[1], Daniel Steil[1], Russell Luke[2], Sabine Steil[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität Göttingen

Orbital imaging (OI) is a powerful method to visualize molecular orbitals in molecule-metal interfaces using angle-resolved photoemission spectroscopy (ARPES) data and phase retrieval algorithms. Here, we will report on our advances in both of these aspects.

So far, successful orbital imaging has been based on the support constraint, for which the shape of the orbital must be known and which can be difficult to estimate. We have developed a sparsity-driven approach to phase retrieval, which uses only the number of non-zero pixels in the orbital and is independent of the actual orbital shape. This algorithm has been applied successfully to both simulated and experimental static ARPES data of different organic molecules.

Our photoemission setup consists of a femtosecond high harmonic generation beamline and a time-of-flight momentum microscope which yields the full momentum- and energy-resolved photoelectron spectrum in a single measurement. This enables us to image multiple molecular orbitals simultaneously. Combined with the sparsity-driven phase retrieval, this setup provides the ideal platform for orbital imaging with great potential to move towards time-resolved measurements.

O 49.3 Tue 13:30 P

Exploring polaron stability and defect structures in $Li_4Ti_5O_{12}$ (LTO) surface: A combined theoretical and experimental approach — •Yu-Te Chan[1], Matthias Kick[2], Cristina Grosu[2,3], Christoph Scheurer[1], and Harald Oberhofer[2] — [1]Fritz Haber Institute — [2]TU München — [3]IEK-9, FZ Jülich

Spinel $Li_4Ti_5O_{12}$ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) by its "zero strain" charge/discharge behavior. Pristine, white LTO possesses poor ionic and electronic conductivity. The latter can be increased by tailoring the sintering protocol to produce oxygen vacancies, resulting in a performant, blue LTO material. Polarons induced by oxygen vacancies have been proposed as one of the origins of the high conductivity. Detailed knowledge about polaron stability, distribution, and dynamics in LTO bulk and surface has been lacking, though. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can play a significant role in the experimentally observed improved conductivities. Moreover we are able to gauge polaronic charge mobility by explicitly calculating polaron hopping barriers.[1,2] In combination with positron lifetime spectroscopy (PALS) data and theoretical positron lifetimes we arrive at a rather complete picture of the bulk vs. surface defect chemistry in LTO particles and their resulting mixed ionic electronic conductivity. [1] M. Kick et al., J. Phys. Chem. Lett. 11 (2020), 2535 [2] M. Kick et al., J. Chem. Phys. 153 (2020), 144701

O 49.4 Tue 13:30 P

Switching current distribution in a STM Josephson junction on a Pb(111) surface with Mn adatoms — •Martina Trahms[1], David Wander[2], J. Rika Simon[1], Nils Bogdanoff[1], Olof Peters[1], Katharina Biel[1], Gaël Reecht[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, Institut Neél, 25 Avenue des Martyrs, 38042 Grenoble, France

Magnetic impurities on superconducting surfaces are expected to locally disturb the superconducting ground state. The critical current of a Josephson junction is a measure of the superconducting order parameter. We employ current-biased Josephson spectroscopy in a scanning tunneling microscope (STM) to measure the junction's switching current which is directly related to the critical current and marks the transition from Cooper-pair tunneling to quasi-particle tunneling. To investigate the activation processes of the switching events, we statistically analyse the switching of a Josephson junction formed between a Pb tip and a Pb adatom on a Pb(111) surface. By adding Mn adatoms to the Pb surface, we show a local reduction of the switching current and thereby a disturbance of the local order parameter due to the magnetic interaction. Additionally, we probe the switching current distribution in close proximity to the Mn atoms.

O 49.5 Tue 13:30 P

Electronic structure and charge density wave properties of $NdTe_3$ — •Henriette E. Lund[1], Alla Chikina[1], Marco Bianchi[1], Davide Curcio[1], Kirstine J. Dalgaard[2], Shiming Lei[3], Martin Bremholm[2], Leslie M. Schoop[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNano), Aarhus University, 8000 Aarhus C, Denmark — [2]Department of Chemistry and Interdisciplinary Nanoscience

Center, Aarhus University, Aarhus, Denmark — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

Rare-earth tritellurides (RTe$_3$) are a group of materials exhibiting high charge carrier mobility and, depending on the rare-earth element R, the materials host either one or two incommensurate charge density waves (CDWs). The electronic properties of RTe$_3$ have previously been investigated by quantum oscillations and angle-resolved photoemission spectroscopy (ARPES), but reconciling the Fermi surface elements observed by both techniques remains an unresolved issue which is complicated by the presence of the CDW and possible additional electronic phase transitions caused by strong magnetic fields.

The goal of the present study is to investigate whether the quantum oscillations reported for NdTe$_3$ can be reconciled with ARPES results. To this end, we refine a tight-binding model to include all relevant interactions and to describe the Fermi surface elements identified by both approaches.

O 49.6 Tue 13:30 P

Metallic Antiferromagnetic Spintronics: Mn2Au a case study — •Sunil Wilfred DSouza[1], Hans-Joachim Elmers[2], Satya Prakash Bommanaboyena[2], Vladimir N Strocov[3], Martin Jourdan[2], and Jan Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Univerzitní 8, CZ-306 14 Pilsen, Czech Republic — [2]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — [3]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen-PSI, Switzerland

The band structure of Mn2Au has been investigated by first-principles density-functional theory calculations based on the Green's function technique. The total density of state reveals contributions mainly from the Au5d and Mn3d states with rigid local moments on the Mn sites. The existence of significant out-of-plane magnetic anisotropy combined with the large strength of short range antiferromagnetic exchange interactions between Mn atoms located at two different Wyckoff positions results in the stabilization of the antiferromagnetic ground state. Two dimensional plots of constant energy surfaces in the Γ-X-Σ plane of the Brillouin zone exibits a 4-fold to 2-fold symmetry breaking as a function of the binding energy at 0.00 eV and 0.25 eV below the Fermi surface. We find that such a symmetry breaking in Mn2Au is arising due to the degeneration of the electronic bands in the presence of external magnetic field indicating a strong spin-orbit coupling interaction. Our results describes the tuning of the magnetic and electronic properties of Mn2Au for spintronic applications.

O 50: Poster Session IV: Tribology: Surfaces and nanostructures II

Time: Tuesday 13:30–15:30 Location: P

O 50.1 Tue 13:30 P

High-throughput ab-initio computation of potential energy surfaces at solid/solid interfaces — •Michael Wolloch[1], Gabriele Losi[2], Omar Chehaimi[3], Mauro Ferrario[2], and M. Clelia Righi[3] — [1]CMP, University of Vienna, Vienna, Austria — [2]FIM, UNIMORE, Modena, Italy — [3]DIFA, University of Bologna, Bologna, Italy

The potential energy surface (PES) characterizes the mechanical properties of an interface to a large extend. It allows the computation of properties like adhesion, shear strength, static friction, and dislocations, among others [1-4]. In the past we have shown that we are able to apply density functional theory to calculate highly accurate PESs for homogeneous interfaces formed by two equivalent surfaces [1,2].

However, the efficient computation of the PES for interfaces consisting of different crystals is exceedingly more complex. Challenges are mainly found in the creation of matching interface structures and the efficient sampling of the interface plane for the total energy calculation.

In this poster we present the algorithm we developed to efficiently and accurately compute the PES of nearly arbitrary interface structures based on the combination of high-symmetry points and interpolation with radial basis functions. A sketch of the full high-throughput workflow is also given.

Part of this work was supported by ERC grant 865633 (SLIDE); [1] Wolloch et al. Sci. Rep. 9, 17062 (2019), [2] Restuccia et al. Comput. Mater. Sci., 154:517-529 (2018), [3] Zilibotti et al. Langmuir 27, 6862 (2011), [4] Mryasov et al. Phys. Rev. B 58, 11927 (1998)

O 50.2 Tue 13:30 P

Nanoscale wear mechanisms on bulk and monolayer molybdenum disulphide — •Alper Özogul[1], Felix Cassin[1], Andrey Turchanin[2], and Enrico Gnecco[1] — [1]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany

We have compared the response of MoS2 in the form of multi- and mono-layers grown on a silica substrate under abrasive wear conditions on the nanoscale [1]. The samples have been scratched with a sharp diamond tip with normal loads in the uN range and scan velocities in the um/s range. The resulting surface structures are characterized by AFM and related to the lateral force acting on the probing tip during scratching. On the bulk crystal distinct stick-slip motion is observed and sequences of chip structures are built up all along the scratch line. Characteristic parameters of this motion, namely the lateral contact stiffness and slip period are found to depend highly on the applied normal force and scratching velocity decreasing exponentially or, respectively, increasing logarithmically with them. Monolayer MoS2 is cracked along the zigzag direction and completely folded over itself while scratching. The time evolution of the lateral force is overall irregular although periodic structures, which possibly originate from rippling of silica substrate, can be recognized. First attempts to analyze the energetics of the complex processes so observed are also discussed.

[1] A. Özogul et al., Phys. Rev. Materials 4 (2020) 033603

O 50.3 Tue 13:30 P

Advancing lubricant materials by first principles material design — •Maria Clelia Righi, Stefan Peeters, Gabriele Losi, Michele Cutini, Edoardo Marquis, and Jacopo Mescitelli — Department of Physics and Astronomy, University of Bologna, Italy

Friction and wear result in massive economic and environmental costs. Optimising lubricant materials is challenging because their performances are ruled by molecular-level processes that occur at the buried interface, which are extremely difficult to monitor by experiments. Simulations can play a decisive role here, in particular those based on quantum mechanics, which is essential to accurately describe the interactions between surfaces in contact and simulate reactions in conditions of enhanced reactivity as those imposed by the mechanical stresses applied. We applied ab initio molecular dynamics (MD), also linked to classical MD in a QM/MM scheme, to understand the functionality of lubricant additives and design new, environment-friendly materials to reduce friction. I will describe i) the in-operando formation of graphene from methane molecules ii) iron lubrication by MoS2, phosphorene and selenium-based compounds.

These results are part of the SLIDE project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme. (Grant agreement No. 865633)

O 51: Poster Session IV: Poster to Mini-Symposium: Free-standing functional molecular 2D materials II

Time: Tuesday 13:30–15:30 Location: P

O 51.1 Tue 13:30 P

Proton and Li-Ion Permeation through Graphene with Eight-Atom-Rings Defects — •Eoin Griffin — Department of Physics and Astronomy & National Graphene Institute, The University of Manchester, Manchester

Defect-free graphene is impermeable to gases and liquids but highly permeable to thermal protons. Atomic-scale defects such as vacancies, grain boundaries and Stone-Wales defects are predicted to enhance graphene's proton permeability and may even allow small ions through, whereas larger species such as gas molecules should remain blocked. These expectations have so far remained untested in experiment. Here we show that atomically thin carbon films with a high density of atomic-scale defects continue blocking all molecular transport, but their proton permeability becomes ~1,000 times higher than that of defect-free graphene. Lithium ions can also permeate through such disordered graphene. The enhanced proton and ion permeability is attributed to a high density of 8-carbon-atom rings. The latter pose approximately twice lower energy barriers for incoming protons compared to the 6-atom rings of graphene and a relatively low barrier of ~0.6 eV for Li ions. Our findings suggest that disordered graphene could be of interest as membranes and protective barriers in various Li-ion and hydrogen technologies.

O 51.2 Tue 13:30 P

From self-assembled monolayers to highly functional substrates for cryo-transmission electron microscopy (cryoTEM) — •Andreas Terfort — University of Frankfurt, Department of Chemistry, Institute of Inorganic and Analytical Chemistry, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany

Major problems for the cryo-transmission electron microscopy (cryoTEM) of proteins are the stabilization of the nm-thick water film and the preservation of the particles within the field of observation without denaturation. Here we report three approaches to produce TEM grids suitable for the task.

1) Covering the supporting carbon films with a hydrophilic film to suppresses adhesion of proteins. This could be extended by introduction of carbon nanotubes, covered by the same kind of molecular film to aid charge dissipation during observation.

2) The cross linking of a polyglycerol-SAM resulted in ultrathin hydrogel membranes, which help the distribution of the unaltered proteins. Self-perforation of the membranes during the deposition process opened windows for an unaltered observation by the electron beam.

3) The modification of the hydrogel membrane with selective binding sites, by formation on-top of carbon nano-membranes, which in turn are obtained by cross-linking of aromatic monolayers by electron-beam irradiation. The bi-layer system is then modified covalent attachment of a selective binding site, which allows for the selective extraction of the analyte from e.g. protein mixtures.

O 51.3 Tue 13:30 P

The impact of domain walls on broken symmetry states in suspended dually-gated bilayer graphene — •Fabian Rudolf Geisenhof[1], Felix Winterer[1], and R. Thomas Weitz[1,2,3,4] — [1]Physics of Nanosystems, Department of Physics, Ludwig-Maximilians-Universität München, Amalienstrasse 54, Munich 80799, Germany — [2]Center for Nanoscience (CeNS), Schellingstr. 4, Munich 80799, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, Munich 80799, Germany — [4]1st Physical Institute, Faculty of Physics, University of Göttingen, Friedrich-Hund-Platz 1, Göttingen 37077, Germany

Bilayer graphene exhibits a rich variety of broken symmetry states due to its various internal degrees of freedom and non-vanishing density of states at the charge neutrality point. Most important for their emergence is the cleanliness of the graphene, however, also the existence of structural and electronic domain walls in bilayer graphene can heavily affect the quantum transport. Here, we present an extensive study on several dual-gated freestanding bilayer graphene devices, giving evidence that domains within a device change its transport properties significantly. Besides suppressing the insulating spontaneous ground state, domain walls alter the electric field dependence of quantum Hall states.

O 51.4 Tue 13:30 P

Crystalline and amorphous graphene from aromatic precursors — •Katayoun Gharagozloo-Hubmann[1], Tibor Lehnert[2], Niclas Sven Mueller[1], Patryk Kusch[1], Ute Kaiser[2], and Stephanie Reich[1] — [1]Department of physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Ulm University, Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Albert Einstein Allee 11, Germany

We study the growth of graphene from (poly)aromatic precursors that react on a substrate while preserving their sp2 structure. These precursors require lower growth temperatures, produce specific types of defects and are self-limited to a monolayer. The growth temperature ($T<500^{\circ}$C) for p-Terphenyl is far below the typical growth temperature ($T>900^{\circ}$C) from the gaseous precursors. Spherical and chromatic aberration-corrected high-resolution transmission electron microscopy and Raman investigations verify the grown structures: Amorphous and crystalline domains are grown from p-Terphenyl molecules. Correlative near field microscopy and spectroscopy (tip enhanced Raman spectroscopy) confirm the co-exist of both domains. Confocal micro-Raman spectra depict the structure observed by high-resolution TEM as well. Larger precursor molecules Di(naphthylen)anthracene led to the growth of polycrystalline graphene. We present a synthesis route, which delivers monolayered 2-D-carbonmaterial with different degree of order. Amorphous, polycrystalline and also crystalline graphene can be produced by modifying the synthesis condition.

O 52: Poster Session IV: Poster to Mini-Symposium: Infrared nano-optics II

Time: Tuesday 13:30–15:30 Location: P

O 52.1 Tue 13:30 P

Local infrared properties of pure antimony in reduced dimension — •Max Dario Siebenkotten[1], Konstantin Wirth[1], Peter Kerres[1], Lisa Schäfer[1], Anne Frommelius[2], Ulrich Simon[2], Matthias Wuttig[1], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]Institute of Inorganic Chemistry, RWTH Aachen

Much progress has been made in recent years in advancing phase-change materials (PCMs) towards becoming a commercial random access memory (RAM) technology [1]. One major remaining issue is that the precise stoichiometry in the region of interest in PCM memory cells still eludes control, particularly when that region is repeatedly switched between its amorphous and crystalline state [2]. Pure antimony is a PCM and recently it has been shown that switching can be achieved when it is confined in reduced dimensions [2].

In this work the infrared optical properties of antimony thin films and nanoparticles are investigated by scattering type scanning near-field optical microscopy (s-SNOM). s-SNOM allows for the study down to the single nanoparticle level. The antimony nanoparticles show distinguishable infrared optical response, at least statistically, between their amorphous and crystalline phase. Confined antimony is found to show pronounced differences to bulk antimony in the infrared, as has been shown for the optical region on thin films before [3].

[1] Kooi, Wuttig, Adv. Mater. 32, 1908302 (2020)
[2] Salinga et al., Nat. Mater. 17, 681-685 (2018)
[3] Cheng et al., arXiv:2008.09007 (2020)

O 52.2 Tue 13:30 P

Vibrational Coupling to Epsilon-Near-Zero Waveguide Modes — •Thomas G Folland[1], Guanyu Lu[2], Autumn Bruncz[2,3], J. Ryan Nolen[2], Marko Tadjer[4], and Joshua D Caldwell[2] — [1]School of Physics and Astronomy, The University of Iowa, Iowa City, Iowa, USA, 52242 — [2]Department of Mechanical Engineering, Vanderbilt University, Nashville, Tennessee 37212, United States — [3]Department of Physics, University of Alabama in Huntsville, Huntsville, Alabama 35899, United States — [4]U.S. Naval Research Laboratory, Washington, D.C. 20375, United States

Epsilon near zero modes offer extreme field enhancement that can be utilized for developing enhanced sensing schemes. Here we fabricate high aspect ratio gratings (up to 24.8 um height with greater than 5 um pitch) of 4H-SiC, with resonant modes that couple to transverse magnetic and transverse electric incident fields. These correspond to metal insulator metal waveguide modes propagating downward into the substrate. The cavity formed by the finite length of the waveguide allows for strong absorption of incident infrared light (>80%) with Q factors in excess of 90, including an epsilon near zero waveguide mode with epsilon = 0.0574 + 0.008i. The localization of the electromagnetic fields within the gap between the grating teeth suggests an opportunity to realize a new platform for studying vibrational coupling in liquid environments, with potential opportunities for enhanced spectroscopies. We show that these modes are supported in anhydrous and aqueous environments and that high aspect ratio gratings coherently couple to the vibrational transition in the surrounding liquid.

O 52.3 Tue 13:30 P

Infrared-visible sum-frequency generation microscopy of phonon polariton resonances in SiC nanorods — •Sören Wasserroth[1], Richarda Niemann[1], Guanyu Lu[2], Martin Wolf[1], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Vanderbilt University, Nashville, USA

Sum-frequency generation (SFG) allows the study of surfaces and inversion broken systems. In a new approach we implemented a wide field sum-frequency microscope combining an infrared free electron laser (IR FEL) as excitation source with visible upconversion. The IR FEL provides a powerful, narrow band, and tunable light source [1]. By direct imaging of the SFG light with a microscope in a wide field scheme without scanning the sample or the focus [2], we achieve a spatial resolution well beyond the infrared diffraction limit.

We use SFG microscopy to image phonon polariton resonances in subdiffractional SiC nanorods. Full spectral mapping of the structures allows spectroscopic identification of the various polariton resonances($\sim 900\ \mathrm{cm}^{-1}$). Additionally, the high spatial resolution of the microscope resolves the modal structure of polaritons within each nanorod. We follow the evolution of the polariton modes by varying the geometrical parameters of the rods. As we demonstrate here, SFG microscopy presents itself as an excellent novel tool to comprehensively study infrared polaritons in subdiffractional nanostructures.

[1] Schöllkopf et al., Proc. of SPIE (2015)
[2] Kiessling et al., ACS Photonics (2019)

O 52.4 Tue 13:30 P

Broken Symmetry of Surface Phonon Polaritons in Monoclinic β-Gallium Oxide — •Nikolai Christian Passler[1], Tom Folland[2], Joseph Matson[3], Xiang Ni[4], Guangwei Hu[4], Martin Wolf[1], Andrea Alu[4], Mathias Schubert[5], Joshua Caldwell[3], and Alexander Paarmann[1] — [1]Fritz-Haber-Institute of the MPG — [2]University of Iowa — [3]Vanderbilt University, Nashville — [4]City University of New York — [5]University of Nebraska

Materials with low crystal symmetry exhibit correspondingly high optical anisotropy - a critical component for manipulating the propagation, polarization, and phase of light. Specifically, polar crystals with strong optical anisotropy in their surface plane can support in-plane hyperbolic surface phonon polaritons (h-SPhPs), featuring highly directional polariton propagation in the surface plane. So far, the investigated material systems for the observation of h-SPhPs comprise uniaxial and biaxial polar crystals with orthogonal optical axes. Yet, in low symmetry Bravais lattices such as monoclinic and triclinic systems a new class of surface polaritons featuring low symmetry are observed. Here we present Otto-type prism coupling experiments of monoclinic β-gallium oxide demonstrating the intrinsic symmetry breaking of the polariton propagation general to this material class. Furthermore, we present a theoretical approach for the description of polaritons in monoclinic crystals, revealing additional directional symmetry breaking in the polariton propagation patterns. Our results offer significant opportunities for topological photonics, as well as for exploring the anisotropic electronic properties for high power electronic devices.

O 52.5 Tue 13:30 P

Extracting the electronic properties of an oxide two-dimensional electron gas by scanning near-field optical microscopy — •Julian Barnett[1], Marc-André Rose[2], Georg Ulrich[3], Martin Lewin[1], Bernd Kästner[3], Regina Dittmann[2], Felix Gunkel[2], and Thomas Taubner[1] — [1]1. Physikalisches Institut (IA), RWTH Aachen — [2]Peter Grünberg Institut, Forschungszentrum Jülich — [3]Physikalisch-Technische Bundesanstalt Berlin

The interface between bulk insulators $SrTiO_3$ and $LaAlO_3$ (LAO/STO) gives rise to a confined and highly conductive two-dimensional electron gas (2DEG) [1], which poses unique analytical challenges, due to its buried and sensitive nature. Scanning near-field optical microscopy (SNOM) was shown to overcome these challenges by measuring the presence of the LAO/STO 2DEG using highly confined optical near-fields [2], opening the possibility for quantitative analysis by comparison to theoretical predictions. We now introduce spectroscopic s-SNOM measurements of the LAO/STO interface [3], showing that we are able to simultaneously disentangle the 2DEG's optical response and discriminate between thin film and substrate contributions. This is possible by using full spectroscopy, phonon-enhancement, and more accurate modeling based on the Finite Dipole Model, allowing us to set the starting point for a wave of similar spectroscopic investigations on other nanoscale layered interfaces.

[1] A. Ohtomo et al., Nature 427, 423 (2004).
[2] W. Luo et al., Nat. Commun. 10, 2774 (2019).
[3] J. Barnett et al., Adv. Funct. Mater. 30(46), 2004767 (2020).

O 53: Poster Session IV: Poster to Mini-Symposium: Frontiers of electronic-structure theory I

Time: Tuesday 13:30–15:30 Location: P

O 53.1 Tue 13:30 P

Broken adiabaticity induced by Lifshitz transition in MoS2 and WS2 single layers — •Dino Novko — Institute of Physics, Zagreb, Croatia

The breakdown of the adiabatic Born-Oppenheimer approximation is striking dynamical phenomenon, however, it occurs only in a handful of layered materials. Here I show that adiabaticity breaks down in doped single-layer transition metal dichalcogenides in a quite intriguing manner. Namely, significant nonadiabatic coupling, which acts on frequencies of the Raman-active modes, is prompted by a Lifshitz transition due to depopulation and population of multiple valence and conduction valleys, respectively. The outset of the latter event is shown to be dictated by the interplay of highly non-local electron-electron interaction and spin-orbit coupling. In addition, intense electron-hole pair scatterings due to electron-phonon coupling are inducing phonon linewidth modifications as a function of doping. Comprehending these intricate dynamical effects turns out to be a key for mastering characterization of electron doping in two-dimensional nano-devices by means of Raman spectroscopy.

O 53.2 Tue 13:30 P

***Ab initio* study of Heat Capacities and Energy Dispersions in Antiferromagnetic L_{10}-type MnPt** — •Kisung Kang, David G. Cahill, and André Schleife — Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

While antiferromagnetic L_{10}-type MnPt has been utilized as a pinning layer to apply exchange bias to a nearby ferromagnetic layer, the detailed physics of magnetism in MnPt is still under the veil. We investigate ground and excited states of antiferromagnetic L_{10}-type MnPt to understand their thermal and magnetic properties through the first-principles density functional theory. Ground-state calculations provide exchange coupling parameters, magnetocrystalline anisotropy, and metallic electronic band structure. Phonon and magnon dispersion curves are obtained from the finite difference method and linear spin-wave theory. At the Γ point a gap is expected in the magnon dispersion. Based on the energy dispersion results, we computed *ab initio* heat capacity for each elementary particle and the total heat capacity. The temperature dependence of the heat capacity at low temperatures originates mostly from phonons. There is almost no contribution from magnons because of the magnon gap and the low density of states in the low energy range. We use a Monte Carlo method based on the stochastic Landau-Lifshitz-Gilbert equation to compute the magnetic heat capacity in the high-temperature regime. Its peak provides the estimation of the Néel temperature, which shows good agreement with the measured value. *Illinois MRSEC NSF DMR-1720633

O 53.3 Tue 13:30 P

Surface Vibrations Enhance Intramolecular Hydrogen Tunneling in (some) Molecular Switches — •Yair Litman[1] and Mariana Rossi[1,2] — [1]MPI for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany. — [2]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Hydrogen atoms in supported molecular-switch architectures can tunnel close to room temperature, which calls for the inclusion of nuclear quantum effects (NQEs) in the calculation of reaction rates even at high temperatures. However, standard approaches to introduce NQEs that rely on standard parametrized dimensionality-reduced models quickly become inadequate in these environments. Here, a paradigmatic molecular switch based on porphycene molecules adsorbed on metallic surfaces is addressed by full-dimensional calculations that combine density-functional theory for the electrons with the semi-classical ring-polymer instanton approximation for the nuclei[1]. Our results show that the double intramolecular hydrogen transfer (DHT) rate can be enhanced by orders of magnitude due to surface fluctuations in the deep tunneling regime. In addition, the origin of an Arrhenius temperature-dependence of the rate below the tunneling crossover temperature, as well as the transition to different regimes, is elucidated. With these considerations, a simple model is proposed to rationalize the temperature dependence of porphycene DHT rates spanning diverse fcc [110] surfaces. [1] Y. Litman, M. Rossi. Phys. Rev. Lett. 125, 216001 (2020)

O 53.4 Tue 13:30 P

The effects of quantum nuclei in metal-molecular interfaces — •Karen Fidanyan[1,2] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Hydrogen-containing molecular adsorbates on platinum-group metals often give rise to situations where the bond strength to the surface and its interplay with nuclear quantum effects (NQE) can substantially change the dynamics and equilibrium of hydrogen dissociation. In this work, we assess by means of density functional theory and path integral molecular dynamics simulations, interfaces involving non-polar molecules (cyclohexane) and polar molecules (water). For the cyclohexane/Rh(111) interface, we show that the H-Rh bond weakens the C-H bond and that NQE are responsible for a geometric isotope effect that is reflected on work-function changes. We further study the importance of simulating nuclear fluctuations including anharmonic effects, concluding that although these contributions play a pronounced role on these interfaces, most of them are concentrated on "classical" degrees of freedom, resulting in minor anharmonic quantum contributions in isotope effects [1]. For water on Pd(111) we investigate hydrogen dissociation under different potential voltage biases and analyze the impact of NQE within a quasi-harmonic approximation throughout the dissociation path.

[1] K. Fidanyan, I. Hamada and M. Rossi, arXiv:2010.03970 (2020)

O 53.5 Tue 13:30 P

Tunnelling with Non-Adiabatic Effects: H-Diffusion in Pd — •Eszter Sarolta Pós[1], Yair Litman[1], and Mariana Rossi[1,2] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Hydrogen diffusion in metals is a fundamental process in areas like energy storage devices and hydrogen separation membranes. However, the accurate theoretical description of it is challenging because (1) nuclear quantum effects (NQEs) such as nuclear tunnelling play an important role even at room temperature due to the light mass of the hydrogen atom; (2) the excitation and relaxation of electron-hole pairs around the Fermi level give rise to non-adiabatic effects (NAEs) that alter the system dynamics. In this work, we present a novel approach that combines the ring polymer instanton formalism [1] with *ab initio* electronic friction [2,3], allowing us to include both NQEs and NAEs in the rate-calculation of H-diffusion between interstitial sites of Pd. Our approach has been implemented into the i-PI code [4] including the spatial dependence of the electronic friction tensor which facilitates the study of nuclear tunnelling on metallic systems with unprecedented realistic first-principles simulations.

[1] J. O. Richardson, *JCP* **144**, 114106 (2016). [2] M. Head-Gordon, J. C. Tully, *JCP* **96**, 3939 (1992). [3] R. J. Maurer, M. Askerka, V. S. Batista, J. C. Tully, *PRB* **94**, 115432 (2016). [4] V. Kapil, *et al.*, *CPC* **236**, 214 (2019).

O 53.6 Tue 13:30 P

Nonadiabatic renormalization of electron-phonon interaction in graphene-based materials — •Nina Girotto and Dino Novko — Institute of Physics, Zagreb, Croatia

Some of the most prominent features of two-dimensional (2D) materials issue from electron-phonon coupling (EPC) and are easily tailored by strain and doping. Phonon-mediated superconductivity is expected in a variety of 2D materials, and because the transition temperature within the Bardeen-Cooper-Schrieffer (BCS) theory increases with increasing EPC, tailoring EPC provides a recipe for a more feasible realization of superconductors. Here, we present density-functional-theory (DFT) calculations of EPC properties of doped 2D systems, specifically highly-doped graphene and hole-doped graphane. Doping equalizes the energy scales of electron transitions and phonon frequencies, but using the adiabatic Born-Oppenheimer approximation, DFT assumes nuclear and electronic motion can be separated. We show that the mentioned approximation is not applicable on studied systems, since the adiabatically obtained phonon spectrum is at significant variance with the one containing nonadiabatic corrections. Nonadiabatic renormalization greatly modifies the EPC strength, which in turn alters the superconducting transition temperature prediction, rendering its calculation more reliable. The importance of including dynamical corrections is indisputable and care should be taken when neglecting nonadiabatic effects as they have a huge impact not only on the magnitude of the EPC strength and the transition temperature, but also on the qualitative understanding of the system in question.

O 53.7 Tue 13:30 P

Polaron and multi-charged states in extended p-conjugated systems: the role of electron correlation. — •Daniele Fazzi[1], Klaus Meerholz[1], and Fabrizia Negri[2] — [1]Institut für Physikalische Chemie, Department Chemie, Universität zu Köln, Greinstr. 4-6. D - 50939 Köln — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi, 2, 40126 Bologna, Italy

Polarons play a crucial role in governing charge and energy transfer in organic functional materials. An accurate description of their electronic structure and electron-phonon couplings is mandatory to assess their response and transport properties.

We report a comprehensive investigation of polarons in ladder-type conjugated polymers [1-3]. Polarons show a polyradicaloid character, as revealed by combining broken-symmetry density functional theory, fragment orbital density analysis, and multireference methods [3]. Electron and hole polarons relaxed on localised states, however showing different structural and electron-phonon coupling properties. Polarons, bipolarons and multi-charged states reveal a complex scenario of quasi-degenerate states, each featuring various spin multiplicity and response properties.

Our study provides insights towards the understanding of doping processes and insulator-to-conductor transitions in ladder-type polymers considered for energy-saving applications.

[1] Wang, S., et al., Adv. Mater. 2018, 30, 1801898. [2] Fazzi D., et al., J. Mat. Chem. C., 2019, 7, 12876-12885. [3] Fazzi D., et al., Adv. Electron. Materials, 2020, 2000786.

O 54: Poster Session IV: Poster to Mini-Symposium: Ultrafast surface dynamics at the space-time limit II

Time: Tuesday 13:30–15:30 Location: P

O 54.1 Tue 13:30 P

Ultrafast nano-imaging of the order parameter in a structural phase transition — •Till Domröse[1], Thomas Danz[1], and Claus Ropers[1,2] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Ultrafast transmission electron microscopy has proven a versatile tool to investigate out-of-equilibrium dynamics in heterogeneous nanostructures on their intrinsic time and length scales [1]. Here, we report on ultrafast dark-field domain mapping in our Göttingen UTEM [2] as a means to image a structural phase transition between two charge density wave (CDW) phases in the correlated material 1T-TaS$_2$ [3]. Selective contrast enhancement enabled by a tailored dark-field aperture array provides real-space sensitivity to the local CDW amplitude with unprecedented simultaneous femtosecond temporal and nanometer spatial resolution. After optical excitation, we observe a global quench of the CDW amplitude, followed by formation, condensation and subsequent spatiotemporal relaxation of domain patterns, ranging from the femtosecond into the nanosecond regime. Accompanying Ginzburg-Landau simulations reproduce key experimental observations, elucidating the order parameter dynamics specifically near domain walls.
[1] A. H. Zewail, Science 328, 187 (2010).
[2] A. Feist et al., Ultramicroscopy 176, 63 (2017).
[3] T. Danz et al., accepted for publication in Science, arXiv:2007.07574

O 54.2 Tue 13:30 P

Determining the orientation of transition dipoles of direct and indirect optical transitions in metals — •Tobias Eul, Michael Hartelt, Eva Prinz, Benjamin Frisch, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center Optimas, University of Kaiserslautern

Understanding the hot electron dynamics and their energy and momentum dissipation mechanisms paves the way to enhance the performance of next-generation electronic and spintronic devices. This understanding can be obtained by the combination of time-resolved photoemission spectroscopy and the recently developed momentum microscopy. However, to properly determine the electron dynamics with these techniques, it is crucial to clearly identify the orbital character of the initial, intermediate and final states that lead to the emission of a photoelectron.

Here, we propose a theoretical framework to predict the nature of the involved electronic states from the cross-correlation signal of a monochromatic 2PPE experiment. Our theory is based on the density matrix formalism, showing a dependence of the ratio between minimum and maximum of the cross-correlation trace and the orientation of the transition dipole with respect to the polarization of the incident light. Our calculations are then compared to momentum microscopy results for direct and indirect optical transitions in Ag(110), using both a phase-averaged and a phase-resolved pump-probe setup with a photon energy of 3.1eV. The comparison shows that the transition dipoles for direct transitions align along the ΓL-direction of the crystal.

O 54.3 Tue 13:30 P

Ultrafast hot electron relaxation in a metallic THz-STM junction — •Natalia Martín Sabanés[1,2], Faruk Krecinic[1], Fabian Schulz[1], Chenfang Lin[1,3], Takashi Kumagai[1,4], Martin Wolf[1], and Melanie Müller[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]IMDEA nanoscience, Madrid, Spain — [3]College of Materials Science and Engineering, Hunan University, Hunan, China — [4]Center for Mesoscopic Sciences, Institute for Molecular Science, Okazaki, Japan

We investigate the ultrafast dynamics of photoexcited hot electrons in a metallic STM junction through modulation of the junction barrier with an ultrabroadband THz field. The ability for phase-resolved quantitative sampling of the THz bias induced in the junction allows to probe the relaxation of hot carriers in the STM on THz sub-cycle time scales. Exact knowledge of the THz voltage is obtained via THz-field-induced modulation of instantaneous photocurrents excited with 8 fs near-infrared (NIR) laser pulses [1-3]. In the presence of a non-instantaneous response, distortions of the original THz waveform occur, from which the ultrafast photocurrent decay can be extracted. Applying a 1D-model for the transmission of thermalized hot electrons to reproduce the distorted THz waveforms, we obtain quantitative information about the electronic temperature in the tip and its ultrafast decay. Our approach provides a new route for non-resonant probing of charge carrier dynamics in photoexcited STM on time scales much shorter than a single THz cycle. [1] L. Wimmer et al., Nat. Phys., 10, 432-436, 2014. [2] M. Müller et al., ACS Photonics, 7(8), 2046-2055, 2020. [3] S. Yoshida et al., ACS Photonics 6, 1356-1364, 2019.

O 54.4 Tue 13:30 P

3-in-1 time-resolved ToF momentum microscopy using FEL and HHG radiation — •N. Wind[1,2], D. Kutnyakhov[2], M. Heber[2], F. Pressacco[2], L. Wenthaus[2], G. Mercurio[3], H. Meyer[1], S. Gieschen[1], K. Bühlmann[4], D. Curcio[5], K. Volckaert[5], S. Däster[4], R. Gort[3], M. Bianchi[5], C. Sanders[5], J. Miwa[5], S. Ulstrup[5], A. Oelsner[6], C. Tusche[7,8], Y.J. Chen[7,8], S.Y. Agustsson[9], D. Vasilyev[9], K. Medjanik[9], G. Brenner[2], S. Dziarzhytski[2], H. Redlin[2], J. Hauer[10], P. Xian[10], M. Dendzik[10], S. Dong[10], L. Rettig[10], F. Diekmann[11], H.J. Elmers[9], J. Demsar[9], P. Hofmann[5], R. Ernstorfer[10],

Y. Acremann[4], M. Martins[1], G. Schönhense[9], W. Wurth[1,2], and K. Rossnagel[2,11] — [1]IEXP, Univ. Hamburg — [2]DESY Hamburg — [3]EuXFEL Schenefeld — [4]ETH Zürich — [5]Univ. Aarhus — [6]Surface Concept GmbH — [7]FZ Jülich GmbH — [8]Univ. Duisburg-Essen — [9]Univ. Mainz — [10]FHI Berlin — [11]CAU Kiel

Time-resolved PES with ultrafast pump and probe pulses is an emerging technique with wide application potential. Combining valence-band and core-level spectroscopy with photoelectron diffraction in a single, ultra-efficient photoelectron detection scheme for electronic, chemical and structural analysis requires soft X-ray pulses of few 10 fs duration at some 10 meV spectral resolution. This is feasible at high-repetition-rate FELs. We present an optimized, versatile setup for the use at FLASH as well as a laboratory HHG source that combines short-pulsed XUV/soft X-ray capabilities with a multidimensional recording scheme for ultrafast photoemission studies of quantum materials.

O 55: Poster Session IV: Poster to Mini-Symposium: Machine learning applications in surface science II

Time: Tuesday 13:30–15:30 Location: P

O 55.1 Tue 13:30 P

Gaussian Approximation Potentials for Surface Catalysis — •Sina Stocker[1,2], Gábor Csányi[3], Karsten Reuter[1,2], and Johannes T. Margraf[1,2] — [1]Technische Universität München, Germany — [2]Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany — [3]University of Cambridge, United Kingdom

Predictive-quality first-principles based microkinetic models are increasingly used to analyze (and subsequently optimize) reaction mechanisms in heterogeneous catalysis. In full rigor, such models require the knowledge of all possible elementary reaction steps and their corresponding reaction barriers. Unfortunately, for complex catalytic processes (such as the generation of ethanol from syngas) the number of possible steps is so large that an exhaustive first-principles calculation of all barriers becomes prohibitively expensive.

To overcome this limitation, we develop a machine learned (ML) interatomic potential to model syngas conversion on Rhodium. This ML potential can be used to determine adsorption energies, geometries and reaction barriers for a large number of adsorbates at a fraction of the computational cost of the underlying first-principles method. Specifically, we use the Gaussian Approximation Potential (GAP) framework and explore iterative training and active learning to minimize the number of reference calculations. Here, the particular challenge lies in selecting representative configurations that adequately characterize the reactivity of molecules on a surface. Different training approaches will be compared.

O 55.2 Tue 13:30 P

Materials genes of heterogeneous catalysis from clean experiments and AI — •Lucas Foppa[1,2], Luca M. Ghiringhelli[1,2], Frank Rosowski[3], Robert Schloegl[1,4], Annette Trunschke[1], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Humboldt-Universität zu Berlin — [3]BASF SE — [4]Max-Planck-Institut für Chemische Energiekonversion

Heterogeneous catalysis is an example of a complex materials function, governed by an intricate interplay of several processes, e.g. the dynamic re-structuring of the catalyst material at reaction conditions and different surface chemical reactions. Modelling the full catalytic progression via first-principles statistical mechanics is impractical, if not impossible. Instead, we show here how an artificial-intelligence approach can be applied, even to an extremely small number of materials, to model catalysis and determine the key descriptive parameters (materials genes) reflecting the processes that trigger, facilitate, or hinder the catalyst performance. We start from a consistent, unparalleled experimental set of "clean data", containing nine vanadium-based oxidation catalysts which were carefully synthesized, fully characterized, and tested according to standardized protocols.[1] By applying the symbolic-regression SISSO approach,[2,3] we identify correlations between the few most relevant materials properties and their reactivity. This approach highlights the underlying physico-chemical processes, and accelerates catalyst design. [1] A. Trunschke, et al., Top. Catal. 63, 1683 (2020). [2] R. Ouyang et al., Phys. Rev. Mater. 2, 083802 (2018). [3] R. Ouyang et al., J. Phys. Mater. 2, 024002 (2019).

O 55.3 Tue 13:30 P

Artificial Intelligence controlls Nanocars across a racetrack — •Bernhard R. Ramsauer[1], Oliver T. Hofmann[1], Grant J. Simpson[2], and Leonhard Grill[2] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Chemistry, University of Graz, Austria

At the world's first nanocar race at CEMES-CNRS, in France, participants had to direct a nanocar across a "racetrack" [1]. In order to control their nanocar, they had to move it using the tip of a STM, albeit without making direct contact with the nanocar.

The physics that govern the molecule's movement and rotation is complex and involves the interaction between the molecule and the tip as well as the molecule and the substrate [2]. Thus, it requires some expertise from humans to manoeuvre the nanocar and predict the outcome of a performed action.

Here, we show how an artificial intelligence (AI) based on reinforcement learning (RL) can be implemented to manipulate single molecules. The AI is implemented in the form of an off-policy RL algorithm, known as the Q-Learning. In a prime example, the AI manoeuvres the nanocar with a success rate of 89%.

Our results can be the basis for more sophisticated techniques of molecular manipulations which allow identification and relocation of single molecules at will, building the basis for future bottom-up constructions of nanotechnology.

[1] Nature Rev. Mater. 2, 17040 (2017)

[2] Nature Nanotech. 12, 604 (2017)

O 55.4 Tue 13:30 P

Configurational polaron energies using machine learning — •Viktor Birschitzky, Michele Reticcioli, and Cesare Franchini — University of Vienna, Faculty of Physics

Polarons are quasiparticles formed by the coupling of excess charge carriers with the phonon field. Polarons form preferentially at surfaces and have a wide range of effects on the chemical and physical properties of the hosting material.[1] First principles calculations of polarons conformational energies typically require large supercells and long molecular dynamics (MD) simulations, making the modeling of multipolaron system within reasonable timescales very challenging. Here, we propose a supervised machine learning scheme based on kernel-regression to solve this problem by learning single polaron energies for the prototypical oxygen-defective rutile $TiO_{2-x}(110)$ surface, where each oxygen vacancy provides two excess electrons. To achieve accurate predictions on an ab initio MD database of polaronic energies[2] a descriptor has been developed, which embodies the interactions between polarons with defects and other localized charge carriers. Our results show that the proposed ML method is able to expand the DFT database with energetically more favorable polaron configurations – improving the convex hull construction – and that generalization at arbitrary polaron concentration and defect types is possible.

[1] C. Franchini et al., Polarons in Material, Nature Review Materials, (2021)

[2] M. Reticcioli et al., Formation and dynamics of small polarons on the rutile TiO_2 surface, Physical Review B, (2018)

O 55.5 Tue 13:30 P

Image-to-graph translation of atomic force microscopy images using graph neural networks — •Niko Oinonen[1], Fedor Urtev[1,2], Alexander Ilin[2], Juho Kannala[2], and Adam Foster[1,3,4] — [1]Department of Applied Physics, Aalto University, Finland — [2]Department of Computer Science, Aalto University, Finland — [3]Graduate School Materials Science in Mainz, Germany — [4]WPI Nano Life Science Institute, Kanazawa University, Japan

The atomic force microscope (AFM) is an important tool in nanoscale science for imaging surfaces and molecules on surfaces. State-of-the-art AFM setups operating in vacuum at low temperatures are able to resolve features on the scale of individual atoms in molecules. However, the process of interpreting the resulting AFM images in some cases can be very challenging even for highly trained experts in the field. We are working towards greater interpretability and greater automation of the processing of AFM images using machine learning methods [1]. We are currently exploring the possibility of directly predicting the atomic structure of the sample as a graph using graph neural networks (GNN) [2]. We propose a GNN model which, conditioned on an AFM image, iteratively constructs the graph of the sample molecule present in the AFM image, following similar work by Li et al. [3]. This is still a work-in-progress, but our initial results are showing promise.

[1] B. Alldritt et al. Sci. Adv. 6(9), eaay6913, 2020.

[2] P. W. Battaglia et al. arXiv:1806.01261.

[3] Y. Li et al. arXiv:1803.03324.

O 55.6 Tue 13:30 P

Inverse problem to AFM imaging with iterative correction loop — •Prokop Hapala[1], Lauri Kurki[2], Niko Oinonen[2], Fedor Urtev[2], Filippo Federici Canova[2], Juho Kannala[2], and Adam S. Foster[2] — [1]Department of Condensed Matter Theory, FZÚ AV ČR, v.v.i. — [2]Department of Applied Physics, Aalto University Espoo, Finland

In the last year we pioneered machine-learning methods for reconstruction of molecular structure from high-resolution AFM images of non-planar organic molecules [1], which opens the way to broader application of this experimental technique for single-molecule analysis [2] e.g. in the pharmaceutical industry. Nevertheless, the robustness of one-shot scheme relying on general-purpose convolutional neural networks (CNN) seems limited as it discards physical insight. We attempt to improve our method by integrating the CNN module together with an image simulation module and interatomic force-field into an iterative feedback loop, which gradually improves the match between reference and simulated image. Such a scheme, with a machine-learned model providing educated trial-move within a global optimization algorithm, can be possibly useful also for solving other difficult inverse problems. [1] Alldritt B., et al., Sci. Adv., vol. 6, no. 9, p. Eaay6913. (2020) [2] Schuler, B., et.al. JACS, 137(31), 9870-9876. (2015)

O 55.7 Tue 13:30 P

Single-Atom Alloy Catalysts Designed by First-Principles Calculations and Artificial Intelligence — Zhong-Kang Han[1], Debalaya Sarker[1], Runhai Ouyang[2], Aliaksei Mazheika[3], Yi Gao[4], and •Sergey V. Levchenko[1] — [1]Skoltech, Moscow, RU — [2]Shanghai University, CN — [3]Technische Universitaet Berlin, DE — [4]Shanghai Advanced Research Institute, Chinese Academy of Sciences, CN

Single-atom metal alloy catalysts (SAACs) have recently become a very active new frontier in catalysis research. However, discovery of new SAACs is hindered by the lack of fast yet reliable prediction of the catalytic properties of the sheer number of candidate materials. In this work, we address this problem by applying a compressed-sensing data-analytics approach parameterized with density-functional inputs. Besides consistently predicting high efficiency of the experimentally studied SAACs, we identify more than two hundred yet unreported promising candidates. Some of these new candidates are predicted to exhibit even higher stability and efficiency than the reported ones. Our study demonstrates the importance of breaking linear relationships to avoid bias in catalysis design, as well as provides a recipe for selecting best candidate materials from hundreds of thousands of transition-metal SAACs for various applications. In addition, we demosntrate how the data-mining approach subgroup discovery can be used to obtain a qualitative understanding of complex symbolic regression models.

O 55.8 Tue 13:30 P

Automated Tip Functionalization and Image interpretation with Machine Learning in Atomic Force Microscopy — Benjamin Alldritt[1], Chen Xu[1], Prokop Hapala[2], Ondrej Krejci[1], •Fedor Urtev[1], Filippo Federici Canova[1,3], Juho Kannala[1], Peter Liljeroth[1], and Adam Foster[1,4,5] — [1]Aalto University, Espoo, Finland — [2]Czech Academy of Sciences, Prague, Czechia — [3]Nanolayers Research Computing Ltd., London, UK — [4]Graduate School Materials Science in Mainz, Germany — [5]WPI Nano Life Science Institute, Kanazawa, Japan

Atomic force microscopy (AFM) is ubiquitous nanoscale characterisation technique to measure a 3D map of surface roughness at atomic resolutions [1]. AFM data interpretation and quantitative analysis for complex mixtures of molecules and bulky 3D molecules can be difficult [2], due to the complex nature of contrast in AFM images, and need significant acceleration and automation to make AFM technique available to a wide range of laboratories and clinics. Here, we introduce a machine learning (ML) approach both for the preparation of AFM experiments and for data interpretation in AFM. For the first objective our method involves a convolutional neural network (CNN) that has been trained to analyse the quality of a CO-terminated tip. For the interpretation of AFM images, we introduce ML image descriptors characterising the molecular configuration, allowing us to predict the molecular structure directly. [1] L. Gross et al., Science, vol. 325, no. 5944, (2009). [2] O. M. Gordon and P. J. Moriarty, Mach. Learn. Sci. Technol., vol. 1, no. 2, (2020).

O 56: Key Note IV

Time: Tuesday 15:30–16:00 Location: R1

Plenary Talk O 56.1 Tue 15:30 R1

Meta-stable intermediates of OER catalysis: connecting their time-resolved spectra to thermodynamic descriptors — •Tanja Cuk, Ilya Vinogradov, Aritra Mandal, Suryansh Singh, and Hanna Lyle — University of Colorado, Boulder, Boulder USA

The intermediate steps of catalytic mechanisms are challenging to identify experimentally, but are critical to understanding the speed, stability, and selectivity of product evolution. In the laboratory, we employ photo-triggered vibrational and electronic spectroscopy to time-resolve the catalytic cycle at a surface, identifying meta-stable intermediates and critical transition states which connect one to another. The focus is on the highly selective oxygen evolution reaction (OER) at the semiconductor (SrTiO3)-aqueous interface, triggered by an ultrafast light pulse in an electrochemical cell. A short summary of past work will be given, which resolved the structure and picosecond formation kinetics of the first meta-stable electron-transfer intermediates (Ti-OH*) of OER. The main topic will concern the recent results that connect the time-resolved kinetics to a thermodynamic free energy difference, (Delta G (OH*)), often used to differentiate the activity of materials. In particular, a Langmuir isotherm as a function of electrolyte pH extracts an effective equilibrium constant for this reaction step using a principal component analysis of the optical spectra. In so doing, reaction conditions that shift equilibria of separable catalytic steps become an important, independent axis to the time & energy axes of the spectroscopy.

O 57: Key Note V

Time: Wednesday 10:00–10:30 Location: R1

Plenary Talk O 57.1 Wed 10:00 R1

Tunneling spectroscopy of magnetic adatoms on superconductors — •Katharina J. Franke — Freie Universität Berlin, Berlin, Germany

Magnetic atoms on superconductors induce an exchange coupling, which leads to states within the superconducting energy gap. We probe these so-called Yu-Shiba-Rusinov (YSR) states of individual adatoms on a Pb surface by scanning tunneling spectroscopy [1]. When the adatoms are brought into sufficiently close proximity, the YSR states hybridize [2] and may lead to the formation of topological states in extended adatom chains [3].

Single-electron tunneling through YSR states requires relaxation of the excited state. At strong tunnel coupling, thermal relaxation is not sufficiently fast and resonant Andreev processes become the dominant tunneling process. We obtain direct evidence of these two transport regimes by inserting GHz radiation into the STM junction and analyzing the photon-assisted tunneling maps [4,5].

[1] M. Ruby, et al., Phys. Rev. Lett. 117, 186801 (2016).
[2] M. Ruby, et al., Phys. Rev. Lett. 120, 156803 (2018).
[3] S. Nadj-Perge, et al., Science 346, 602 (2014).
[4] O. Peters, et al., Nature Phys. 16, 1222 (2020).
[5] S. Acero Gonzalez, et al., Phys. Rev. B 102, 045413 (2020).

O 58: Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces II

Time: Wednesday 10:30–12:30 Location: R1

Invited Talk O 58.1 Wed 10:30 R1

Simulating interfacial water with neural network potentials — •Christoph Dellago[1], Oliver Wohlfahrt[1], and Marcello Sega[2] — [1]University of Vienna, Faculty of Physics, Vienna, Austria — [2]Forschungszentrum Jülich, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Nürnberg, Germany

The strong, directed network of hydrogen bonds of water lies at the heart of its rich phase diagram and numerous anomalous properties and is responsible for the peculiar structure of its liquid/vapor interface. Detailed insights into the molecular structure and dynamics of bulk and interfacial water have been gleaned from first principles simulations, which provide an unbiased description of water at the atomic level and yield information on the underlying molecular forces. However, the computational cost of such simulations is still daunting, particularly for interfacial systems that require relatively large systems sizes as they suffer from finite size effects more than bulk systems. Recently, artificial neural networks have been proposed to overcome these limitations, yielding the accuracy of first principles simulations at a fraction of their computational cost. In this talk, I will report on the structural and thermodynamic properties of the water/vapor interface obtained using a neural network potential trained for bulk and interfacial water. In particular, I will discuss the liquid/vapor coexistence curve and its size dependence as well as the structure of the interface in terms of density profiles and molecular orientations.

O 58.2 Wed 11:00 R1

Modelling solvation at dielectric interfaces — •Jakob Filser[1], Markus Sinstein[1], Konstantin Jakob[1], Karsten Reuter[2], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

Modelling solvation effects is a complex challenge in molecular simulations. The difficulty lies in unravelling classical electrostatic, quantum mechanical, nuclear, entropic and other free energy contributions in liquid systems. In reality these contributions interact with each other and a simplistic separation is not possible. Modelling this full complexity by accounting for all relevant degrees of freedom explicitly is often computationally intractable. Therefore, approximations are necessary. The family of implicit solvation models treats only the solute on an explicit, atomistic level and summarizes the degrees of freedom of all or all but few solvent molecules in a structurless dielectric medium.

The presence of dielectric interfaces in the system further complicates things. Different models which predict similar energies in bulk solvent can predict substantially different behaviour at a dielectric interface. We systematically construct a method which can implicitly model dielectric interfaces. It describes a solvent only by three parameters, the first of which is experimentally known: The relative permittivity, a dimensionless interaction distance and an effective interfacial tension with the explicit system. First predictions are compared to experimental results as well as predictions from explicit solvent models for an octanoic acid surfactant on water droplets.

Invited Talk O 58.3 Wed 11:20 R1

Surface activity of hydroxide and the hydrated proton — •Ellen Backus — Institut für Physikalische Chemie, Wien, Österreich — Max-Planck-Institute für Polymerforschung, Mainz, Deutschland

The behavior of hydroxide and hydrated protons, the auto-ionization products of water, at surfaces is important for a wide range of applications and disciplines. Despite of its importance, the likelihood of surface adsorption of either of those two ions is controversially discussed in literature. By determining the onset concentration of surface adsorption at the water-air surface of hydrated protons and hydroxide ions, we can determine the relative surface-activity. To this order, we perform surface-sensitive vibrational sum frequency generation spectroscopy - basically providing the vibrational spectrum of just the interfacial layer - on the O-H stretch vibration. We will discuss how spectral changes in the response from hydrogen bonded molecules can be related to the surface adsorption of the hydrated ions. Moreover, changes in the spectral signature of the so-called free OH molecule sticking out in the air are used to determine the adsorption free energy of the proton.

O 58.4 Wed 11:50 R1

Vibrational Dynamics of Interfacial Ice Ih and Liquid Water — •Prerna Sudera[1], Jenée D. Cyran[2], Malte Deiseroth[1], Marc-Jan van Zadel[1], Mischa Bonn[1], and Ellen Backus[3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Baylor University, Waco, Texas, USA — [3]University of Vienna, Vienna, Austria

The dynamics of vibrational energy relaxation and dissipation at surfaces of aqueous systems is relevant for chemical conversion occurring at the surface of those systems: the energy flow pathways determine the likelihood of a reaction taking place on the surface. Subtle differences in energy dissipation mechanism can account for different photo-chemical activities of water and ice surfaces, relevant for atmospheric processes. We excite water and ice at 3100 and 3300 cm-1, the low- and high-frequency regions of the water stretch band, with femtosecond infrared excitation pulses of 150 cm-1 bandwidth and probe over the entire O-H stretch region with Sum Frequency Generation spectroscopy. Our results show extremely rapid spectral diffusion for both ice and water on sub-100 fs timescales, before vibrational relaxation and thermal redistribution of excess energy on several hundreds of fs timescales. The non-hydrogen bonded water molecules show relaxation dynamics on a picosecond timescale with ice being slower than water. By comparing the observed relaxation dynamics of water molecules at the surface of single-crystalline ice and the water-air interface, we discuss the potential implications of the results for chemical dynamics at the two surfaces.

O 58.5 Wed 12:10 R1

Mass transfer of water at organic aerosol interfaces — •Matus E. Diveky, Michael Gleichweit, Sandra Roy, and Ruth Signorell — Laboratory of Physical Chemistry, ETH Zürich, Vladimir-Prelog-Weg 2, CH-8093 Zürich, Switzerland

Interfacial mass transport plays a crucial role in defining growth rates of aerosols. To properly assess the potential of aerosols to behave as condensation nuclei, it is of paramount importance to unravel the kinetics of mass transport through the interface. The important parameter defining the probability of a gas-phase molecule accommodating to the surface upon collision is called mass accommodation coefficient. Despite the widespread relevance of accommodation coefficients, values for many important systems are still lacking.

We employ Photothermal Single-Particle Spectroscopy (PSPS) to investigate the water accommodation on miscible organic aerosol particles. Such systems remain largely uncharted despite the abundance of organic matter and gas-phase water molecules in the atmosphere. The PSPS technique combines photoacoustic spectroscopy with modulated Mie scattering performed simultaneously on a single-particle level.

Through a careful droplet manipulation inside an optical trap, we study the temperature and relative humidity dependence of the mass accommodation coefficient of water on organic miscible droplets. Our results hint at a negative correlation between accommodation coefficient and temperature. Lastly, we argue that the PSPS technique can be used to restrict the lower limit of the mass accommodation of water on liquid water.

O 59: Mini-Symposium: Coherent band structure engineering with light I

Time: Wednesday 10:30–12:30 Location: R2

Invited Talk O 59.1 Wed 10:30 R2

TBA — •Netanel Lindner — Technion, Haifa

O 59.2 Wed 11:00 R2

Electronic Liquid Gyro-Crystals — •Iliya Esin[1,2], Gaurav Gupta[2], Erez Berg[3], Mark Rudner[4], and Netanel Lindner[2] — [1]California Institute of Technology, Pasadena, USA — [2]Technion, Haifa, Israel — [3]Weizmann Institute of Science, Rehovot, Israel — [4]University of Copenhagen, Copenhagen, Denmark

We show that coherent time-periodic driving can be used to induce non-equilibrium correlated states with spontaneously broken symmetry in lightly doped semiconductors. In the presence of a resonant driving field, the system spontaneously develops quantum liquid crystalline order featuring extreme anisotropy whose directionality rotates as a function of time. The phase transition occurs in the steady state of the system achieved due to the interplay between the coherent external drive, electron-electron interactions, and dissipative processes arising from the coupling to phonons and the electromagnetic environment. We obtain the phase diagram of the system using numerical calculations that match predictions obtained from a phenomenological treatment and discuss the conditions on the system and the external drive under which spontaneous symmetry breaking occurs. Our results demonstrate that coherent driving can be used to induce novel non-equilibrium quantum phases of matter with dynamical broken symmetry.

Invited Talk O 59.3 Wed 11:15 R2

Engineering emergent states in quantum materials with classical and quantum light — •Michael Sentef — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Light-matter coupling enables the coherent manipulation of quantum states. For classical light, this is known as Floquet engineering, with potential applications ranging from engineered photon-photon interactions in Rydberg gases to Floquet topological states in a variety of platforms. In the limit of quantum light, quantum-electrodynamical cavities could enable the creation of polaritonic light-matter hybrid states, again ranging across platforms, from polaritonic chemistry with molecules to cavity superconductivity in quantum materials.

In this talk, I will discuss the status of our understanding of light-matter engineering of emergent states in quantum materials. I will show examples for the manipulation of fundamental interactions (Hubbard U) and their potential role in experiments on light-induced superconductivity [1,2] and dynamical phase transitions [3,4] driven by classical light, and discuss the quantum-to-classical crossover of Floquet engineering of the spin-exchange interaction [5].

[1] Buzzi et al., Phys. Rev. X 10, 031028 (2020). [2] Tindall et al., Phys. Rev. Lett. 125, 137001 (2020). [3] Tancogne-Dejean et al., Phys. Rev. Lett. 121, 097402 (2018). [4] Beaulieu et al., arXiv:2003.04059. [5] Sentef et al., Phys. Rev. Research 2, 033033 (2020).

O 59.4 Wed 11:45 R2

Tracking topological signatures by time- and angle-resolved photoemission spectroscopy — •Michael Schüler — Stanford Institute for Materials and Energy Sciences (SIMES), SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

The impressive progress in high-resolution and multi-dimensional angle-resolved photoemission (ARPES) allows insights into the nature of the quantum states in the solid itself. We will discuss how topological properties are manifest in circular dichroism in ARPES. Based on state-of-the-art calculations, we demonstrate how momentum-resolved Berry curvature can be mapped out for prototypical two-dimensional materials. Furthermore, topological properties can be induced by tailored light. However, realizing the induced Floquet-Chern insulator state and tracing clear experimental manifestions has been a challenge. We tackle this gap between theory and experiment by employing microscopic nonequilibrium Green's functions (NEGF) calculations including realistic electron-electron and electron-phonon scattering. Combining our nonequilibrium calculations with an accurate one-step theory of photoemission allows us to establish a direct link between the build-up of the topological state and the dichroic pump-probe photoemission signal.

O 59.5 Wed 12:00 R2

Electromagnetic dressing of the electron energy spectrum at high momenta — •David Schmitt[1], Marius Keunecke[1], Marcel Reutzel[1], Alexander Osterkorn[2], Tridev A. Mishra[2], Christina Möller[1], Wiebke Bennecke[1], G. S. Matthijs Jansen[1], Daniel Steil[1], Salvatore R. Manmana[2], Sabine Steil[1], Stefan Kehrein[2], and Stefan Mathias[1] — [1]1. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Institut für Theoretische Physik, Georg- August-Universität Göttingen, Göttingen, Germany

The coherent manipulation of quantum states is a promising route towards new emerging phases of solids. The concept of *Floquet engineering* has been used in various theoretical approaches. However, the experimental identification of such light dressed eigenstates is challenging. In this contribution, we discuss the generation of photon dressed sidebands throughout the full surface Brillouin zone when probed with two-color time- and angle-resolved photoelectron spectroscopy. We put special focus onto the differentiation of the laser-assisted photoelectric effect, the generation of Flouqet-Bloch bands, and scattering amplitude between both cases at large in-plane momenta, i.e. at the edges of the surface Brillouin zone.

O 59.6 Wed 12:15 R2

Time-Resolved Plasmoemission Spectromicroscopy — •Pascal Dreher, David Janoschka, Jan-Henrik Herrig, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

Photoemission in intense light fields has received a lot of attention in the past and the coherent interaction of electrons with the field after the emission process has been revealed. Within a solid, strong nonperturbative interactions of the intense driving light field with the electronic band structure can also occur under suitable driving conditions. Ultimately, observing such dressing of electronic bands by light requires electronic state resolution as well as precise control over the intense periodic driving field.

Here, we explore nanofocusing of femtosecond surface plasmon polariton (SPP) pulses on flat surfaces in combination with time- and angle-resolved photoemission spectromicroscopy as a possible route towards strong-field control over electronic states within a solid. We observe coherent nonlinear electron emission from the Au(111) Shockely surface state into SPP-dressed free-electron final states by the absorption of up to seven SPP quanta. The ponderomotive shift of the observed electron spectra is used to determine the transient field strength in the nanofocus. We present first results on time-resolved plasmoemission spectroscopy, which provides us with direct access to the coherent nonlinear dynamics of electrons within the intense SPP nanofocus.

O 60: Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems I

Time: Wednesday 10:30–12:30 Location: R3

Invited Talk O 60.1 Wed 10:30 R3

Rashba effect and chiral magnetism: some insights from density functional theory — •Gustav Bihlmayer — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1) Forschungszentrum Jülich, D-52425 Jülich, Germany

Both, the Rashba effect and the Dzyaloshinskii-Moriya interaction (DMI) rely on inversion symmetry breaking and spin-orbit coupling (SOC) effects. While the qualitative behavior of both is easily described on a model level, quantitative insights in strength and sign are not so easy to obtain. Density functional theory (DFT) offers an effective tool to study these effects on an ab initio level. E.g. it was found that oxygen coverage changes both, the sign of the Rashba constant on a metal surface [1], and that of the DMI in a magnetic thin film [2]. We shortly discuss the interplay of magnetism and the Rashba effect and questions about the size and sign of the Rashba constant. These findings will be connected to recent models on so-called Rashba- and SOC-mediated DMI. DFT calculations of simple trilayer systems based on a Co/Pt interface show that the DMI can not only vary by a factor of 2 – 3, but also change sign depending on the inclusion of a third element [3]. We acknowledge discussions and collaborations with H. Jia, B. Zimmermann, and M. Hoffmann and funding by the Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 "Skyrmionics".

[1] O. Krupin et al., New J. Phys. **11**, 013035 (2009)
[2] A. Belabbes et al., Sci. Rep. **6**, 24634 (2016)
[3] H. Jia et al., Phys. Rev. Mater. **4**, 024405 (2020)

Invited Talk O 60.2 Wed 11:00 R3

Synthetic chiral magnets and domain wall logic circuits — •Pietro Gambardella — Department of Materials, ETH Zurich

The ability to engineer the interactions in assemblies of nanoscale magnets is central to the development of artificial spin systems and spintronic technologies. Following the emergence of the Dzyaloshinskii-Moriya interaction (DMI) in thin film magnetism, new routes have been opened to couple nanomagnets via strong chiral interactions, which is complementary to the established dipolar and exchange coupling mechanisms. In this talk, we show how two-dimensional synthetic antiferromagnets, skyrmions, and artificial spin systems can be realized by simultaneous control of the DMI and magnetic anisotropy in ultrathin magnetic films. In addition, we show that the combination of DMI and current-induced spin-orbit torques can be exploited to achieve field-free switching of synthetic magnetic elements as well as all-electric operation of domain wall logic circuits.

Invited Talk O 60.3 Wed 11:30 R3

Zero-field magnetic skyrmions in model-type systems studied with STM — •Kirsten von Bergmann — Department of Physics, University of Hamburg, Germany

Magnetic skyrmions can be stabilized in thin films by interface-induced Dzyaloshinskii-Moriya interactions that compete with exchange interactions. Such skyrmions can become lowest energy states in applied magnetic fields but are often only metastable configurations in zero magnetic field.

We have studied the magnetic properties of two different ultra-thin magnetic film systems on Ir(111) using spin polarized STM [1]. Depending on the material properties we find both zero-field skyrmions that are stabilized by neighboring skyrmions or by the rim of the film, and isolated zero-field skyrmions [2,3]. In both systems these skyrmions can be found in the virgin state, meaning that up- and down-skyrmions can coexist. Ab-initio calculations in combination with spin dynamics simulations shed light on the origin, and different stabilization mechanisms are revealed for the two different film systms.

[1] K. von Bergmann et al., J. Phys.: Cond. Mat. 26, 394002 (2014).
[2] S. Meyer et al., Nature Commun. 10, 3823 (2019).
[3] M. Perini et al., Phys. Rev. Lett. 123, 237205 (2019).

Invited Talk O 60.4 Wed 12:00 R3

Spin Orbit driven effects in Graphene-FM systems — •Paolo Perna — IMDEA Nanociencia, 28049 Madrid, Spain

A major challenge for future spintronics is to develop suitable spin transport channels with superior properties such as long spin lifetime and propagation length. Graphene can meet these requirements, even at room temperature [1], but other active properties, such as magnetic order and large spin-orbit coupling (SOC), need to be incorporated into graphene [2]. Taking advantage of the fast motion of perpendicular magnetic anisotropy (PMA) chiral spin textures can satisfy the demands for high-density data storage, low power consumption and high processing speed [3], while the presence of graphene enables the possibility to electrically tune the magnetic properties [4]. Here, I report on high quality, epitaxial graphene/Co(111)/HM(111) stacks grown on (111)-oriented insulating oxide crystals which exhibit enhanced PMA for Co layers up to 4 nm thick and left-handed Néel-type chiral DWs stabilized by interfacial Dzyaloshinskii-Moriya interaction (DMI) localized at both graphene/Co and Co/HM interfaces with opposite sign [4,5]. While the DMI at Co/HM side is due to the intrinsic SOC, the sizeable DMI experimentally found at the Gr/Co interface has Rashba origin [5]. The active magnetic texture is protected by the graphene monolayer and stable at 300 K in air, and, since it is grown on an insulating substrate, amenable to be controlled electrically [3]. [1] Nat. Nanotech. 9, 794 (2014). [2] Nat. Nanotech. 8, 152 (2013). [3] https://nanociencia.imdea.org/sographmem/ [4] Nano Lett. 18(9), 5364 (2018). [5] ACS Appl. Mat.&Int., 12, 4088 (2020).

O 61: Poster Session V: Oxide and insulator surfaces: Structure, epitaxy and growth I

Time: Wednesday 10:30–12:30 Location: P

O 61.1 Wed 10:30 P

High Pressure Oxidation of Copper on Au(111) - A Route towards Bulk-like Cuprous Oxide Films — •Alexander Gloystein[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

As low-pressure oxidation is inefficient to grow Cu2O films of more than monolayer thickness, Cu slabs were oxidized on Au(111) at 50 mbar of oxygen. The procedure results in bulk-like Cu2O films with (111) termination, as concluded from XPS, LEED and STM. Their surface shows a (sqrt3 x sqrt3)R30° reconstruction, also known from bulk crystals. Using DFT, it is assigned to an array of Cu4O nano-pyramids that occupy every third Cu-O six ring of the bulk-cut (111) surface and remove the majority of its dangling bonds. Electronically, the films exhibit a p-type conductance behavior with the valence-band maximum located directly at EF. At high temperature, the films decay into Cu2O(111) crystallites and a Cu3O2 surface oxide, the latter resembling the Cu-O monolayer formed upon low-pressure Cu oxidation.

O 61.2 Wed 10:30 P

First-Principles Characterisation of the Diamond(110) Surface Oxygenation State — •Shayantan Chaudhuri[1], Samuel Hall[1], Benedikt Klein[1,2], Andrew Logsdail[3], Julie Macpherson[1], and Reinhard Maurer[1] — [1]University of Warwick, Coventry, United Kingdom — [2]Diamond Light Source, Didcot, United Kingdom — [3]Cardiff University, Cardiff, United Kingdom

Diamond is a material that possesses numerous properties and has applications in a variety of fields. When grown via chemical vapour deposition, the growth rate of the (110) face is typically much faster than the other two dominant crystallographic orientations: (111) and (100). Due to its fast growth rate, both polycrystalline and nanocrystalline diamond have been shown to have a predominant (110) texture. Despite the (110) surface having so much apparent importance, there has been a lack of both experimental and theoretical studies on this surface. Diamond surfaces are typically cleaned in a way prior to use that renders their surfaces oxygen-terminated, which can have numerous effects on the properties exhibited by the diamond. For this reason, it is important to be able to determine the oxygenation state of the (110) surface. Using density functional theory, we determine that the phase diagram of the diamond(110) surface is dominated by a highly stable phase of coexistent carbonyl and ether groups, while peroxide groups become more stable at lower temperatures and higher pressures. Our findings are corroborated by comparing simulated core-level binding energies and vibrational frequencies to experiment.

O 61.3 Wed 10:30 P

Surface reconstructions: challenges and opportunities for the growth of perovskite oxides — Giada Franceschi, Michael Schmid, Ulrike Diebold, and •Michele Riva — Institute of Applied Physics, TU Wien, Austria

Achieving atomically flat and stoichiometric films of complex multicomponent oxides is crucial for integrating these materials in emerging technologies. While pulsed laser deposition (PLD) can in principle produce these high-quality films, experiments often show rough surfaces and nonstoichiometric compositions.

To understand the cause, we follow the growth at the atomic scale from its early stages, using STM. We focus on SrTiO$_3$(110) and La$_{0.8}$Sr$_{0.2}$MnO$_3$(110) films. For both, the non-stoichiometries introduced during growth accumulate at the surface. As a result, their surface structure evolves along phase diagrams of surface structure vs. composition [1,2,3]. This can drastically degrade the surface morphology: pits develop on reconstructed areas with different sticking [4]; ill-defined oxide clusters nucleate when the non-stoichiometry introduced is too large to be accommodated in the surface by changing its structure. On the positive side, one can take advantage of the high sensitivity of surface structures to composition deviations to grow films with thickness of several tens of nanometers retaining atomically flat surfaces, and with stoichiometry control better than 0.1% [1].

[1] Phys. Rev. Mater. **3**, 043802 (2019). [2] J. Mater. Chem. A **8**, 22947 (2020). [3] arXiv:2010.05205 (2020). [4] Phys. Rev. Res. **1**, 033059 (2019).

O 61.4 Wed 10:30 P

Thermal (in)stability of the bulk-terminated SrTiO$_3$(001) surface — •Igor Sokolović[1], Giada Franceschi[1], Zhichang Wang[1], Jian Xu[1], Jiří Pavelec[1], Michele Riva[1], Michael Schmid[1], Ulrike Diebold[1], and Martin Setvín[1,2] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

The assumption of bulk-terminated perovskite oxide surfaces is common in most studies in literature, mostly based on (1×1) diffraction patterns observed in LEED or RHEED. The same is true for the prototypical SrTiO$_3$(001) perovskite surface, but the only direct evidence of an unreconstructed SrTiO$_3$(001) surface comes from our previous study [1], where it was obtained by cleaving single crystals, and studying the atomically flat surfaces with ncAFM. These surfaces consist of both (1×1)-terminated SrO and TiO$_2$ terminations, each covered with intrinsic polarity-compensating point defects. Neither of these two terminations is stable upon heating to 500 °C in UHV as clearly shown by ncAFM, despite the (1×1) LEED pattern and no shifts in XPS [2]. The (1×1) termination was also not observed by ncAFM on TiO$_2$-terminated surfaces prepared by traditional wet-chemistry, which likewise exhibit the (1×1) LEED pattern [2]. These clear evidence that the (1×1) LEED diffraction patterns can originate from subsurface layers below a disordered surface should be taken into account, since the common assumption of a pristine and unreconstructed SrTiO$_3$(001) might not be warranted. [1] Sokolović *et al.*, Phys. Rev. Mater. 3, 034407 (2019), [2] Sokolović *et al.*, arXiv:2012.08831 (2020).

O 61.5 Wed 10:30 P

Role of apical oxygen in oxide thin films — •Judith Gabel[1], Matthias Pickem[2], Philipp Scheiderer[3], Marius Fuchs[3], Berengar Leikert[3], Martin Stübinger[3], Lenart Dudy[4], Jan M. Tomczak[2], Giorgio Sangiovanni[3], Karsten Held[2], Tien-Lin Lee[1], Michael Sing[3], and Ralph Claessen[3] — [1]Diamond Light Source, United Kingdom — [2]TU Wien, Austria — [3]Universität Würzburg, Germany — [4]Synchrotron SOLEIL, France

Owing to their complex phase diagram, transition metal oxides are an interesting playing field for fundamental research but also open up a gateway to novel electronic functionalities. Oxide thin films are of particular importance as they bring along additional parameters to tune the phase diagram. The films are commonly assumed to be stoichiometric and to have an abrupt surface. Using the example of the prototypical correlated metal SrVO$_3$, we demonstrate here that this description overlooks an essential ingredient, apical oxygen adsorbing at the surface, which has to be considered for an accurate description of oxide thin films. The oxygen adatoms, which form even under UHV, change the film stoichiometry and are shown to severely alter the intrinsic electronic structure. They can affect the doping level of the film as well as the energetic order of the atomic orbitals and may lead to the formation of an electronically and magnetically dead surface layer. We demonstrate that, in the presence of apical oxygen, the thickness-dependent metal-insulator transition observed in SrVO$_3$ can no longer be categorized as a purely bandwidth-controlled Mott transition as previously understood.

O 61.6 Wed 10:30 P

A Large Unit Cell Quasicrystal Approximant derived from SrTiO$_3$ on Pt(111): A LEED, STM and STS Study — •Oliver Krahn, Sebastian Schenk, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The discovery of a two-dimensional dodecagonal oxide quasicrystal (OQC) formed from BaTiO$_3$ on Pt(111) has pushed the field of ultrathin ternary oxides on metal supports [1]. The OQC structure is based on atomic arrangements in vertices of triangles, squares and rhombuses. Periodically repeated patches of the OQC tiling are known as approximants. In this contribution, we present the largest approximant observed so far, emerging in ultrathin SrTiO$_3$ on Pt(111), homogenously covering the entire substrate surface. As derived from low-temperature scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), its unit cell spans an area of (44 × 43)Å^2. Inside the unit cell, 48 Ti atoms are seen by STM, which form the vertices of 48 triangles, 18 squares and 6 rhombuses. Interestingly, this structure can be understood as a unit cell doubling of a previously reported approximant resulting from a glide mirror symmetry [2]. Detailed studies of the electronic structure by scanning tunneling spectroscopy (STS) reveal the metallic behaviour of the film around the Fermi energy and the independence of the local electronic structure from different vertex configurations in the unoccupied states regime.

[1] S. Förster, O. Krahn et al., Phys. Status Solidi B **257**, 1900624 (2020)
[2] S. Schenk et al., J. Phys.: Condens. Matter **29**, 134002 (2017)

O 61.7 Wed 10:30 P

Subtle differences between periodic and aperiodic 2D ternary oxides determined from photoemission spectroscopy — •Loi Vinh Tran, Maniraj Mahalingam, Oliver Krahn, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The discovery of oxide quasicrystals (OQCs) in two-dimensional ternary oxides on metal support has triggered many studies in this field in recent years [1,2]. Here, for the first time, the single-phase preparations of approximants in a periodic hexagonal wagon-wheel structure (WW) and a six-membered ring (6Net) network structure are reported, which are known from mixed phases [3]. This enables a side-by-side comparison between the aperiodic OQC and two distinct periodic superstructures of the same material by means of X-ray, UV photoemission spectroscopy (XPS, UPS). These periodic structures together with the OQC system are distinguished in terms of stoichiometry, workfunction, and atomic density measured by XPS, UPS and STM. Changes in workfunctions from 3.8, via 4.0, to 4.2 eV for the OQC, WW, and 6Net structures, respectively, are observed. On the other hand, XPS reveals a decreasing Ba:Ti ratio for the same sequence of structures as well as the atomic density measured by STM. The implications of these observations on different structural properties of BaTiO3 will be discussed.

O 61.8 Wed 10:30 P

Charge Deposition on SrTiO3 as a Model for Spacecraft Surface Charging — •Mirco Wendt[1], Franziska Dorn[1], Regina Lange[1], Jens Berdermann[2], Ingo Barke[1], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock, Germany — [2]Institute for Solar-Terrestrial Physics, German Aerospace Center (DLR), 17235 Neustrelitz, Germany

Differential charging due to high energy particle bombardment is a common reason for hardware degradation and sensor errors in spacecrafts. As a model for studying charge accumulation and dynamics, we propose SrTiO3, a transparent oxide with charges deposited by utilising the electron beam of a scanning electron microscope (SEM). In a first step, we show that charges deposited on SrTiO3 (100) surfaces can be observed in ambient environment by force microscopy methods (AFM). Using a plate capacitor model [1], we also estimate the total deposited charge and charge density. To meet the conditions at medium earth orbit and to address more extended life times, in situ AFM-SEM studies in UHV environment are set up.

[1] A. Berkowitz, et al, Appl Phys Lett 74, 472 (1999)

O 61.9 Wed 10:30 P

Metal-supported two-dimensional ternary oxides: A case study of $BaTiO_x$ on Pd(111) — •Friederike Wührl, Sebastian Schenk, Oliver Krahn, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The discovery of a quasicrystalline phase in ultrathin films of $BaTiO_x$ (BTO) on Pt(111) opened a new field of research on ternary oxides on metal substrates [1]. The dodecagonal oxide quasicrystal (OQC) shows up in a two-dimensional wetting layer, for which atomically-resolved scanning tunneling microscopy (STM) images show the Ti subgrid decorating the vertices of three tiling elements with equal edge lengths: square, triangle and rhombus [2]. To elucidate the role of the substrate on the formation of OQCs, we report here on a growth study of ultrathin BTO films on Pd(111). Upon annealing in UHV at 930 K to 1030 K, reduced BTO forms long-range ordered two-dimensional layers encapsulating the Pd substrate. In these wetting layers a series of structures has been identified by means of STM and LEED. Depending on the preparation conditions, the different structures follow triangle-rhombus, triangle-square or in case of the largest ones triangle-square-rhombus tilings. They can be classified according to their atom density per unit area. Although the largest unit cell, which covers an area of (2.6 x 6.4) nm^2, host a complex triangle-square-rhombus tiling, an aperiodically ordered structure has not been detected on Pd(111).

[1] S. Förster *et al.*, Nature **502**, 215 (2013)
[2] S. Förster *et al.*, Phys. Status Solidi B, 1900624 (2019)

O 62: Poster Session V: Organic molecules on inorganic substrates: electronic, optical and other properties I

Time: Wednesday 10:30–12:30 Location: P

O 62.1 Wed 10:30 P

Plasmon-driven motion of an individual molecule — •Tzu-Chao Hung, Brian Kiraly, Julian Strik, Alexander Khajetoorians, and Daniel Wegner — Institute for Molecules and Materials, Nijmegen, The Netherlands

Combining scanning tunneling microscopy (STM) and spectroscopy (STS) with STM-induced light emission, we demonstrate that nanocavity plasmons injected a few nanometers away from a molecule can induce molecular motion. For this, we studied the rapid shuttling motion of zinc phthalocyanine molecules adsorbed on ultrathin NaCl films. Single-molecule luminescence spectra from molecules anchored to a step edge were compared with isolated molecules adsorbed on the free surface. We found that the azimuthal modulation of the Lamb shift is almost two times larger compared to isolated molecules. A remotely induced rapid shuttling motion of isolated molecules by plasmon-exciton coupling can explain the difference. Plasmon-induced molecular motion may open an interesting playground to bridge the nanoscopic and mesoscopic world by combining molecular machines with nanoplasmonics to control directed motion of single molecules without the need for a local probe.

O 62.2 Wed 10:30 P

Application of laser PEEM to a biological system: Geobacter sulfurreducens — •Franz Niklas Knoop, Gerhard Lilienkamp, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

Recently, multi-photon photoelectron emission microscopy (nP-PEEM) was successfully applied to the spectromicroscopy of porphyrin thin films and exciton-plasmon coupling in nanoplasmonic-porphyrin hybrid systems by tuning the laser wavelength for multi-photon excitation in resonance with the molecular S_0 -> S_2 transition (Soret band) [1]. Here, we report on our laser-PEEM study of a biological system, the bacterium Geobacter sulfurreducens. This anaerobic bacterium features membrane-associated and extracellular cytochromes containing iron porphyrins. In contrast to porphyrin films of ZnTPP or MgTPP, near-Soret excitation of photoelectrons from Geobacter sulfurreducens results in pronounced dependencies of the photoemission on irradiation time indicating laser-induced, irreversible changes of the bacteria. An initial decrease of the photoemission can be related to an irreversible photo-induced oxidation of the cytochromes while a strong increase for longer periods of irradiation is shown to be caused by thermal effects. PEEM excitation spectra of the exposed bacteria also show the degenerative effect of the exciting laser pulses.

[1] K. Stallberg, G. Lilienkamp, W. Daum, J. Phys. Chem. C **121**, 13833 (2017).

O 62.3 Wed 10:30 P

First-principles simulation of core-level spectroscopy to reveal the nature of chemical bonding at metal-organic interfaces — •Samuel J. Hall, Benedikt P. Klein, and Reinhard J. Maurer — Department of Chemistry, University of Warwick, Coventry, United Kingdom

X-ray photo-emission spectroscopy XPS and near-edge adsorption fine structure spectroscopy (NEXAFS) experiments are routinely used to characterise the chemical environment and the valence electronic structure of organic materials and metal-organic interfaces. In the past, certain spectral changes upon adsorption of molecules to surfaces have been connected to changes in chemical bonding and charge distribution, however complex overlapping spectra of multiple species often complicate such an interpretation. Through the use of Density Functional Theory (DFT) calculations, we study two molecular isomers, azulene and naphthalene, adsorbed on three different metal(111) surfaces. These six systems fall into three distinct regimes of molecule-metal chemical bonding. Our core-level spectroscopy simulations connect the changes seen in the spectra with different levels of chemical bonding and decompose these signatures into initial core state and final valence state contributions. We analyse the effect of charge transfer, electronic hybridisation and dispersion effects, all with the aim to provide new insights to experimental spectral analysis.

O 62.4 Wed 10:30 P

Benchmarking ab-initio methods to predict non-adiabatic charge transfer at metal-organic interfaces — •Daniel Corken, Nicholas D.M. Hine, and Reinhard J. Maurer — University of Warwick, Coventry , United Kingdom

State-resolved molecular beam scattering experiments have shown that small molecules scattering from metal surfaces exhibit non-adiabatic behaviour whereby charge is dynamically transferred from the metal to the molecule, creating a transient anion. Understanding chemical dynamics of molecule-metal systems is essential for designing the next generation of heterogeneous catalysts. Such dynamical non-adiabatic charge-transfer is not captured by ground state Density Functional Theory or classical dynamics and the explicit anionic excited-state and coupling constants between states need to be described. Metal-organic interfaces feature a continuum of electronic states rendering conventional excited state methods prohibitively expensive. Here we assess three approximate and computationally efficient methods to predict excited states at metal surfaces: The use of an applied electric field, constrained DFT, and the linear-expansion-Delta-Self-Consistent-Field method. For the prototypical system of CO on Au(111), we compare the methods based on how accurately they predict excited-state energy landscapes and their computational efficiency and numerical robustness, with the aim to identify an excited state method to perform non-adiabatic dynamics simulations for charge transfer systems in the future.

O 62.5 Wed 10:30 P

How molecular composition affects molecular double bond switching at metal surfaces: Azobenzene vs. Benzalaniline vs. Stilbene on Ag(111) — •Martin Lea[1], David A. Duncan[2], and Reinhard J. Maurer[1] — [1]University of Warwick, Coventry, United Kingdom, CV4 7AL — [2]Diamond Light Source, Didcot, United Kingdom, OX11 0DE.

Photoswitches are a class of organic molecules which have shown prevalence within the field of nanotechnology; the ability to reversibly convert between two geometric states as a response to light absorption has shown prospects for molecular-based electronics applications, transistors, and storage devices. Integration of such organic molecules in devices requires adsorption upon a metal surface, which often leads to quenching of the molecules switching ability. Adsorption of the prominent photoswitch azobenzene upon metallic substrates has shown that the switching behavior observed in both gas and solution phases does not translate to the interface, as the surface modifies the energy landscape. In this work we explore whether this same deactivation effect is consistent with other similar molecular switch architectures. Using dispersion-corrected density functional theory, we explore the consequences of metal adsorption for a series of homologic molecules with central double bonds of varying composition: azobenzene, benzalaniline and stilbene. We compare minimum energy paths and electronic structure characteristics to unveil how molecular architecture can affect switching capabilities at surfaces.

O 62.6 Wed 10:30 P

Application of periodic energy decomposition analysis to metallic systems — •Jan-Niclas Luy[1], Benedikt P. Klein[2], J. Michael Gottfried[2], and Ralf Tonner[1] — [1]Fakultät für Chemie und Mineralogie, Universität Leipzig, Germany — [2]Fachbereich Chemie, Philipps Universität Marburg, Germany

The Energy Decomposition Analysis (EDA) is a wavefunction based bonding analysis scheme that enjoys significant popularity in the molecular chemistry community [1]. Recently the method has been extended to surfaces and solids [2] and applied to organic surface chemistry [3]. It was shown that localized, covalent bonds in a periodic system can be interpreted in a similar fashion as their 0D molecular counterparts. Adsorption of organic molecules on transition metal surfaces, however, requires a more nuanced description [4]. In addition to covalent bonds, interactions are often characterized by large charge transfer, polarization and dispersion contributions. While for many alternant aromats dispersion dominates on Cu(111), orbital interactions can be identified in non-alternant cases. With the more reactive Pt(111) surface, both types form strong chemisorptive bonds that show donor/acceptor and shared-e^- character.

[1] M. von Hopffgarten and G. Frenking, *WIREs Comput Mol Sci* **2012**, *2*, 43.
[2] M. Raupach, R. Tonner, *J. Chem. Phys.* **2015**, *142*, 194105.
[3] L. Pecher, S. Laref, M. Raupach and R. Tonner, *Angew. Chem. Int. Ed.* **2017**, *56*, 15150.
[4] B. P. Klein *et al.*, *Phys. Rev. X* **2019**, *9*, 011030.

O 62.7 Wed 10:30 P

Imaging Charge Localization in a Conjugated Oligophenylene — •Laerte Patera[1,2], Fabian Queck[1], and Jascha Repp[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department of Chemistry, Technical University of Munich, 85748 Garching, Germany

Polaron formation in conjugated polymers has a major impact on their optical and electronic properties. In polyphenylenes, the molecular conformation is determined by a delicate interplay between electron delocalization and steric effects. Injection of excess charges is expected to increase the degree of conjugation, leading to structural distortions of the chain. Here we investigated at the single-molecule level the role of an excess charge in an individual oligophenylene deposited on sodium chloride films. By combining sub-molecular-resolved atomic force microscopy with redox-state-selective orbital imaging, we characterize both structural and electronical changes occurring upon hole injection. While the neutral molecule exhibits a delocalized frontier orbital, for the cationic radical the excess charge is observed to localize, inducing a partial planarization of the molecule. These results provide direct evidence for self trapping of the excess charge in oligophenylenes, shedding light on the interplay of charge localization and structural distortion.

O 62.8 Wed 10:30 P

Controlling long-distance motion of single molecules on Ag(111) — •Donato Civita, Grant J. Simpson, and Leonhard Grill — Institute of Chemistry, University of Graz, Austria

The motion of single molecules adsorbed on solid surfaces is of fundamental importance in various fields as heterogeneous catalysis, film growth processes, and on-surface polymerization. However, the motion of adsorbed molecules is usually a diffusive process with random changes in the direction of motion, and thus limited control. Here, we show how the motion of single di-bromo-ter-fluorene molecules on a Ag(111) surface can be controlled over distances of more than 100 nm with picometric precision [1]. The molecule moves strictly in one dimension across the surface, driven by an interplay of van der Waals and electrostatic interactions, which are used to repel and attract the molecule. The large spatial extension of the motion, and its astonishing confinement allow the direct measurement of the molecular speed, and to realize a sender-receiver experiment where a single molecule is transferred between two independent STM tips. These results suggest how a single molecule may be aimed toward a stationary target to study chemical reactions in relation to momentum and orientation of the reagent.

[1] D. Civita, M. Kolmer, G. J. Simpson, A.-P. Li, S. Hecht, L. Grill, Control of long-distance motion of single molecules on a surface, Science, Vol. 370, Issue 6519, pp. 957-960 (2020).

O 62.9 Wed 10:30 P

Controlled Manipulation of Single Molecules on an Ag(111) Surface — •Julia Lanz, Donato Civita, and Leonhard Grill — Single Molecule Chemistry, Institute of Chemistry, University of Graz

Thermal motion of molecules at surfaces is a stochastic process which makes it complicated to control the molecular trajectory. Here, we have used scanning tunneling microscopy under ultrahigh vacuum conditions to manipulate individual molecules to move controllably across a flat Ag(111) surface, kept at low temperatures of about 7 K. The controlled motion of single molecules gives deeper understanding of the relation between molecular motion and the chemical as well as geometrical properties of the molecules and the surface. Vertical manipulation provides insight into the dependence of molecular motion on conformational changes. Upon lateral manipulation the molecules follow the STM tip in a precise fashion. This occurs preferably in pairs, which will be discussed in view of intermolecular interaction.

O 63: Poster Session V: Electron-driven processes at surfaces and interfaces

Time: Wednesday 10:30–12:30 Location: P

O 63.1 Wed 10:30 P

Quantifying the breakdown of electronic friction theory during molecular scattering of NO from Au(111) — •Connor L. Box[1], Yaolong Zhang[2], Rongrong Yin[2], Bin Jiang[2], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, United Kingdom — [2]Department of Chemical Physics, University of Science and Technology of China, Hefei, China

The multiquantum vibrational energy loss recorded during molecular scattering from metallic surfaces is a testament to the breakdown of the Born-Oppenheimer approximation. Vibrational state-to-state scattering of NO on Au(111) has been one of the most studied examples in this regard, providing a testing ground for developing various nonadiabatic theories. However, the exact failings compared to experiment and their origin from theory are not established for any system because dynamic properties are affected by many compounding simulation errors of which the quality of nonadiabatic treatment is just one. We use a high dimensional machine learning representation of energy and electronic friction tensor to minimize errors that arise from quantum chemistry.[1,2] This allows us to perform a comprehensive quantitative analysis of the performance of molecular dynamics with electronic friction in describing state-to-state scattering. We find that electronic friction theory accurately predicts elastic and single-quantum energy loss, but underestimates multi-quantum energy loss and overestimates molecular trapping at high vibrational excitation. Our analysis reveals potential remedies to these issues. [1] R. Yin et al, J. Phys. Chem. Lett, 2019 [2] C. L. Box et al, JACS Au, 2020

O 63.2 Wed 10:30 P

Superoxide formation near DMSO/Cu(111) interfaces — •Angelika Demling[1,2], Sarah B King[3], and Julia Stähler[1,2] — [1]Institut für Chemie, Humboldt-Universität zu Berlin, Berlin — [2]Fritz-Haber-Institut der MPG, Berlin — [3]Department of Chemistry, University of Chicago, Chicago

DMSO is a common non-aqueous solvent with the potential to be used in lithium-oxygen batteries due to its ability to catalyze the superoxide formation [1]. In this study we investigate the electron dynamics in DMSO films on Cu(111) using time- and angle-resolved two-photon photoemission and disentangle the individual steps of charge transfer leading to superoxide formation: Electrons are injected from the metal to the DMSO, where they form small polarons on sub-picosecond time scales. The subsequent trapping extends the electronic lifetimes to several seconds [2]. Under co-adsorption of O_2 another intermediate state arises, whose binding energy is in good agreement with electrochemical data of superoxide [3]. A phenomenological model reproduces the time-dependent data and shows that trapped electrons act as precursors for the superoxide. Further, our data suggests that more superoxide is formed on the surface than in the bulk of DMSO after diffusion.

These results may contribute to a basic understanding of charge transfer processes in novel battery systems.

[1] K. M. Abraham, J. Electrochem. 162, A3021 (2015)
[2] S. B. King et al., J. Chem. Phys., 150, 041702 (2019)
[3] Donald T. Sawyer et al., J. Electroanal. Chem. 12, 90-101 (1966)

O 63.3 Wed 10:30 P

Investigations of polarons in hematite $\alpha - Fe_2O_3(1\bar{1}02)$ by means of nC-AFM and KMC — •Jesús Redondo[1], Pavel Kocán[1], Giada Franceschi[2], Florian Kraushofer[2], Michele Riva[2], Gareth S. Parkinson[2], Michael Schmid[2], Ulrike Diebold[2], and Martin Setvin[1,2] — [1]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Applied Physics, TU Wien, Austria

Polarons are known to strongly influence the catalytic activity and the electronic, magnetic and structural properties of transition metal oxides and halide perovskites. The study of polaron formation and dynamics is fundamental to understanding the actual mechanisms and yields of catalytic reactions in these materials. A new method for the investigation of electron- and hole- polarons is demonstrated. Charge carriers are injected with the atomic force microscope (AFM) tip into the $\alpha - Fe_2O_3(1\bar{1}02)$ surface. The injected charges form a cloud of charged particles trapped in the lattice. This cloud expands due to electrostatic interactions and thermally activated polaron hopping. Controlled annealing the sample and characterization by Kelvin probe force microscopy (KPFM) provides information on polaron dynamics that is compared to kinetic Monte Carlo (KMC) simulations.

The work was supported by projects GACR 20-21727X and GAUK Primus/20/SCI/009

O 63.4 Wed 10:30 P

Ultrafast lattice dynamics and microscopic energy flow in 3d ferromagnets — •Daniela Zahn[1], Florian Jakobs[2], Yoav William Windsor[1], Hélène Seiler[1], Thomas Vasileiadis[1], Tim Butcher[3], Yingpeng Qi[1], Dieter Engel[4], Unai Atxitia[2], Jan Vorberger[3], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [4]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin, Germany

The response of ferromagnets to laser excitation is governed by the interplay of electronic, magnetic and lattice degrees of freedom. The lattice plays an important role in the magnetization dynamics, since it drains energy from the electrons and absorbs angular momentum. Here, we study the lattice response of the 3d ferromagnets nickel, iron and cobalt directly using femtosecond electron diffraction. We compare the experimental results to spin-resolved DFT calculations combined with energy flow models. While the conventional two-temperature model is not in agreement with the experimental results, a consistent description of the laser-induced dynamics is achieved with energy-conserving atomistic spin dynamics simulations. Our results provide a clear picture of the microscopic energy flow between electronic, magnetic and lattice degrees of freedom on ultrafast timescales.

O 63.5 Wed 10:30 P

Transient reflectivity in nonequilibrium warm dense gold — •Pascal D. Ndione[1], Sebastian T. Weber[1], Dirk O. Gericke[2], and Baerbel Rethfeld[1] — [1]Department of Physics and OPTIMAS Research Center, Technische Universität Kaiserslautern — [2]CFSA, Department of Physics, University of Warwick

Ultrashort and intense laser pulses can induce strong modification of materials properties such as optical parameters determining the amount of absorbed energy in time. After excitation with lasers of high energy, the electrons thermalize fast to a hot Fermi distribution. Yet, the band occupation numbers are still in strong nonequilibrium as particle exchange between the bands takes longer than energy exchange.

We study excitation of gold with optical photons. Only the $5d$ and $6sp$ bands are considered to be active. We present a density-resolved approach coupled with a two-temperature model to follow the nonequilibrium band occupation. A Drude-Lorentz formalism is used to calculate the dielectric function of the heated system. We simulate the temporal evolution of a probe reflectivity up to delay time of 6 ps. Our predictions reveal over time a strong compensation of damping mechanisms for the electrons and phonons. The good agreement between simulation and time-resolved measurements suggests a good understanding of the experimental data and the underlying physical processes, which has been interpreted differently as a lack of dynamics on the subpicosecond timescale.

O 64: Poster Session V: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Wednesday 10:30–12:30 Location: P

O 64.1 Wed 10:30 P

Adlayer influence on Dirac-type surface state at W(110) — •Pascal Jona Grenz[1], Danny Thonig[2,3], Marcel Holtmann[1], Koji Miyamoto[4], Shiv Kumar[4], Eike Schwier[4,5], Taichi Okuda[4], Jürgen Henk[6], and Markus Donath[1] — [1]University of Münster, Germany — [2]Uppsala University, Sweden — [3]Örebro University, Sweden — [4]Hiroshima Synchrotron Radiation Center, Japan — [5]University of Würzburg, Germany — [6]Martin Luther University Halle-Wittenberg, Germany

In a combined experimental and theoretical study, we investigated how Fe and Co adlayers on W(110) affect the Dirac-type surface state (DSS). Angle-resolved photoelectron spectroscopy data show an increase in binding energy of 75 meV and 107 meV for Fe and Co, respectively. To identify the origin of the energy shift, we performed first principle calculations of the surface electronic structure. The inward surface relaxation of the uncovered W(110) surface is lifted by the adlayers. This structural change is one reason of the energy shift of the DSS. Furthermore, the Fe and Co adlayers lead to a reduced charge distribution of the DSS at the vacuum side, which results in an additional energy shift of the DSS.

O 64.2 Wed 10:30 P

Spin and Orbital Angular Momentum observed by Linear Dichroism: Interplay of Inversion Symmetry Breaking and Spin-Orbit Coupling — •Maximilian Ünzelmann[1], Hendrik Bentmann[1], Tim Figgemeier[1], Raphael Crespo Vidal[1], Thiago R. F. Peixoto[1], Henriette Maass[1], Chul-Hee Min[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

The formation of spin- and orbital angular momentum (SAM and OAM) for electronic states in non-centrosymmetric crystal-structure environments is shaped by a complex interplay of inversion symmetry breaking (ISB) and spin-orbit coupling (SOC) as well as their characteristic energy scales [1]. This phenomenology plays an important role in many modern quantum materials, such as topological insulators and Weyl semimetals [2,3]. Devising experimental approaches to access SAM and OAM is thus of fundamental interest. By means of spin- and angle-resolved photoemission we have investigated the photoelectron spin polarization and the linear dichroism (LD) [4] in various materials with spin-polarized surface states. Our results suggest that LD is linked to the OAM [5] in regimes dominated by either SOC or ISB.

[1] V. Sunko et al., Nature 549, 492 (2017)
[2] M. Schüler et al., Sci. Adv. 6, eaay2730 (2020)
[3] M. Ünzelmann et al., arXiv:2012.06996 (2020)
[4] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017)
[5] M. Ünzelmann et al., Phys. Rev. Lett. 124, 176401 (2020)

O 64.3 Wed 10:30 P

Unconventional Surface Conductivity in Correlated Honeycomb Transition Metal Oxide Mott Insulators — •Thomas Dziuba[1], Máté Stark[1], Ina Pietsch[2], Philipp Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Experimentalphysik, Universität Augsburg, Germany

The correlated honeycomb transition metal oxides attract large attention for the theoretical prospect of topological non-triviality as well as being a possible realization of the magnetic Kitaev exchange model. The Mott insulating sodium iridate Na2IrO3 is prototypical among these materials with the potential to bridge the field of strongly correlated systems with topology [1]. By using home-built STM and STS combined with macroscopic conductivity measurements of freshly cleaved Na2IrO3 surfaces in UHV we measure the properties provided by the sample surface. We report on the rather unconventional linear-dispersion in-gap conductivity found by tunneling spectroscopy. The addressability of such states strongly depends on the electronic properties of the probe and local surface structures. We will further discuss the found conductivity of the Na2IrO3 surface in the light of macroscopic measurements, complementing previous (bulk) results [2]. We thank the Deutsche Forschungsgemeinschaft for financial support via projects 220179758 (SPP 1666) and 107745057 (TRR 80).

[1] Phys. Rev. B 91, 041405(R) (2015), [2] Phys. Rev. B 82, 064412 (2010)

O 64.4 Wed 10:30 P

Surface electronic structure of CsSnBr3perovskite — •Jonas Hauner, Janek Rieger, Daniel Niesner, and Thomas Fauster — Friedrich-Alexander-Universität, Erlangen, Deutschland

Lead and tin halide based semiconductors with the perovskite structure show high dynamic disorder, i.e. local and instantaneous deviations from the ideal perovskite structure. These are expected to be larger for tin than for lead halide perovskites. Resulting local orientation of electric dipoles may drive unusual physical phenomena like dynamical Rashba or polaronic effects. While lead-based compounds are studied extensively, reports of tin-based compound surfaces are limited. We carried out angle-resolved photoelectron spectroscopy and two-photon photoelectron spectroscopy (2PPE) on (001) surfaces of $CsSnBr_3$. The valence band maximum is found close to the Fermi level and thus the surfaces are p-doped. The valence band dispersion is consistent with a hole effective mass of $m^* < 0.2\ m_e$. Two unoccupied states are found by 2PPE.

O 64.5 Wed 10:30 P

Surface atomic and electronic structure of $CsPbBr_3$ — •Janek Rieger, Tilman Kisslinger, M. Alexander Schneider, Thomas Fauster, and Daniel Niesner — Lehrstuhl für Festkörperphysik, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Staudtstr. 7, D-91058 Erlangen, Germany

Lead-halide-based semiconductors with the perovskite structure (LHPs) and the empirical formula ABX_3 (where A = Cs, CH_3NH_3, B = Pb and X = I, Br, Cl) tend to form stable (001) surfaces, which can exhibit AX and BX_2 surface terminations. A giant Rashba splitting of the valence bands backfolded to the $\bar{\Gamma}$ point could be observed for the BX_2 termination, but not for the AX-terminated surfaces of organic-inorganic LHPs (A = CH_3NH_3) [1].

For a systematic study of the interplay between surface atomic and electronic structure of purely inorganic LHPs, we carried out low-energy electron diffraction (LEED), scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES) on $CsPbBr_3$. From our STM and LEED results we can identify the prevalence of two different surface terminations for different preparations. The different terminations exhibit distinct spectral features in photoemission spectroscopy. ARPES results indicate no Rashba splitting and no band backfolding of the valence bands for the CsBr termination in line with earlier observations [2].

[1] J. Yang et al., Phys. Rev. B **102**, 245101 (2020).

[2] M. Puppin et al., Phys. Rev. Lett. **124**, 206402 (2020).

O 64.6 Wed 10:30 P

Strong anisotropy in the ballistic transport regime on Pd(110) — •Markus Leisegang, Robert Schindhelm, Jens Kügel, and Matthias Bode — Experimentelle Physik 2, Physikalisches Institut, Universität Würzburg

Atomic-scale charge transport is not only of significant fundamental interest but also highly relevant for numerous technical applications. However, experimental methods which are capable of detecting charge transport at the relevant single digit nanometer length scales are scarce. Here we report on molecular nanoprobe (MONA) [1] experiments on Pd(110) where we utilize the charge carrier-driven switching of a single cis-2-butene molecule [2] to detect ballistic transport properties over length scales of a few nanometers. Our data demonstrate a striking angular dependence with a dip in charge transport along the [1-10]-oriented atomic rows and a peak in the transverse [001] direction. The narrow angular width of both features and distance-dependent measurements suggest that the nanometer-scale ballistic transport properties of metallic surfaces are significantly influenced by the atomic structure.

[1] M. Leisegang et al. Nano Letters 18, 2165-2171 (2018)

[2] Y. Sainoo et al. Phys. Rev. Lett. 95, 246102 (2005)

O 65: Poster Session V: Solid-liquid interfaces: Reactions and electrochemistry II

Time: Wednesday 10:30–12:30 Location: P

O 65.1 Wed 10:30 P

Modelling of Lithium Whisker Dissolution — •Martin Werres[1,2], Arnulf Latz[1,2,3], and Birger Horstmann[1,2,3] — [1]Helmholtz Institute Ulm for Electrochemical Energy Storage, Ulm, Germany — [2]German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart, Germany — [3]Ulm University, Institute of Electrochemistry, Ulm, Germany

In the search for next generation batteries, lithium metal anode research experiences a refreshed attention due to its high theoretical energy density. Focus lies on enhancing the durability of lithium metal anode batteries and eliminating safety concerns. The battery capacity fades over cycling due to continous SEI buildup, consuming lithium and electrolyte, and the formation of inactive lithium, which is electrically disconnected from the anode. As the surface of the anode is highly irregular and tends to form whisker during charging, experiments show that during discharge, the tip of the whisker is not dissolved and a droplet stays behind inside the SEI shell. We developed a generalized phase-field model of the dissolution in order to gain insights in the droplet formation process.

Utilizing non-equilibrium thermodynamics, our phase-field model describes the dissolution of a single lithium whisker by taking the surface tension of lithium metal into account, and the interaction between lithium and the SEI. We are able to predict the nucleation of a Reyleigh instability behind the tip, leading to the formation of an electronically isolated lithium metal droplet.

O 65.2 Wed 10:30 P

Nanostructuring Cu tunes CO(2)R selectivity through the mass transport of products: the example of acetate — •Hendrik H. Heenen[1], Georg Kastlunger[1], Haeun Shin[2], Sean Overa[2], Joseph A. Gauthier[3], Feng Jiao[2], and Karen Chan[1] — [1]Department of Physics, Technical University of Denmark — [2]Department of Chemical and Biomolecular Engineering, University of Delaware — [3]Department of Chemical Engineering, Stanford University

Nanostructured Cu catalysts have increased the yield of and lowered the overpotential for high value C-C coupled (C_{2+}) products in electrochemical CO reduction (CORR). With this type of catalyst also the selectivity among C_{2+} products has changed where acetate has emerged as a major product depending strongly on alkalinity and catalyst structure. This striking selectivity dependence is far from being understood. In this work, we elucidate the mechanism towards acetate using an *ab-initio* derived microkinetic model coupled to mass transport as well as loading experiments. We find that acetate selectivity is only dependent on local mass transport properties of the catalyst and not founded in changes of the intrinsic activity of Cu. The selectivity mechanism originates in the transport of ketene away from the catalyst surface. This unprecedented mechanism may also explain similar selectivity fluctuations observed for other saturated intermediates like CO and acetaldehyde. Our proposed mechanism explains changes in selectivity of acetate with potential, pH, and catalyst roughness which are the basis for design principles of a selective CORR operation.

O 65.3 Wed 10:30 P

Surface pH estimation during electrochemical CO_2 reduction in a non-RDE setup — •David Egger, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The electro-chemical CO_2 reduction reaction (CO_2RR) represents a promising route to renewable fuels. CO_2RR in aqueous electrolyte solutions is hampered by the loss of faradaic efficiency due to the competing hydrogen evolution reaction (HER) either by the reduction of hydronium ions or water. The latter lead to a pH increase towards the electrode surface under high current operating conditions. This shift in electrode pH can significantly influence the active catalytic state and stability of the electrode. Yet, the crucial surface pH is neither experimentally easily accessible, nor can it be simply obtained from bulk equilibrium thermodynamics.

Here, we present a semi-empirical approach to estimate the surface pH at a planar electrode from experimental electrode currents at a range of different nominal bulk pHs. By solving a 1-D simplified Poisson-Nernst-Planck equation to account for mass transport and chemical kinetics, the current approach works even outside a rotating disc electrode setup. We apply it to corresponding CO2RR data at molybdenum carbide provided alongside *in situ* XPS measurements and show that only after surface pH correction the XPS compositional information can be brought into agreement with the Pourbaix diagram obtained from *ab initio* thermodynamics.

O 65.4 Wed 10:30 P

Anodic Polarization of Electrodes at High Potentials in Alkaline Electrolytes — •Evelyn Artmann, Lukas Forschner, Vincent Pramod Menezes, Mohamed Elnagar, Ludwig Kibler, Timo Jacob, and Albert K. Engstfeld — Institute of Electrochemistry, University of Ulm, Germany

Polarization of electrodes in aqueous electrolytes at anodic potentials in the range of a few to several hundred volts has a significant impact on the structural properties of the electrodes as well as on the products formed in the solution [1-2]. This opens up interesting opportunities for applications, e.g. electrocatalyst design.

In this work we report on the I-U characteristics and the structural properties of Pt, Au and Cu wire electrodes during anodic polarization between the stability region of water and anodic Contact Glow Discharge Electrolysis (aCGDE) in alkaline electrolyte. The structural changes of the electrodes were characterized by means of scanning electron microscopy (SEM) and electrochemical measurements. The latter suggest potential dependent oxide formation on Au and Cu. The nature of the formed oxides is discussed based on X-ray photoelectron spectroscopy (XPS) measurements.

An important finding is that the structural properties of the electrodes also depend on how quickly the electrodes were removed from the electrolysis solution. We will discuss in how far the electrolysis products affect the structure formation after the anodic treatment.

[1] G. Saito, T. Akiyama, J. Nanomater., 10 (2015) 1.

[2] A. Allagui et. al., Electrochim. Acta, 93 (2013) 137.

O 65.5 Wed 10:30 P

Increasing stability, efficiency, and fundamental understanding of lithium-mediated electrochemical nitrogen reduction — •Vanessa J. Bukas[1], Suzanne Z. Andersen[1], Michael J. Statt[2], Sarah G. Shapel[1], Jakob B. Pedersen[1], Kevin Krempl[1], Mattia Saccoccio[1], Debasish Chakraborty[1], Jakob Kibsgaard[1], Peter C. K. Vesborg[1], Jens K. Nørskov[1], and Ib Chorkendorff[1] — [1]Technical University of Denmark — [2]Stanford University, USA

Lithium-mediated nitrogen reduction is a proven method to electrochemically synthesize ammonia; yet the instability and low efficiency of this process have so far limited its practical application. One major obstacle against improving the Li-mediated approach is that very little is understood about the mechanism. We develop here a kinetic model that highlights mass transport limitations as a very important factor to the resulting faradaic efficiency. Our results reproduce experimental trends for varying conditions of N_2 pressure or H^+ availability and show that the relative diffusion rates of reacting Li^+, N_2, and H^+ species are key to selectively forming ammonia. On the basis of this understanding, we develop a potential-cycling strategy which can recover 'catalytic' high-energy electrons from unused metallic Li that was deposited at the electrode surface. This is shown experimentally to improve the stability of the system, alleviate the need for continuously replenishing the electrolyte with Li salts, and lead to a significant increase in both faradaic and energy efficiency [1].
[1] Andersen *et al.*, Energy Environ. Sci. **13**, 4291 (2020)

O 65.6 Wed 10:30 P

Light assisted electrodeposition of Ni catalysts on p- doped Si(111) for photoelectrochemical water reduction — •David Ostheimer[1], Mario Kurniawan[2], Lara Eggert[2], Thomas Hannappel[1], and Andreas Bund[2] — [1]Fundamentals of Energy Materials, Ilmenau University of Technology, Germany — [2]Electrochemistry and Electroplating, Ilmenau University of Technology, Germany

The development of efficient and inexpensive (photo-)electrocatalysts plays an important role to enhance the hydrogen evolution reaction for photoelectrochemical water-splitting. In the present work, nickel particles were electrochemically deposited on a p-type Si-(111) substrate under illumination. Different parameters have been varied to obtain beneficial morphologies and particle sizes. We show that they can be tailored by using either a potentiostatic method (resulting in large particles) or a galvanostatic deposition method (small particles), while the distribution of the particles on the surface is strongly influenced by the electrodeposition time. The particles size and the coverage including the surface roughness were investigated using atomic force microscopy. A relation between the surface morphology and catalytic activity was analyzed by comparing photocurrents of various samples. A dense particle coverage can block the incident light and thus limit the photoabsorption of the p-Si. This can be observed especially for samples with large catalyst particle sizes. Specimens with smaller nickel particles show a significant improvement of the photoactivity compared to samples with larger particles.

O 65.7 Wed 10:30 P

Quantum Chemical Assessment of well-defined Catalysts for the Oxygen Reduction Reaction — •Christopher Ehlert[1,2], Anna Piras[1,2], and Ganna Gryn'ova[1,2] — [1]Heidelberg Institute for Theoretical Studies (HITS gGmbH),Heidelberg, Germany — [2]Interdisciplinary Center for Scientific Computing, Heidelberg University, Heidelberg, Germany

The Oxygen Reduction Reaction (ORR) is an important electrochemical process taking place at the negatively charged cathode with applications in fuel cells and metal-air batteries. The bare reduction shows a rather sluggish reaction kinetics requiring catalysts to achieve larger electrical currents. Precious metal Pt-alloys show good performance and serve as a reference, however their rareness, high prices and poor long-term durability inhibit large-scale applications.

In a recent study, Kahan et. al.(doi:10.1021/acs.chemmater.8b04027) investigated six well defined (co)doped polyaromatic hydrocarbons (PAHs), or nanographene sheets. In this study, we investigate the catalytic reaction pathways of the proposed PAHs from the physisorbed oxygen towards the chemisorbed minimum by density functional theory. For the neutral catalysts, the potential energy surface scans show fully repulsive or energetically unfavorable situations. We therefore suggest that the initial chemisorption occurs via negatively charged catalysts, which is confirmed by exergonic reaction energetics.

O 66: Poster Session V: 2D Materials: Electronic structure, excitations, etc. I

Time: Wednesday 10:30–12:30 Location: P

O 66.1 Wed 10:30 P

Selective Oxygen Functionalization of the h-BN/Rh(111) Nanomesh — •Eva Marie Freiberger, Florian Späth, Fabian Düll, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität, Erlangen, Germany

2D materials such as the graphene analogue hexagonal boron nitride (h-BN) are interesting due to their unique structural, chemical and electronic properties. The morphology of a supported h-BN layer strongly depends on the underlying crystal surface. In the case of Rh(111) as substrate, a Moiré with pore and wire regions evolves, also known as nanomesh. Chemical modification, e.g. covalent functionalization with hydrogen and oxygen, of Ni(111) supported h-BN has already been reported. In the case of the h-BN nanomesh on Rh(111), such functionalization is especially interesting since the pores and wires may show different reactivity towards functionalization enabling spatially defined modification of h-BN.

Herein, we present detailed studies on the adsorption of molecular oxygen on the h-BN nanomesh on Rh(111). Using synchrotron radiation-based in situ high-resolution X-ray photoelectron spectroscopy we are able to provide a deep insight in this system regarding the adsorption behavior and the thermal stability of the covalent functionalization. Oxygen functionalization is performed via a supersonic molecular beam and is found to be an activated process occurring selectively in the pores of h-BN. The adsorbed oxygen is proposed to bind molecularly to two boron atoms in the pores of the Moiré. It is stable up to about 650 K.

O 66.2 Wed 10:30 P

Unconventional superconductivity mediated by spin fluctuations in single-layer NbSe2 — Wen Wan, Paul Dreher, Rishav Harsh, Francisco Guinea, and •Miguel M. Ugeda — Donostia International Physics Center (DIPC), Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain.

Van der Waals materials provide an ideal platform to explore superconductivity in the presence of strong electronic correlations, which are detrimental of the conventional phonon-mediated Cooper pairing in the BCS-Eliashberg theory and, simultaneously, promote magnetic fluctuations. Despite recent progress in understanding superconductivity in layered materials, the glue pairing mechanism remains largely unexplored in the single-layer limit, where electron-electron interactions are dramatically enhanced. Here we report experimental evidence of unconventional Cooper pairing mediated by magnetic excitations in single-layer NbSe2, a model strongly correlated 2D material. Our high-resolution spectroscopic measurements reveal a characteristic spin resonance excitation in the density of states that emerges from the QP coupling to a collective bosonic mode. This resonance, observed along with higher harmonics, gradually vanishes by increasing the temperature and upon applying a magnetic field up to the critical values, which sets an unambiguous link to the superconducting state. Furthermore, we find clear anticorrelation between the energy of the spin resonance and its harmonics and the local superconducting gap, which invokes a pairing of electronic origin associated with spin fluctuations.

O 66.3 Wed 10:30 P

A full gap above the Fermi level: the charge density wave of monolayer VS2 — •Camiel van Efferen[1], Jan Berges[2], Joshua Hall[1], Erik van Loon[2], Stefan Kraus[1], Arne Schobert[2], Tobias Wekking[1], Felix Huttmann[1], Eline Plaar[1], Nico Rothenbach[3], Katharina Ollefs[3], Lucas Machado Arruda[4], Nick Brookes[5], Gunnar Schönhoff[2], Kurt Kummer[5], Heiko Wende[3], Tim Wehling[2], and Thomas Michely[1] — [1]UzK, Köln, Germany — [2]UB, Bremen, Germany — [3]UDE, Duisburg, Germany — [4]FUB, Berlin, Germany — [5]ESRF, Grenoble, France

We present experimental evidence, via scanning tunneling microscopy and spectroscopy, of a $2/3\Gamma K$ charge density wave (CDW) in monolayer VS2. The CDW is shown to be stable at room temperature, and causes a full CDW gap in the unoccupied states of VS2. Unlike conventional CDWs, which undergo a metal-insulator transition, creating a gap at the Fermi level, the CDW in VS2 induces a topological metal-metal Lifshitz transition. Our ab initio calculations show anharmonic coupling of transverse and longitudinal phonons to be essential for the formation of the CDW and the full gap above the Fermi level. Additionally, x-ray magnetic circular dichroism reveals the absence of net magnetization in this phase, pointing to a coupled CDW-antiferromagnetic ground state.

O 66.4 Wed 10:30 P

Charge Transfer of Twist-Angle-Dependent Phosphorene-Graphene Hetero-bilayers. — •el-abed Haidar — The University of Sydney, Sydney, Australia

Twistronics is the study of the changes to the electronic properties of two-dimensional material bilayers due to rotational stacking, or twisting. In this work we explore the impact of twisting on the vertical charge transfer in a graphene-phosphorene bilayer using density-functional theory. We examine different twist angles and find significant drop in charge transfer when the twist changes from zero to greater than zero degrees. Such interesting feature can have major impacts in enriching two dimensional twistronics concepts especially their electronic properties.

O 66.5 Wed 10:30 P

Electronic structure and charge density wave in monolayer NbS_2 — •Timo Knispel[1], Jeison A. Fischer[1], Daniela Mohrenstecher[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], and Thomas Michely[1] — [1]Institute of Physics II, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institute of Theoretical Physics, Bremen Center for Computational Materials Science, University Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

We investigated monolayer 1H-NbS_2 grown in-situ on Gr/Ir(111) by high resolution scanning tunneling microscopy and spectroscopy at temperatures down to 0.4K. The characteristic 3x3 CDW pattern is present only in the monolayer, but absent in the bilayer. We analyze the CDW gap, contrast inversion in the dI/dV maps towards both sides of the gap and the suppression of the CDW pattern in the gap. Furthermore, quasiparticle interference is observed at island edges and defects and enables us to measure the dispersion of the hole-like pocket around the Γ-point. Density of states, dispersion around the Γ-point and the properties of the CDW are compared to density functional theory calculations.

Support from the Deutsche Forschungsgemeinschaft, SFB 1238 (project number 277146847, subprojects A01 and B06) is gratefully acknowledged.

O 66.6 Wed 10:30 P

Metal-to-insulator transition in MoS_2 by contactless chemical gating — •Wouter Jolie[1,2], Clifford Murray[1], Camiel van Efferen[1], Jeison A. Fischer[1], Carsten Busse[2], Hannu-Pekka Komsa[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Microelectronics Research Unit, University of Oulu, Finland

We present an effective way to gate semiconducting transition metal dichalcogenides without changing their direct chemical environment. The principle is demonstrated for MoS_2 on graphene on Ir(111). Intercalation of oxygen (europium) between graphene and Ir(111) removes (adds) charge in graphene, leading to a strong gating effect in MoS_2. Using scanning tunneling microscopy, we show that removing charge with oxygen leads to a 450 meV shift of the MoS_2 band gap with respect to the Fermi level. Adding charge with europium shifts the conduction band below the Fermi energy, accompanied by a band gap reduction of 700 meV due to renormalization. In addition, we find that gating also shifts the one-dimensional band present in MoS_2 mirror twin boundaries, which can be used as gating sensors.

O 66.7 Wed 10:30 P

Surface and interface effects in oxygen deficient $SrMnO_3$ thin films grown on $SrTiO_3$ — •Moloud Kaviani and Ulrich Aschauer — Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland

Complex oxide functionality, such as ferroelectricity, magnetism or superconductivity, is often achieved in epitaxial thin-film geometries. Oxygen vacancies tend to be the dominant type of defect in these materials but a fundamental understanding of their stability and electronic structure has so far only been established in the bulk or strained bulk, neglecting interfaces and surfaces present in the thin-film geometry. We investigate here by first-principles calculations, oxygen vacancies in the model system of a $SrMnO_3$ (SMO) thin-film atop a $SrTiO_3$ (STO) (001) substrate. We establish structural and electronic differences compared to bulk SMO that, in addition to misfit strain result also from under-coordination at the film surface. We then study the stability and electronic structure of oxygen vacancies in both the thin-film and the substrate, showing that electrostatics render oxygen vacancies more stable towards the film surface. As opposed to bulk SMO, we observe only partial reduction of Mn^{4+} to Mn^{3+} and for oxygen vacancies in SrO layers, a reduction of Mn only in the layer below the vacancy. We relate this to crystal field changes at the surface, that strongly alter the defect chemistry in the film. Our results show that surface and interface effects lead to significant differences in stability and electronic structure of oxygen vacancies in thin-film geometries compared to the (strained) bulk.

O 66.8 Wed 10:30 P

Mechanism of Self-Intercalation in Niobium Disulphide Monolayers on Gr/Ir(111) — •Daniela Mohrenstecher[1], Timo Knispel[1], Carsten Speckmann[2], Jeison Fischer[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Physics of Nanostructured Materials, University of Vienna, 1090 Wien, Austria

For 2D layered TMDCs the intercalation of native metal atoms into the van-der-Waals gap under metal excess conditions is a well-known phenomenon [1] and may result in covalently bonded materials that may exhibit phenomena like ferromagnetic order or spin-frustrated Kagome lattices [2]. Here we report self-intercalation for in-situ grown NbS_2 monolayers on Gr/Ir(111) .The process utilizes Nb atoms that are already present in the material and traverse from the pristine material into the van-der-Waals gap between NbS_2 and graphene during post-growth annealing.

Our quantitative coverage analysis based on scanning tunneling microscopy images indicates a conversion of Nb from the pristine material into the intercalated phase containing a stoichiometry of $Nb_{5/3}S_2$, featuring a $\sqrt{3} \times \sqrt{3}$ R30° superstructure. Moreover, self-intercalation suppresses the charge density wave of the NbS_2 monolayer. Using tunneling spectroscopy dramatic changes are found in the electronic structure self-intercalated compared to pristine non-intercalated layers.

[1] Jellinek et al. Nature 185, 376 - 377 (1960)
[2] Zhao et al. Nature 581 171-177 (2020)

O 66.9 Wed 10:30 P

The role of surface termination in the electronic, magnetic and catalytic properties of hematene: a computational study — •Mahdi Ghorbani-Asl, Yidan Wei, and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

Very recently, a new class of non-van der Waals 2D materials including hematene have been successfully exfoliated from their non-layered crystal counterparts.[1] Using density functional calculations, we have systematically studied the stability, electronic and magnetic properties of 2D α-Fe_2O_3 nanosheets and their functionalized derivatives.[2] Our results show that not only that different surface passivation with hydrogen on hydroxyl groups may exist but also passivation with the former group significantly facilitates the stability of material under ambient conditions. The hydrogenated sheets are found to be a half-metal, whereas the fully hydroxylated sheets are antiferromagnetic semiconductors. We show that the reduced dimensionality and defects on the hematene surface can also enhance the catalytic activity of the material for the oxygen evolution reaction.[3]

[1] A. Puthirath Balan, S. Radhakrishnan, C. F. Woellner, et al. Nat. Nanotechnol. 13, 602 (2018).

[2] Y. Wei, M. Ghorbani-Asl, and A. V. Krasheninnikov, J. Phys. Chem. C 124, 22784 (2020).

[3] B. Mohanty, Y. Wei, M. Ghorbani-Asl, A.V. Krasheninnikov, et. al, J. Mater. Chem. A 8, 6709 (2020).

O 66.10 Wed 10:30 P

Electronic properties of metal (Fe, Co, Ni, V) / $MoSe_2$ 2D-heterostructures. — •Lyes Mesbahi[1], Omar Messaoudi[1], Hamid Bouzar[1], and Samir Lounis[2] — [1]Laboratoire de Physique et Chimie Quantique (LPCQ), Mouloud Mammeri University, BP 17 RP, 15000 Tizi-Ouzou, Algeria — [2]Peter Grunberg Institut and Institute for Advanced Simulation, Forschungszentrum Julich & JARA, D-52425 Julich, Germany

We present a comparative first principles investigation of the electronic properties of 2D systems consisting of a $MoSe_2$ monolayer with a transition metal overlayer : Fe, Co, Ni and V. Our calculations show that Fe-$MoSe_2$ and Co-$MoSe_2$ are half-metallic ferromagnets with bandgaps of 0.94 eV and 0.74 eV, respectively, for one of the spin channels. Moreover, Ni-$MoSe_2$ converges into a semiconductor with an indirect bandgap of 0.68 eV. Interestingly, V-$MoSe_2$ turns out to be an anti-ferromagnetic material with a gapless dirac-cone located 0.20 eV below the Fermi level. The combined effect of time-reversal symmetry breaking and the effect of spin-orbit coupling induced by Mo, lead to non-degenerate K and K' valleys, which renders these heterostructures good candidates for diverse spintronic applications.

O 66.11 Wed 10:30 P

Atomic-scale characterization of few-layer Cr5Se8 — •Paul Dreher[1], Wen Wan[1], Carmen Gonzalez Orellana[2], Max Ilyn[2], Javier Herrero-Martin[3], Pierluigi Gargiani[3], Marco Gobbi[4], Santiago Blanco-Canosa[4], and Miguel Ugeda[1] — [1]Donostia International Physics Center, Donostia - San Sebastián, Spain — [2]Centro de Física de Materiales (CSIC-UPV/EHU) — [3]ALBA Synchrotron Light Source — [4]CIC Nanogune

The realization of magnetic order at the two-dimensional limit is currently a priority for Materials Science. In this arena, transition metal chalcogenides have emerged as candidate magnetic 2D materials with unprecedented robust chemical stability, which could enable their integration in durable, flexible magnetic devices. Here we perform combined atomic-scale structural and electronic characterization of few layer Cr5Se8 with its mesoscopic magnetic characterization. We have studied the atomic, electronic and magnetic structure of MBE-grown few-layer Cr5Se8 on graphene substrates (BLG/SiC(0001) and HOPG) by means of 4.2K-STM/STS and XMCD measurements. STM imaging reveals that Cr5Se8 present both Se- and Cr-terminations, the latter showing a 2x2 periodicity in the Cr plane stable up to room temperature. Both terminations exhibit a semiconducting behavior with an accused layer-dependent gap value maximized at 1.2 eV for three layers. Lastly, our XMCD measurements are compatible with a weak ferromagnetic ground state down to 2K.

O 66.12 Wed 10:30 P

Elelctronic structure and bonding of h-BN on Pt(110) — •Marco Thaler[1], Dominik Steiner[1], Alexander Menzel[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Institute of Applied Physics and Center for Computational Materials Science, University of Technology, Vienna, Austria

The electronic properties and substrate interaction of single domain hexagonal boron nitride (h-BN) grown on structurally incommensurable Pt(110) were investigated by density functional theory (DFT), angle-resolved photoemission spectroscopy (ARPES), and work function measurements. DFT calculations show that the h-BN-substrate interaction is dominated by nonlocal van der Waals forces. However, locally, a covalent bond forms between on-top N and Pt atoms, forcing the Pt(110)-surface to adapt to the adlayer in the form of a (1xn)-m.r. reconstruction. In addition, the covalent bond gives rise to a peak in the local density-of-states at the Fermi level within the h-BN band gap and generally to hybridization of h-BN and substrate bands in the calculated band structure. In contrast, the experimental band dispersion coincides well with band structure calculations for a free-standing h-BN monolayer. We attribute the difference to correlation effects, i.e. the confinement of the photo-hole within the h-BN monolayer. Considerable correlation is also indicated by the appearance of a flat band in the σ manifold. The Moiré structure causes the appearance of umklapp bands in the ARPES data, differing in nature from Moiré-induced replica bands observed in e.g. Ru(0001) or Rh(111).

O 66.13 Wed 10:30 P

Highly ordered metallic phase of Indium on SiC(0001) — •Jonas Erhardt, Maximilian Bauernfeind, Simon Moser, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg D-97074, Germany

Indium thin films attract attention due to diverse electronic properties, which feature for instance a two-dimensional electron gas (2DEG) [1] and superconductivity [2] in the 2D limit or Dirac-electrons in a triangular lattice [3]. Here, we present a combined angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling microscopy (STM) study of ultrathin (~ 2 monolayers) epitaxial indium films on silicon carbide (SiC). STM reveals a Kagome-like superstructure with a lattice constant of approximately 2.1 nm assigned as a $(4\sqrt{3} \times 4\sqrt{3})\mathrm{R}30^\circ$ reconstruction. Additionally, ARPES as well as scanning tunneling spectroscopy (STS) show a metallic band structure with a pronounced electron pocket, indicative of a 2DEG. Interestingly, STS further reveals negative differential conductance, which is in contrast to the canonical interpretation of the dI/dV signal as local density of states and is possibly related to substrate effects.

[1] E. Rotenberg *et al.*, Phys. Rev. Lett. **91**, 246404 (2003).
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010).
[3] M. Bauernfeind *et al.*, (unpublished)

O 67: Poster Session V: Ultrafast electron dynamics at surface and interfaces I

Time: Wednesday 10:30–12:30 Location: P

O 67.1 Wed 10:30 P

Improved projection-operator diabatization for electron transfer on periodic surfaces — •Simiam Ghan[1], Karsten Reuter[1,2], and Harald Oberhofer[1] — [1]Chair for Theoretical Chemistry, Technical University of Munich, Garching, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We discuss the recently-proposed[1] projection-operator diabatization method POD2GS for calculating electronic coupling in donor-acceptor charge transfer systems. The new scheme offers accurate electronic couplings by constructing diabats which remain localized on their respective fragments, as demonstrated for the Hab11 benchmark suite with molecular dimers.

Here, we apply this improved scheme to explore electron transfer from photoexcited adsorbates to surfaces, a problem for which the original POD method has been widely used. Specifically, we report results for the case of monolayers of core-hole excited Argon on ferromagnetic substrates, where accurate spin-dependent electron transfer lifetimes have been measured experimentally. Aspects of periodic boundary conditions in the electron transfer model are discussed; in particular, we examine the validity of the Γ-point approximation which is commonly used with POD models for electron transfer on surfaces.

[1] S. Ghan *et al.*, J. Chem. Theory Comput. **16**, 7431 (2020).

O 67.2 Wed 10:30 P

The ambivalent competition of Coulomb and van-der-Waals interactions in Xe-Cs$^+$ aggregates on Cu(111) surfaces — •John Thomas[1], Cord Bertram[1,2], Janos Daru[2], Ping Zhou[1], Dominik Marx[2], Karina Morgenstern[2], and Uwe Bovensiepen[1] — [1]Physik, Universität Duisburg-Essen — [2]Chemie, Ruhr-Universität Bochum

The properties of heterogeneous interfaces are important because of their fundamental and technological perspectives. We aim at understanding the contributions of the Coulomb and van-der-Waals interactions in Xe-Cs$^+$ aggregates on Cu(111). By combining time-resolved Two-Photon Photoelectron Spectroscopy (2PPE), Scanning Tunneling Microscopy (STM), and coupled cluster calculations, we investigate the microscopic structure and the ultrafast dynamics excited by photo-induced electron transfer. We observe by time-resolved 2PPE that adsorption of Xe results in a fivefold increase of the Cs 6s electron lifetime, an effect attributed to the repulsion of the Cs 6s wave function by the electron density of Xe. Furthermore, we observe by STM that the Cs$^+$...Cs$^+$ distance shrinks from 2-7 nm to 1-3 nm for the aggregates compared to bare Cs$^+$/Cu(111). The adsorption of Xe on Cs/Cu(111) results in a dual, i.e. attractive or repulsive, response of Xe depending on the positive or negative charge of the respective counterparticle, which emphasizes the dominant role of the Coulomb interaction between an alkali and a noble gas atom on the Cu(111).

This work was supported by the Cluster of Excellence RESOLV, funded by the Deutsche Forschungsgemeinschaft.

O 67.3 Wed 10:30 P

Ultrafast Dynamics of Hot Electrons and Holes by Femtosecond Photoelectron Spectroscopy in Au/Fe/MgO(001) — •Florian Kühne[1], Yasin Beyazit[1], Detlef Diesing[2], Ping Zhou[1], and Uwe Bovensiepen[1] — [1]University of Duisburg-Essen, Physics — [2]University of Duisburg-Essen, Chemistry

Optically excited electrons and holes are of particular interest in solid state physics, because they allow a microscopic understanding of interactions in non-equilibrium states. Here we aim at discerning electronic relaxation by local inelastic processes and non-local transport. To analyze the ultrafast dynamics of charge carriers in the vicinity of the Fermi energy E_F, femtosecond time-resolved linear photoelectron spectroscopy was applied and we report on results obtained by using 1.55 eV pump and 6 eV probe photons on Au/Fe/MgO(001), complementary to previous work in Beyazit et al., PRL **125**, 076803 (2020). In case of the back side pumping, hot electrons are excited in the Fe, are injected into Au and propagate to the surface, where they are probed by photoelectron emission spectroscopy. We observe a positive shift in the time delay of the transient intensity increasing with d_Au in comparison to the front pump data, which is attributed to transport effects in Au. The analyzed electron distribution in the vicinity of E_F indicates a symmetric excitation of electrons and holes. It can be described by a Fermi-Dirac distribution function. We estimate a maximum increase in the electron temperature by 50 K, which builds up within 100fs and then decays by energy transfer to phonons.

This work was funded by the DFG through the CRC 1242.

O 67.4 Wed 10:30 P

Ultrafast laser-induced electronic dynamics of perylene@MoSe$_2$ monolayer — •Matheus Jacobs[1], Jannis Krumland[1], and Caterina Cocchi[1,2] — [1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Carl von Ossietzky Universität Oldenburg Institut für Physik, Oldenburg, Germany

Hybrid interfaces formed by atomically thin semiconductors, such as transition-metal dichalcogenides, and physisorbed organic molecules have received considerable attention in the last years due to their potential for opto-electronic applications. In particular, interfacial charge transfer in the earliest stage of the photoexcitation plays a crucial role in the electronic and optical response of these systems[1]. Therefore, it is of great relevance to gain insight into the dynamics of the involved processes. In the framework of real-time time-dependent density functional theory, we investigate the ultrafast electronic dynamics at the interfaced formed by perylene physisorbed on a MoSe$_2$ monolayer. We monitor the evolution of the electrons in k-space when the hybrid system is excited by a resonant time-dependent electric field. Our results provide a valuable starting point to explore further relevant effects, such as vibronic coupling.

[1] M. Jacobs *et. al.*, Advances in Physics: X 5, 1749883(2020)

O 67.5 Wed 10:30 P

Pump-probe second harmonic spectroscopy of molecule/metal interfaces — Jinghao Chen, Ping Zhou, Uwe Bovensiepen, and •Andrea Eschenlohr — Faculty of Physics, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Achieving a microscopic understanding of charge transfer dynamics and the relaxation of optically excited electrons and holes at molecule/metal interfaces requires an interface-sensitive analysis on the respective femtosecond timescales. Second harmonic spectroscopy (SHS) [1] is such an interface-sensitive probe in centrosymmetric materials. We employ a non-collinear optical parametric amplifier in the visible wavelength range (1.9-2.5 eV) for pump-probe SHS with <20 fs pulse duration. A prototypical molecule/metal interface is prepared by adsorption of iron octaethylporphyrin (FeOEP) molecules on Cu(001) [2] and analyzed *in situ* in ultrahigh vacuum. We find a molecule-induced resonance at about 2.2 eV fundamental photon energy in the second harmonic spectrum of one monolayer of FeOEP/Cu(001). At this resonance, we observe a markedly slower relaxation time of the pump-induced changes in SHS compared to the bare Cu(001) surface, which indicates an increased lifetime of the electronic molecular state.

We thank H. Wende, J. Güdde and E. Riedle for valuable experimental advice, and the German Research Foundation for funding via SPP 1840 QUTIF and Sfb 1242.

[1] T. F. Heinz, C. K. Chen, D. Ricard, and Y. R. Shen, Phys. Rev. Lett. **48**, 478 (1982); U. Höfer, Appl. Phys. A **63**, 533 (1996).

[2] H. C. Herper et al., Phys. Rev. B **87**, 174424 (2013).

O 67.6 Wed 10:30 P

Energy transfer during resonant neutralization of hyperthermal protons at an aluminum surface studied with time-dependent density functional theory — •Lukas Deuchler and Eckhard Pehlke — Christian-Albrechts-Universität Kiel

Knowledge about the charge and energy transfer between an ion and a surface is crucial for the description of the plasma-surface interaction. In the present work, we report results from TDDFT based Ehrenfest molecular dynamics (MD) simulations for energy and charge transfer for a proton (H^+) with initial kinetic energy 2 eV – 50 eV incident normally on an Al(111) surface [1]. Simulations have been performed with the Octopus code [2]. The Al-surface is represented by an Al-cluster.

As pointed out by Winter [3], energy and angle shifts observed in the energy distribution of the scattered projectile should provide a means to experimentally estimate the neutralization distance. In this poster, we present the difference in initial kinetic energy between an H^+ and an H^0 projectile which is required to yield identical exit velocities of the H after neutralization. Notably, this difference changes sign within the studied range of kinetic energies.

[1] L. Deuchler and E. Pehlke, Phys Rev B **102**, 235421 (2020).

[2] X. Andrade et al., Phys. Chem. Chem. Phys. **17**, 31371 (2015).

[3] H. Winter, J. Phys.: Condens. Matter **8**, 10149 (1996).

O 67.7 Wed 10:30 P

Relaxation and Transport Processes of Hot Electrons in Au/Fe/MgO(001) — •Yasin Beyazit[1], Ping Zhou[1], Florian Kühne[1,2], Jan Philipp Meyburg[2], Detlef Diesing[2], and Uwe Bovensiepen[1] — [1]Faculty of Physics, University Duisburg-Essen — [2]Faculty of Chemistry, University Duisburg-Essen, Germany

This work presents an energy resolved analysis of relaxation and transport processes of excited electrons in the time domain. By employing femtosecond laser pulses with 2 eV pump energy and pulse width less than 35 fs we excite hot electrons in epitaxially grown Au/Fe/MgO(001). The photo-excited electrons exhibit local and nonlocal dynamics which lead to relaxation and transport processes of charge carriers. We perform time-resolved two photon photoelectron spectroscopy (tr-2PPE) with a particular excitation scheme; back side pumping and front side probing. The hot electrons are excited in the buried Fe layer 2 eV above the Fermi level E_F and experience subsequently spatiotemporal transport through the Fe-Au interface towards the Au surface and local inelastic relaxation. By analysis of the relaxation dynamics as a function of Au film thickness we determine the electron lifetimes of bulk Au and Fe and distinguish the relaxation in the heterostructures constituents. Furthermore, we show that the hot electrons propagate through the Au in a superdiffusive regime [1]. Additional measurements allow us to discuss contributions of secondary electrons. This study was funded by the DFG through SFB 1242. [1] Beyazit et al., PRL 125, 076803 (2020)

O 68: Poster Session V: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces I

Time: Wednesday 10:30–12:30 Location: P

O 68.1 Wed 10:30 P

Stability of radical-functionalized gold surfaces by self-assembly and on-surface chemistry — •Tobias Junghöfer, Ewa Malgorzata Nowik-Boltyk, and Maria Benedetta Casu — Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie, 72076 Tübingen, Germany

Organic radical thin films are of great interest for organic electronics such as spin filtering devices, data storage devices, and as quantum bits for quantum computing devices. Here we present the functionalisation of a gold substrate by using a derivative of the perchlorotriphenylmethyl (PTM) radical. PTM is a very chemically and thermally stable radical. We investigate the gold/PTM derivative interface by using soft X-ray techniques, such as X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Our results show that the functionalisation is successful under specific preparation conditions. The radical is still intact and keeps its magnetic character at the interface. Our findings are a significant step forward on the implementation of organic radicals in molecularbased devices with different properties and applications as energy, sensing, imaging, memories, and spintronics.

O 68.2 Wed 10:30 P

Chemical Doping of Individual Polynuclear Molecular Magnets on Surfaces — •Fabian Paschke[1], Vivien Enenkel[1], Tobias Birk[1], Jan Dreiser[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Swiss Light Source, 5232 Villigen PSI, Switzerland

The controlled deposition, characterization and manipulation of single molecule magnets (SMMs) on surfaces is one of the crucial topics to investigate with regard to their possible implementation as units in future electronic and spintronic devices. Fe_4 derivatives are among the most investigated SMMs showing a giant spin and a variety of quantum mechanical phenomena. We showed that a flat derivative of this SMM is suitable for defined adsorption on decoupling monatomic layers of *h*-BN and graphene [1,2]. We proved the robust molecular magnetism to be retained on a global and single molecule scale, even on metallic substrates [2-4]. In order to manipulate electronic and magnetic properties of individual SMMs chemical doping with alkali atoms has shown to be a feasible technique [5]. Unfortunately, large polynuclear compounds like Fe_4 can host numerous adsorption sites for dopants. Here we present successful chemical doping with a defined adsorption configuration for the prototypical Fe_4 SMM and study the effect on its electronic and magnetic properties.

[1] P. Erler et al., Nano Lett. 15, 4546 (2015). [2] L. Gragnaniello et al., Nano Lett. 17, 7177 (2017). [3] F. Paschke et al., ACS Nano 13, 780 (2019). [4] F. Paschke et al., Quantum Mater. Res. 1:e200002 (2020). [5] C. Krull et al., Nat. Mat. 12, 337 (2013).

O 68.3 Wed 10:30 P

An atomic Boltzmann machine capable of self-adaption — Brian Kiraly[1], •Elze J Knol[1], Werner MJ van Weerdenburg[1], Hilbert J Kappen[2], and Alexander A Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [2]Donders Institute, Radboud University, Nijmegen, the Netherlands

To move beyond the current hybrid approaches to hardware-based artificial neural networks, new architectures, linking physical phenomena to machine learning models, are needed. Here, we realized an atomic Boltzmann machine capable of self-adaption using atomic manipulation with a scanning tunneling microscope. We utilized the concept of orbital memory, derived from single Co atoms on black phosphorus, as the building blocks of the prerequisite multi-well energy landscape. Namely, when gating two Co atoms simultaneously, there is a finite probability in each of the four possible states. This multi-well behavior persists for larger ensembles. Additionally, we found that the coupling between Co atoms is anisotropic, which we exploited to build synapses capable of tuning the neurons' energy landscape, and to introduce two inherent timescales: a fast neural timescale and a slow synaptic timescale. Finally, we observed self-adaption of the synaptic weights in response to external electrical stimuli, opening a path to on-chip learning in atomic-scale machine learning hardware.

B. Kiraly et al., arXiv:2005.01547v2 (2020)

O 68.4 Wed 10:30 P

Tunneling anisotropic magnetoresistance of Pb and Bi adatoms and dimers on Mn/W(110) — •Soumyajyoti Haldar, Mara Gutzeit, and Stefan Heinze — Institute of Theoretical Physics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Noncollinear magnetic structures at transition-metal interfaces are very promising candidates for spintronics applications [1]. A Mn monolayer on W(110) is a prominent example which exhibits a noncollinear cycloidal spin-spiral ground state with an angle of about 173° between neighboring spins. This allows to rotate the spin-quantization axis of an adatom or dimer quasicontinuously and is ideally suited to explore the angular dependence of the tunneling anisotropic magnetoresistance (TAMR) using scanning tunneling microscopy. Here [2], using density functional theory, we explored the TAMR effect of Pb and Bi adatoms and dimers adsorbed on this surface as these elements have a very strong spin-orbit coupling. Pb and Bi adatoms and dimers show a large TAMR up to 60% due to strong spin-orbit coupling (SOC) and the hybridization of $6p$ orbitals with $3d$ states of the magnetic layer. For dimers the TAMR also depends sensitively on the dimer orientation with respect to the crystallographic directions of the surface due to bonds formation with the surface and the symmetry of the SOC induced mixing.

[1] A. Fert et al. Nat. Nanotechnol. **8**, 152 (2013). [2] S. Haldar et al. Phys. Rev. B **100**, 094412 (2019)

O 68.5 Wed 10:30 P

Local electronic structure of lanthanide metallofullerene single-molecule magnets

— •Tobias Birk[1], Fabian Paschke[1], Alexey Popov[2], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstr. 20, 01069 Dresden, Germany

Dimetallofullerenes with single-electron lanthanide-lanthanide (Ln-Ln) bonds are new promising single-molecule magnets with exceptional robustness and high blocking temperatures up to 25 K [1]. These molecules are well suited for STM based magnetization relaxation and spin excitation measurements due to their high blocking temperature and exceptional stability.

Here we present the first successful deposition of the lanthanide metallofullerene single-molecule magnet $Dy_2@C_{80}(CH_2Ph)$ on graphene/Ir(111) using electrospray deposition (ESD). Scanning tunneling microscopy (STM) and spectroscopy (STS) measurements are performed in order to study ordering behavior and electronic properties on this weak coupling substrate. The observation of LUMO resonances in combination with varying topographic appearances reveal different adsorption configurations of the molecules on the surface. Additional comparison between molecules with Dy and Er atoms as magnetic centers show a shift in LUMO energies proving that electron tunneling mediated by the single-electron Ln-Ln bond is possible.

[1] F. Liu et al. Nat Commun 10, 571 (2019).

O 68.6 Wed 10:30 P

Complete reversal of the atomic unquenched orbital moment by a single electron

— •Rasa Rejali[1], David Coffey[1], Jeremie Gobeil[1], Jhon W. González[2], Fernando Delgado[3], and Alexander F. Otte[1] — [1]Delft University of Technology, Delft, The Netherlands — [2]Universidad Técnica Federico Santa María, Valparaíso, Chile — [3]Universidad de La Laguna, Santa Cruz de Tenerife, Spain

Efforts to downscale information storage to the single-atom limit have largely focused on readily probing and manipulating the spin of single magnetic atoms adsorbed on surfaces. This emphasis on the spin is primarily due to orbital quenching combined with spin-orbit coupling: the orbital angular momentum of these systems is often diminished due to the local symmetry of the surface, and what remains of it typically delineates the direction of the electron spin. This limits the scope of information processing based on these atoms to essentially one magnetic degree of freedom: the spin. By coordinating a Fe atom atop the fourfold symmetric nitrogen binding site of the $Cu_2N/Cu_3Au(100)$ surface, we gain independent access to both the spin and orbital degrees of freedom. We demonstrate a full rotation of the orbital moment, without altering the spin state of the atom; and a distinct spin excitation, which does not affect the orbital moment. The full inversion of the unquenched moment is a seemingly forbidden transition (Δm = 4) that defies the selection rules that apply to the spin (Δm = 1); we justify this apparent violation of momentum conversation in terms of the Einstein-de Haas effect.

O 68.7 Wed 10:30 P

Hyperfine fields of magnetic adatoms on ultrathin insulating films

— •SUFYAN SHEHADA[1,2], Manuel dos Santos Dias[1], Filipe Souza Mendes Guimarães[1], Muayad Abusaa[3], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Department of Physics, Arab American University, Jenin, Palestine — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Individual nuclear spin states can have very long lifetimes and could be useful as qubits. Promising steps in this direction were realized on MgO/Ag(001) via STM detection of the hyperfine interaction (HFI) of Fe and Ti adatoms [1] and the electrical control of the nuclear polarization of Cu adatoms [2]. Here, we report on systematic first-principles calculations of the HFI for $3d$ adatoms (Sc–Cu) atop ultra-thin insulators (MgO, NaF, NaCl, h–BN and Cu_2N) [3]. We analyze the trends and the dependence of the computed HFI on the filling of the magnetic s and d-orbitals of the adatoms and on bonding type and strength with the substrate. Finally, we identify promising candidates for future experimental investigations with scanning probe techniques.

–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] Willke *et al.*, Science **362**, 336 (2018); [2] Yang *et al.*, Nat. Nanotechnol. **13**, 1120 (2018); [3] Shehada et al. ArXiv:2012.11639.

O 69: Poster Session V: Poster to Mini-Symposium: Infrared nano-optics III

Time: Wednesday 10:30–12:30 Location: P

O 69.1 Wed 10:30 P

Nano-scale analysis of Phase Change Material thin films using a Scattering-type Scanning Near-field Optical Microscope (s-SNOM)

— •Oxana Maurer, Julian Barnett, Konstantin Wirth, Lisa Schäfer, Matthias Wuttig, and Thomas Taubner — Institute of Physics (IA), RWTH Aachen

Phase Change Materials (PCMs) possess two or more different states with a distinct contrast in optical and electrical properties. The states can be switched in a reversible and non-volatile manner, leading to applications in optical and electrical data storage, but also in photonics and thermoelectrics. PCMs exhibit a bonding mechanism referred to as metavalent bonding (MVB)[1], which is characterised by a competition between electron localisation and delocalisation. Based on theoretical calculations, indications of MVB seem to persist down to the 2D limit [2], e.g GeTe shows PCM properties down to a few bilayers and its band gap is increasing for decreasing film thickness. To verify this, the optical near-field response of ultrathin PCM films are investigated with a scattering-type Scanning Near-field Optical Microscope (s-SNOM). Until now, a fundamental understanding of band gap effects on the s-SNOM contrast is lacking. Therefore, our measurements are combined with theoretical modelling to gain insight into the s-SNOM contrast changes introduced by band gaps.

[1] B. J. Kooi, M. Wuttig (2020) Adv. Mater. 32, 1908302

[2] I. Ronneberger, et al. (2020) Adv. Mater. 30, 2001033

O 69.2 Wed 10:30 P

Infrared super-resolution microscopy of phonon polariton modes by sum-frequency generation

— •Richarda Niemann[1], Sören Wasserroth[1], Guanyu Lu[2], Christopher R. Gubbin[3], Martin Wolf[1], Simone De Liberato[3], Joshua D. Caldwell[2], and Alexander Paarmann[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Vanderbilt University, Nashville, USA — [3]University of Southhampton, Southhampton, UK

Nanophotonics is based on the subdiffractional localization of light by surface polariton modes. Its devices enable the modulation of light matter interaction on the nanometer scale by specifically designed subdiffractional nanostructures. Inherently, though, the spatial resolution for optical characterization of the polaritonic modes is limited by the diffraction limit. Here, we demonstrate a novel approach that overcomes this limitation by using Infrared-Visible Sum-Frequency Generation (IR-VIS-SFG) wide-field microscopy.

After the first SFG microscopy study of a nanophotonic system [1], we here demonstrate subdiffractional spatial resolution of <1 μm when imaging phonon polariton modes in SiC nano pillar structures at a wavelength of $\lambda \approx 11$ μm using the wide-field approach. The wide tunability of the infrared free-electron laser [2] used as the infrared light source enables full spectral mapping of the polaritonic modes in various simple subdiffractional structures, providing access to the polariton mode formation for the first time.

[1] Kiessling et al., ACS Photonics, (2019)

[2] Schöllkopf et al., Proc. of SPIE (2015)

O 69.3 Wed 10:30 P

Plasmonic antenna coupling to hyperbolic phonon polaritons for sensitive and fast mid-infrared photodetection with graphene

— •Sebastian Castilla[1], Ioannis Vangelidis[2], Varun-Varma Pusapati[1], Jordan Goldstein[3], Tetiana Slipchenko[4], Luis Martin-Moreno[4], Dirk Englund[3], Klaas-Jan Tielrooij[5], Rainer Hillenbrand[6], Elefteris Lidorikis[2], and Frank Koppens[1] — [1]ICFO - The Institute of Photonic Sciences, Castelldefels (Barcelona), Spain — [2]University of Ioannina — [3]Massachusetts Institute of Technology — [4]University of Zaragoza — [5]Catalan Institute of Nanoscience and Nanotechnology (ICN2) — [6]CIC nanoGUNE

In this work, we show the realization of a new concept room temperature ultrafast infrared photodetector that exceeds any commercial technology. It has a response time of <15 nanoseconds (setup limited), while at the same time showing excellent sensitivity: we extracted a NEP down to 82 pw/$\sqrt{Hz}$ at 6 μm. Our approach consists in exploiting the efficient coupling of plasmonic antennas with hyperbolic phonon-polaritons (HPPs) in hBN for highly concentrate mid-infrared light into a graphene pn junction in order to overwhelm its low absorption and small photoactive area. The antennas plasmonic resonances spectrally overlap within the upper reststrahlen band of hBN (6-7 μm), thus launching efficiently these HPPs and guiding them with constructive interferences towards the photodetector active area. These experimental results are in excellent quantitatively agreement with a novel multiphysics model, which includes optical, thermal and electrostatic simulations.

O 69.4 Wed 10:30 P

Spectrally resolved near-field response of mid-IR phonon-polariton antennas — •Andrea Mancini[1], Christopher R. Gubbin[2], Rodrigo Berté[1], Francesco Martini[2,3], Alberto Politi[2], Emiliano Cortés[1], Yi Li[1,4], Simone De Liberato[2], and Stefan A. Maier[1,5] — [1]Chair in Hybrid Nanosystems, Nanoinstitute Munich, LMU München, Germany — [2]School of Physics and Astronomy, University of Southampton, United Kingdom — [3]Istituto di Fotonica e Nanotecnologie - CNR, Via Cineto Romano, Italy — [4]School of Microelectronics, Southern University of Science and Technology, Shenzhen, China — [5]Department of Physics, Imperial College London, United Kingdom

As the optical behavior of metals approaches the one of perfect conductors at longer wavelengths, the efficiency of plasmonic antennas for light confinement is reduced in the infrared (IR) range. Efficient field confinement in the mid-IR, which can be particularly useful for ultra-sensitive and chemically-selective spectroscopy of molecular vibrations, can be achieved with antennas supporting localized surface phonon polaritons. Due to the presence of evanescent waves that do not propagate, far-field measurements cannot fully characterize the behavior of antennas in the near-field region. We employ scattering-scanning near field optical microscopy to unveil the spectral near-field response of 3C-SiC antenna arrays. We compare far-field and near-field spectra, and demonstrate the existence of a mode with no net dipole moment, absent in far-field spectra, but of importance for applications that exploit the heightened electromagnetic near fields.

O 70: Poster Session V: Poster to Mini-Symposium: Frontiers of electronic-structure theory II

Time: Wednesday 10:30–12:30 Location: P

O 70.1 Wed 10:30 P

The coordination corrected enthalpies method in AFLOW — •Rico Friedrich[1,2], Marco Esters[1], Corey Oses[1], Stuart Ki[1], Maxwell J. Brenner[1], David Hicks[1], Michael J. Mehl[1], Mahdi Ghorbani-Asl[2], Arkady Krasheninnikov[2], Cormac Toher[1], and Stefano Curtarolo[1,3] — [1]Center for Autonomous Materials Design, Duke University, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

The AFLOW database and software leverages *ab initio* calculations for autonomous materials design [1]. The predictive power critically relies on accurate formation enthalpies - quantifying the thermodynamic stability of a compound. For polar materials such as chalcogenides (*e.g.* oxides), pnictides (*e.g.* nitrides), and halides, standard semi-local DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. Here, we introduce AFLOW-CCE: a tool where users can input a structure file of their system and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN formation enthalpies are provided. The results can be used for the computational design of *e.g.* 2D materials.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).

O 70.2 Wed 10:30 P

Non-perturbative modelling of exciton-phonon interactions in organic semiconductors — •Antonios M. Alvertis[1], Timothy J.H. Hele[2], and Bartomeu Monserrat[3] — [1]Cavendish Laboratory, University of Cambridge, J.,J.,Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Department of Chemistry, University College London, 20, Gordon Street, London WC1H 0AJ, United Kingdom — [3]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

The optoelectronic response of organic semiconductors is dominated by excitons, which often strongly interact with phonons. This makes perturbation theory insufficient for describing exciton-phonon interactions in these materials. Here we present a non-perturbative methodology for accurately capturing exciton-phonon interactions to all orders, combining finite differences methods for phonons with GW-BSE or TD-DFT calculations for crystalline or isolated systems respectively. We show that exciton spatial delocalisation is the main parameter controlling the magnitude of its coupling to phonons and reveal the microscopic mechanism of exciton temperature- and pressure-dependence in molecular crystals. Furthermore, accounting for nuclear quantum motion is found to be critical for achieving quantitative accuracy in the prediction of exciton energies, both for single molecules and periodic systems. Overall, we provide a unified picture of exciton-vibration interactions in organic semiconductors, reconciling the complementary views of finite molecular clusters and periodic molecular solids.

O 70.3 Wed 10:30 P

Ultrafast control of material optical properties via the infrared-resonant Raman effect — •Guru Khalsa, Nicole Benedek, and Jeffrey Moses — Cornell University, Ithaca, NY, USA

The Raman effect - the inelastic scattering of light by lattice vibrations - provides an important tool for conversion of light from one color to another in optical physics, and is ubiquitous in materials characterization because of its fundamental connection to crystal symmetry. The Raman effect is dominated by changes to the electronic susceptibility in the UV and visible frequency ranges. However, in the mid- and far-IR, nonlinear contributions to the lattice polarization provide additional Raman pathways, which have been little explored.

Using a combination of theory and first-principles calculations, we derive and evaluate symmetry relations and complete expressions for the Raman effect in insulating crystalline materials including all electronic and lattice-mediated pathways. We show that when infrared-active phonons are resonantly excited, the Raman effect may be dominated by direct changes to the lattice polarizability induced by Raman phonons. Applying this approach to the archetypal perovskite SrTiO3, we show that this infrared-resonant Raman effect can induce optical symmetry breaking and giant refractive index shifts that are tailored by the incident light polarization and which infrared active phonons are excited. (arXiv:2011.02010)

O 70.4 Wed 10:30 P

Non-Perturbative Theory of Charge Transport in Crystalline Solids — •Christian Carbogno and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Our understanding of charge transport in crystalline solids predominantly relies on the Boltzmann transport equation. However, its perturbative approximations for the nuclear dynamics and for its coupling to the electrons can be inaccurate in complex materials [1]. We present an alternative, non-perturbative *ab initio* Green-Kubo approach based on a new formulation of the flux viz. polarization. It can be evaluated via *ab initio* molecular dynamics and only requires gauge-fixed properties. At variance with Berry phase approaches [2], it can thus be evaluated for (semi-)conductors at finite temperatures featuring thermal electronic excitations. We demonstrate our methodology by calculating the electrical conductivity for 2D honeycomb lattices as well as for the harmonic material Si and the anharmonic perovskite $SrTiO_3$. Furthermore, we systematically compare to non-perturbative Kubo-Greenwood calculations and discuss why the latter approach has so far only been numerically applicable for materials with strong structural disorder [3], i.e., when the dispersion in reciprocal space is negligible.

[1] M. Zacharias, M. Scheffler, and C. Carbogno, *Phys. Rev. B* **102**, 045126 (2020).
[2] R. D. King-Smith and D. Vanderbilt, *Phys. Rev. B* **47**, 1651 (1993).
[3] B. Holst, M. French, and R. Redmer, *Phys. Rev. B* **83**, 235120 (2011); C. Di Paola, *et al.*, *Phys. Rev. Research* **2**, 033055 (2020).

O 70.5 Wed 10:30 P

Uncovering the Relationship Between Thermal Conductivity and Anharmonicity with Symbolic Regression — •Thomas Purcell, Matthias Scheffler, Luca Ghiringhelli, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Quantitatively understanding the link between anharmonicity and thermal conductivity, κ, is pivotal to the search for better thermal insulators. While it is qualitatively known that more anharmonic materials have a lower κ, until recently, no quantitative measure of anharmonicity existed. Here we present descriptors of κ based on our new measure of anharmonicity, σ^{A} [1]. We find the analytical expressions with symbolic regression, via the sure-independence screening and sparsifying operator (SISSO) method [2]. To better capture the nonlinearities in

the correlation between κ and σ^{A}, we introduce an automatic scaling and shifting of the input data when generating new features like $\exp(\alpha x + a)$. Using our new strategy, we generate expressions that are competitive with those previously reported in the literature using only a third of primary the features [3], and reduce the test error of the models when compared to traditional SISSO. Finally, we discuss the implications of the new models on future materials design.
[1] F. Knoop, et al. Phys. Rev. Mat. 4. 083809 (2020)
[2] R. Ouyang, et al. Phys. Rev. Mat. 2. 083802 (2018)
[3] L. Chen, et al., J. Com. Mat. Si. 170. 109155 (2019)

O 70.6 Wed 10:30 P

Excited Electron Enhanced Defect Diffusion in MgO under Ultrafast Laser Irradiation — •Yifan Yao and Andre Schleife — University of Illinois, Urbana-Champaign

Electronic excitation of defect states has been predicted to enhance ion diffusion via manipulating the explicit electron distribution. Due to the induced non-linear excitation, the ultrafast laser can offer a novel opportunity to control the electron dynamics in materials. Hence, a detailed understanding of laser-materials interaction is vital for manufacturing with nanoscale precision but still remains unclear, due to its non-linear and non-equilibrium character. Here, we use oxygen vacancy migration in MgO as an example to study the ion diffusion in laser-irradiated materials. We apply real-time TDDFT, which can accurately describe such nonlinear effects, to calculate the time-evolution of the occupation number under different laser frequencies and intensities. Comparison to the distribution of hot electrons following proton irradiation can provide insights into how diffusion enhancement can be achieved by the transient localized electron dynamics and how it depends on specific laser parameters.

We acknowledge ONR N00014-18-1-2605 for financial support.

O 70.7 Wed 10:30 P

Modelling the structural and charge transport properties of merocyanine single-crystals — •Nora Gildemeister[1], Fabrizia Negri[2], Klaus Meerholz[1], and Daniele Fazzi[1] — [1]Insitut für Physikalische Chemie, Department Chemie, Universität zu Köln, Greinstr. 4-6, D - 50939 Köln — [2]Dipartimento di Chimica, Università di Bologna, via F. Selmi 2, 40126 Bologna, Italy

Merocyanines are highly polar organic π-conjugated molecules investigated for their self-assembly and optoelectronic properties. The accurate description of their molecular, electronic and vibrational structure remains a challenge due to strong electron correlation effects and long-range inter-molecular interactions. [1-2]

We report a comprehensive analysis modelling intra- and inter-molecular charge transport properties for a library of different donor-acceptor units and lateral groups. We found that constrained DFT is an effective embedding method to correctly assess the molecular and electronic structure in single crystals. Charge mobilities were computed within the semiclassical nonadiabatic electron-transfer theory by analysing different single crystals and highlighting the impact of side groups and casting conditions. Computed and experimental values are in good agreement. Our modelling suggests that charge diffusion is maximized when dipolar molecules are packed in slipped anti-symmetric pairs, arranged in 2D interconnected architectures. [3]

[1] C. Brückner, et al., J. Phys. Chem. C 2015, 17602-17611. [2] D. Bialas, et al., J. Phys. Chem. C 2019, 123, 30, 18654-18664. [3] N. Gildemeister, et al. Paper in preperation.

O 71: Mini-Symposium: Machine learning applications in surface science I

Time: Wednesday 13:30–15:30 Location: R1

Opening remarks

Invited Talk O 71.1 Wed 13:45 R1

Machine learning for novel functional materials — •Pascal Friederich — Karlsruhe Institute of Technology, Germany

During the last decade, machine learning (ML) algorithms were increasingly applied to questions in the physical sciences, e.g. to automate labs, to accelerate simulations, and to solve inverse problems such as the design of new materials. This talk will show our recent work on combining ML models with conventional tools to accelerate simulations and to obtain new scientific insight. Firstly, we show that ML enables the analysis of energy disorder in amorphous organic semiconductors which is of high relevance to understand charge transport in devices such as OLEDs.[1] Secondly, we will show how ML models can accelerate ab-initio photodynamics simulations of small molecules to unprecedented simulation times of 10 ns and more.[2] Thirdly, we will show how a combination of graph representations and basic ML regression models can provide scientific insight into organic electronics as well as quantum optical experiments in a highly intuitive and human interpretable way.[3]

[1] The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS, P. Friederich, S. Leon, J. D. Perea Ospina, L. Roch and A. Aspuru-Guzik, MLST, 2020. [2] Nanosecond Photodynamics Simulations of a cis-transIsomerization are Enabled by Machine Learning, J. Li, P. Reiser, A. Eberhard, P. Friederich, and S. A. Lopez, DOI: 10.26434/chemrxiv.13047863.v1, 2020. [3] Scientific intuition inspired by machine learning generated hypotheses, P. Friederich, M. Krenn, I. Tamblyn, A. Aspuru-Guzik, arXiv:2010.14236, 2020.

O 71.2 Wed 14:15 R1

Automated Tip Functionalization and Image interpretation with Machine Learning in Atomic Force Microscopy — Benjamin Alldritt[1], Chen Xu[1], Prokop Hapala[2], Ondrej Krejci[1], •Fedor Urtev[1], Filippo Federici Canova[1,3], Juho Kannala[1], Peter Liljeroth[1], and Adam Foster[1,4,5] — [1]Aalto University, Espoo, Finland — [2]Czech Academy of Sciences, Prague, Czechia — [3]Nanolayers Research Computing Ltd., London, UK — [4]Graduate School Materials Science in Mainz, Germany — [5]WPI Nano Life Science Institute, Kanazawa, Japan

Atomic force microscopy (AFM) is ubiquitous nanoscale characterisation technique to measure a 3D map of surface roughness at atomic resolutions [1]. AFM data interpretation and quantitative analysis for complex mixtures of molecules and bulky 3D molecules can be difficult [2], due to the complex nature of contrast in AFM images, and need significant acceleration and automation to make AFM technique available to a wide range of laboratories and clinics. Here, we introduce a machine learning (ML) approach both for the preparation of AFM experiments and for data interpretation in AFM. For the first objective our method involves a convolutional neural network (CNN) that has been trained to analyse the quality of a CO-terminated tip. For the interpretation of AFM images, we introduce ML image descriptors characterising the molecular configuration, allowing us to predict the molecular structure directly. [1] L. Gross et al., Science, vol. 325, no. 5944, (2009). [2] O. M. Gordon and P. J. Moriarty, Mach. Learn. Sci. Technol., vol. 1, no. 2, (2020).

O 71.3 Wed 14:30 R1

Automatic image evaluation of aberration-corrected HRTEM images of 2D materials. — •Christopher Leist, Haoyuan Qi, and Ute Kaiser — Central Facility for Electron Microscopy,of Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany

Aberration-corrected high-resolution transmission electron microscopy (HRTEM) allows for unambiguous elucidation of atomic structures down to sub-Angstrom scale. By determining the positions of each single atom, the distribution and local variation of bond lengths and angles can be evaluated statistically. However, conventional image analysis methods, e.g., handcrafted filter kernels, often requires heavy user supervision and tremendous time cost, posing strong limitations on the data volume for statistical analysis. The incompetence in handling big data volume also incurs the risk of user-induced selection bias, leading to overestimation of low-probability phenomena. Here, we developed a neural network of U-net architecture for automatic analysis of atomic positions in HRTEM images. A combination of networks can be applied to automatically evaluate image series, including automatic exclusion of image regions unusable for evaluation. This method results in large statistics thus reducing the impact of individual errors. The networks are trained with simulated data which reduces user bias and gives a time inexpensive way of generating the required training data. Its implementation on various 2D carbon materials is compared to one another. The distribution of bond angles in CVD graphene, determined by this method, shows excellent agreement with literature.

O 71.4 Wed 14:45 R1

Active Discovery of Organic Semiconductors — •Christian Kunkel[1,2], Johannes T. Margraf[1], Ke Chen[1], Harald Oberhofer[1], and Karsten Reuter[1,2] — [1]Chair for Theoretical Chemistry and Catalysis Research Center — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft

Improving charge-transport of organic semiconductors (OSCs) for electronic applications is usually tackled by empirical structural tuning of promising compounds. Howver, the versatility of organic molecules generates a rich design space whose vastness dictates efficient search strategies. We thus here present an active machine learning (AML) approach that explores this virtually unlimited design space iteratively. Judging suitability of OSC candidates by charge injection and mobility-related descriptors, the AML approach iteratively queries first-principle evaluation on well-selected molecules. We first optimize the approach in a fully characterized, but truncated molecular test space, gaining deep methodological insight about its exploratory behavior. Outperforming a conventional computational funnel, the devised algorithm can thereby successfully leverage its gradually improving knowledge and focus on promising regions of the design space. When subsequently lifting the artificial truncation, high-performance candidates are constantly found while the algorithm meanders ever more deeply through the endless OSC design space. The demonstrated high efficiency in the detection of candidate compounds with superior charge conduction properties highlights the usefulness of autonomously operating systems for a targeted OSC design.

Invited Talk O 71.5 Wed 15:00 R1

Theory-informed Machine Learning for Surface and Interface Structure Reconstruction from Experimental Data — Eric Schwenker[1,2], Chaitanya Kolluru[1,3], Marcel Chlupsa[1], Arun Mannodi Kanakkithodi[1], Richard Hennig[3], Pierre Darancet[1,2], and •Maria Chan[1,2] — [1]Argonne National Laboratory, Lemont, USA — [2]Northwestern University, Evanston, USA — [3]University of Florida, Gainsville, USA

Determining atomistic structure at surfaces and interfaces is challenging because metastable surfaces/interfaces are likely accessible under realistic conditions, rendering energy-only searches insufficient, and experimental data often give incomplete information. Therefore, neither theory nor experimental data alone is sufficient to determine these structures. In this talk, we will discuss how we use machine learning to combine experimental and theory-based data to determine surface and interface structures.

O 72: Mini-Symposium: Coherent band structure engineering with light II

Time: Wednesday 13:30–15:30 Location: R2

Invited Talk O 72.1 Wed 13:30 R2

On the survival of Floquet-Bloch states in the presence of scattering — •Isabella Gierz — University of Regensburg, Institute for Experimental an Applied Physics

Floquet theory has spawned many exciting possibilities for electronic structure control. The experimental realization in solids, however, still largely remains pending. Despite the enormous potential for future applications, the influence of scattering on the formation of Floquet-Bloch states remains poorly understood. Here we combine time- and angle-resolved photoemission spectroscopy (tr-ARPES) with time-dependent density functional theory (TDDFT) and a simple two-level system with dissipation to investigate the survival of Floquet-Bloch states in the presence of scattering. We find that Floquet-Bloch states will be destroyed if scattering — activated by electronic excitations — prevents the Bloch electrons from following the driving field coherently. The two-level system also shows that Floquet-Bloch states reappear at high field intensities where energy exchange with the driving field dominates over energy dissipation to the bath. Our results clearly indicate the importance of long scattering times combined with strong driving fields for the successful realization of various Floquet phenomena.

O 72.2 Wed 14:00 R2

Ultrafast spin-dependent band structure renormalization of a molecular/2D semiconductor heterostructure by the formation of interlayer excitons — •Benito Arnoldi[1], Sebastian Hedwig[1], Sara Zachritz[2], Oliver L.A. Monti[2,3], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics, University of Kaiserslautern, Erwin-Schroedinger-Strasse 46, Kaiserslautern 67663, Germany — [2]Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721, United States — [3]Department of Physics, University of Arizona, Tucson, Arizona 85721, United States

Engineering the spin-dependent band structure of atomically thin materials with ultra-short light pulses offers the intriguing possibility to control spin and charge carrier functionalities on smallest length and fastest time-scales. Here, we explore the transient band structure dynamics of a heterostructure between C_{60} and WSe_2 after optical excitation with fs light pulses. The ultrafast charge carrier dynamics of the interface is investigated by time-, spin- and angle-resolved photoemission spectroscopy. Resonant optical excitation of the molecular layer instantaneously results in the formation of excitons within the C_{60} layer. These excitons transform within 200 fs into interlayer excitons, which are trapped at the heterostructure interface for 14 ps. Most interestingly, the formation of the interlayer excitons coincides with a transient spin-dependent renormalization of the valence band structure of WSe_2. This transient spin texture modification is attributed to the charge transfer character to the interlayer excitons at the interface.

O 72.3 Wed 14:15 R2

Ultrafast Dynamical Lifshitz Transition — •Samuel Beaulieu[1,2], Shuo Dong[1], Nicolas Tancogne-Dejean[3], Maciej Dendzik[1,4], Tommaso Pincelli[1], Julian Maklar[1], R. Patrick Xian[1], Michael Sentef[3], Martin Wolf[1], Angel Rubio[3,5], Laurenz Rettig[1], and Ralph Ernstorfer[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Université de Bordeaux - CNRS - CEA, CELIA, UMR5107, F33405 Talence, France — [3]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Department of Applied Physics, KTH Royal Institute of Technology, Electrum 229, SE-16440, Stockholm, Kista, Sweden — [5]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010

Fermi surface is at the heart of our understanding of metals and strongly correlated many-body systems. An abrupt change in the Fermi surface topology, also called Lifshitz transition, can lead to the emergence of fascinating phenomena like colossal magnetoresistance and superconductivity. Combining time-resolved multidimensional photoemission spectroscopy with state-of-the-art TDDFT+U simulations, we introduce a novel scheme for driving an ultrafast Lifshitz transition in the correlated type-II Weyl semimetal T_d-$MoTe_2$. We demonstrate that this non-equilibrium topological electronic transition finds its microscopic origin in the dynamical modification of the effective electronic correlations.

Invited Talk O 72.4 Wed 14:30 R2

Light-induced anomalous Hall effect in graphene — •James McIver — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Optical driving has been proposed as a means of engineering topological properties in topologically trivial systems. One proposal for such a "Floquet topological insulator" is based on breaking time-reversal symmetry in graphene through a coherent interaction with circularly polarized light [1]. This was predicted to lift the degeneracy of the Dirac point, opening a topological band gap in the resulting photon-dressed band structure accompanied by the formation of dressed chiral edge states [2]. In this talk, I will report on our recent observation of a light-induced anomalous Hall effect in monolayer graphene driven by an intense femtosecond pulse of circularly polarized light [3]. We probed electrical transport using an ultrafast device architecture based on photoconductive switches. The dependence of the anomalous Hall effect on a gate potential used to tune the equilibrium Fermi level revealed multiple features that reflect a Floquet-engineered topological band structure. This included an approximately 60 meV wide conductance plateau centered at the Dirac point, where a gap of equal magnitude was predicted to open. We found that when the Fermi level was tuned within this plateau, the estimated anomalous Hall conductance saturated around 1.8 +/- 0.4 e^2/h. [1] T. Oka & H. Aoki. Phys. Rev. B 79, 081406 (2009) [2] T. Kitagawa et al. Phys. Rev. B 84, 235108 (2011) [3] J.W. McIver et al. Nature Physics 16, 38 (2020)

O 72.5 Wed 15:00 R2

Observing Light-Induced Floquet Band Gaps in the Longitudinal Conductivity of Graphene — •Lukas Broers[1,2] and Ludwig Mathey[1,2,3] — [1]Center for Optical Quantum Technologies, University of Hamburg, 22761 Hamburg, Germany — [2]Institute for Laser Physics, University of Hamburg, 22761 Hamburg, Germany — [3]The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We propose optical longitudinal conductivity as a realistic observable to detect light-induced Floquet band gaps in graphene. These gaps manifest as resonant features in the conductivity, when resolved with respect to the probing frequency and the driving field strength. We demonstrate these features via a dissipative master equation approach which gives access to a frequency- and momentum-resolved electron distribution. This distribution follows the light-induced Floquet-Bloch bands, resulting in a natural interpretation as occupations of these bands. Furthermore, we show that there are population inversions of the Floquet-Bloch bands at the band gaps for sufficiently strong driving field strengths. This strongly reduces the conductivity at the corresponding frequencies. Therefore our proposal puts forth not only an unambiguous demonstration of light-induced Floquet-Bloch bands, which advances the field of Floquet engineering in solids, but also points out the control of transport properties via light, that derives from the electron distribution on these bands.

Open discussion

O 73: Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems II

Time: Wednesday 13:30–15:30 Location: R3

Invited Talk O 73.1 Wed 13:30 R3

Theoretical insights into Dzyaloshinskii-Moriya interaction in nanostructures based on transition metals, oxides and 2D materials — •Mairbek Chshiev — Univ. Grenoble Alpes, CNRS, CEA, Spintec, Grenoble, France

Spin-orbit coupling (SOC) based phenomena at interfaces comprising ferromagnetic (FM) and nonmagnetic (NM) metals, oxides (O) and/or 2D materials have been of major interest [1,2]. Here we elucidate microscopic mechanisms of Dzyaloshinskii-Moriya interaction at FM/NM [3,4], FM/O [4,5] and FM/2D [6,7] interfaces. In particular, we show that while the DMI at FM/NM interfaces is governed by Fert-Levy model [3], in case of FM/O or FM/graphene interfaces the DMI is mainly due to Rashba SOC [4,6]. In addition, several approaches for DMI enhancement are presented [4] that allowed observation of room temperature skyrmions [5]. Possibility of controlling DMI by voltage (VCDMI) at NM/FM/O [4,8] or by hydrogenation at FM/graphene interfaces [7] are discussed as well. Finally, DMI mechanisms and potential of realizing skyrmion states in 2D magnets are discussed [9,10].

[1] B. Dieny and M. Chshiev, Rev. Mod. Phys. 89, 025008 (2017); [2] S. Roche et al, 2D Materials 2, 030202 (2015); [3] H. X. Yang et al, Phys. Rev. Lett. 115, 267210 (2015); [4] H. X. Yang et al, Sci. Rep. 8, 12356 (2018); [5] O. Boulle et al, Nat. Nanotech. 11, 449 (2016); [6] H. X. Yang et al, Nat. Mater. 17, 605 (2018); [7] B. Yang et al, Phys. Rev. B 101, 014406 (2020); [8] T. Srivastava et al, Nano Lett. 18, 4871 (2018) [9] J. Liang et al, Phys. Rev. B 101, 184401 (2020); [10] T.-E. Park et al, arXiv:1907.01425.

O 73.2 Wed 14:00 R3

Prospecting chiral multi-site interactions in prototypical magnetic systems — •Manuel dos Santos Dias[1], Sascha Brinker[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Atomistic spin models can successfully explain the properties of magnetic materials once the relevant magnetic interactions are identified. Recently, new types of chiral interactions that generalize the Dzyaloshinskii-Moriya interaction have been proposed [1,2,3,4]. Here, we present a systematic construction of a generalized spin model containing isotropic and chiral multi-site interactions, motivated by a microscopic model, and their symmetry properties are established. We show that the chiral interactions arise solely from the spin-orbit interaction and that the multi-site interactions do not have to follow Moriya's rules, unlike the Dzyaloshinskii-Moriya interaction [1,4]. We then report on density functional theory calculations for prototypical magnetic systems, Cr, Mn, Fe and Co trimers and tetrameters on the Re(0001), Pt(001), Pt(111) and Au(111) surfaces. The multi-site interactions are substantial in magnitude and cannot be neglected when comparing the energy of different magnetic configurations.

[1] S. Brinker, M. dos Santos Dias and S. Lounis, New J Phys **21**, 083015 (2019); [2] A. Lászlóffy *et al.*, Phys Rev B **99**, 184430 (2019); [3] S. Grytsiuk *et al.*, Nat Commun **11**, 511 (2020); [4] S. Brinker, M. dos Santos Dias and S. Lounis, Phys Rev Research **2**, 033240 (2020)

O 73.3 Wed 14:20 R3

DMI in intercalated Pt/Co/graphene thin films: localization in reciprocal and real space — Maria Blanco-Rey[1,2], Mikhail Otrokov[3,4,2], Andres Arnau[4,1,2], and •Jorge I. Cerda[5] — [1]Universidad del Pais Vasco UPV/EHU, Spain — [2]Donostia International Physics Center DIPC, Spain — [3]Ikerbasque Foundation, Spain — [4]Centro de Fisica de Materiales CFM, CSIC-UPV/EHU, Spain — [5]Instituto de Ciencia de Materiales de Madrid ICMM, CSIC, Spain

The Dzyaloshinskii-Moriya interaction (DMI) of Pt(111)/Co and Pt(111)/Co/G films (G=graphene), with face-centered tetragonal Co, has been studied by first-principles calculations in two thickness regimes. For ultrathin Co we find that interlayer additivity of the DMI breaks down and the D-vectors acquire a sizable out-of-plane component. For 5ML Co, DMI localizes at the interfaces and is mainly contributed by the Pt/Co interface. Indeed, an spectral analysis in reciprocal space shows the largest DMI contributions at the crossings of highly-dispersive Pt substrate bands with Co-d bands. Interestingly, the Co/vaccum interface chirality, which is the same as in Pt/Co and smaller in energy by only one order of magnitude, is switched by the effect of graphene. We find that, to account for the DMI energy in this system, a model that includes at least second nearest-neighbour lateral Co-Co interactions is needed.

Invited Talk O 73.4 Wed 14:40 R3

Dzyaloshinskii-Moriya Interaction in magnetic layered systems — •Albert Fert — CNRS-Thales, Palaiseau, France

I will be the moderator of the mini-Symposium Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems. The DMIs are generated by the combination of the spin-orbit coupling and the breaking of inversion symmetry by the interfaces of the layered systems. There are related to the Rashba interactions generated by the same conditions. We will discuss the relation between DMI and Rashba in the different situations of metal/metal or metal/oxide interfaces and van der Waals interfaces.

O 74: Poster Session VI: Oxide and insulator surfaces: Structure, epitaxy and growth II

Time: Wednesday 13:30–15:30 Location: P

O 74.1 Wed 13:30 P

Reduction of the α-$Fe_2O_3(1\bar{1}02)$ surface to Fe_3O_4 — •Erik Rheinfrank[1], Giada Franceschi[1], Igor Sokolović[1], Jesús Redondo[2], Pavel Procházka[3], Nishant Kumar[3], Ondřej Man[3], Jan Michalička[3], Jan Čechal[3], Michael Schmid[1], Gareth S. Parkinson[1], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic — [3]CEITEC, Brno, Czech Republic

Iron oxides list among the most abundant compounds in Earth's crust and are involved in many natural processes as well as in a wide range of applications. To understand their fundamental surface-chemical properties it is crucial to reproducibly prepare atomically well-defined surfaces in a controlled environment. Here we report on the local reduction of the α-$Fe_2O_3(1\bar{1}02)$ surface by two processes. First, by annealing in ultra high vacuum (UHV) at 450 °C and subsequent sputtering and annealing in low 10^{-6} mbar O_2 at 450 °C, and second, by annealing in UHV at 600 °C. Atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS) reveal that both routes lead to the formation of boulder-like magnetite inclusions. Once they are created, the preferential removal of oxygen by sputtering enhances their formation instead of removing them. A pristine hematite surface can be recovered by exposure to higher oxygen pressures (1 mbar) at ~ 850°C. The nature of these Fe_3O_4 inclusions was studied by low-energy electron microscopy (LEEM) and low-energy electron diffraction (LEED).

O 74.2 Wed 13:30 P

Fe_3O_4 (001) near-surface diffusion observed by nuclear resonant scattering (NRS) — •Steffen Tober[1,2], Jan-Christian Schober[1,2], Esko Erik Beck[1,2], Guilherme Dalla Lana Semione[1,2], Simon Chung[1,2], Kai Schlage[1], Olaf Leupold[1], Ilya Sergeev[1], René Steinbrügge[1], Hans-Christian Wille[1], Heshmat Noei[1], Vedran Vonk[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron, Hamburg — [2]Universität Hamburg, Fachbereich Physik

Elevated temperature cation transport processes influence the structure and stoichiometry in the near surface region of magnetite (Fe_3O_4) (001) which is of crucial importance for the performance of magnetite-based catalysts and devices [1,2]. Near surface transport was studied by stepwise annealing of a homoepitaxially grown $^{57}Fe_3O_4$ layer on a (001) oriented Fe_3O_4 single crystal, monitored by nuclear resonant reflectivity (NRR) and time spectra (TS) after each step. Site selective depth profiles obtained from simultaneous fitting of NRR and TS indicate transport from 470 K on. Diffusion constants estimated from the ^{57}Fe depth profiles were in good agreement with previous results [4], while the site-selectivity of NRS revealed notable differences in the transport of oct- and tet coordinated cations enabling a more precise description of the diffusion process.

[1] Arndt et al. Chem. Comm. 1, 92 (2019) [2] Arndt et al. Surf. Sci. 653, 76 (2016) [3] Andreeva et al., Mosc. Univ. Phys. Bull. 63, 132 (2008) [4] Tober et al., Phys Rev Research. 2, 023406 (2020)

O 74.3 Wed 13:30 P

Strongly Strained VO_2 Thin Film Growth — •Simon Fischer[1], Jan Ingo Flege[2], Michael Foerster[3], Lucia Aballe[3], Jens Falta[1], and Jon-Olaf Krisponeit[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus, Germany — [3]ALBA Synchrotron Light Facility, Barcelona, Spain

The semiconductor-metal transition temperature of VO_2 strongly shifts as a result of strain applied along the rutile *c* axis, making it interesting for various switching applications, as smart coatings and as sensors. In the past, this has been demonstrated, for instance, through the application of epitaxial strain on TiO_2 substrates.

We extend this tailoring approach by utilizing the much larger lattice mismatch of 8.78 % occurring in the VO_2/RuO_2 system for orientations where the *c* axis lies in-plane. Depositing vanadium oxide by atomic oxygen-supported reactive MBE on an oxidized Ru(0001) template, we have grown VO_2 thin films on single domain RuO_2 islands with distinct orientations. Locally resolved electron spectroscopy was used to ascertain the correct stoichiometry of the grown VO_2 films on all template island types. Low energy electron diffraction reveals the VO_2 films to grow indeed fully strained on RuO_2(110) but fully relaxed on RuO_2(100).

Hence, the presented template allows for simultaneous access to a remarkable strain window ranging from bulk-like structures to regions of massive tensile strain.

O 74.4 Wed 13:30 P

XPS and UPS investigation of an ALD prepared Al_2O_3/ZnO heterojunction — •Christoph Janowitz[1], Ali Mahmoodinezhad[1], Franziska Naumann[2], Paul Plate[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

The band alignment of two large band gap oxides was studied by a combination of XPS and UPS using consecutive sputter steps to unravel the electronic structure and elemental composition of each layer and the interface region. An Al_2O_3/ZnO heterointerface (10 nm Al_2O_3 on 59 nm ZnO) was grown on top of a Si single crystal substrate by consecutive thermal and plasma-assisted atomic layer deposition (ALD) respectively. The valence band maximum of Al_2O_3 was found to be 1.1 eV below that of ZnO, the conduction band minimum 2.3 eV above, resulting in a type-I staggered heterojunction. A reduction of ZnO to elemental Zn in the interface region was detected by the apparent shoulder of the Zn 2p and 2s core levels and by the Zn LMM Auger. This suggests an ALD interface formation mechanism different from previous models identified for other heterointerfaces.

O 74.5 Wed 13:30 P

Functional ultra-thin oxide films deposited by atomic layer deposition on structured substrates — •Carlos Morales[1], Ali Mahmoodinezhad[1], Andreas Markus Schubert[2], Christian Wenger[2], Karsten Henkel[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Strasse 1, D-03046 Cottbus, Germany — [2]IHP - Leibniz-Institut für innovative Mikroelektronik, IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

In the last decades, atomic layer deposition (ALD) has gained prominence in the materials and surface science communities owing to its high potential for integration as a scalable process in microelectronics. ALD's largest strengths are its well-controlled layer-by-layer deposition and growth conformity on 3D structures. Yet, the ALD technique is also well known to lead to amorphous and defective, non-stoichiometric thin films, resulting in modified materials properties that may even preferentially be used in certain applications. To study these issues, we have developed an in-situ ALD reactor attached to an X-ray photoelectron spectroscopy (XPS) system, capable of switching between both pump and flow-type operation. This novel tool allows to cover the entire range of compounds and recipes used in ALD, thus clarifying the role of such defects at different deposition stages, growth conditions and film/substrate interfaces. To exemplify these sorts of studies, we show the deposition of Al2O3 5-10 nm films on nanostructured Si, and their use as substrates for functional CeOx ALD deposits.

O 74.6 Wed 13:30 P

Phase diagrams of Co_3O_4 and Mn_3O_4 surfaces under different experimental conditions — •Maria Fernanda Juarez[1], Hui Yin[1,2], and Axel Gross[1] — [1]Ulm University, Ulm, Germany — [2]South China University of Technology, Guangzhou, P. R. China

In spite of the many advantageous features of the zinc-air batteries (ZABs), one of the basic problems for its uses is the slow kinetics of oxygen evolution and reduction reactions (OER and ORR) [1]. In recent years many effort has devoted to solve this problem by finding new electrocatalysts that promote both reactions or by changing the experimental conditions and thence the reaction mechanism[2].

Presently, Mn and Co oxides are among the most active electrochemical catalysts. By doping or by introducing oxygen vacancies, the electronic configuration of the metal ions can be modified, changing their interaction with the adsorbed species and leading to modifications in the catalytic activity.

It is the objective of this work to determine the proper surface structure of Mn_3O_4 and Co_3O_4 (111) surfaces under the experimental conditions of operating ZABs: oxidating or reducting environments and non-alkaline electrolytes. Using the concept of the computational hydrogen electrode [3], we will obtain the equilibrium structures as a function of potential and OH^- concentration. As hydroxyls are strongly interacting with water, the presence of water will be taken into account.

[1] D. Yang *et al.* Elect. Energy Rev. (2019) 2:395.
[2] Sun *et al.* Science (2021) 371:46.
[3] Norskøv *et al.* J. Phys. Chem. B (2004) 108:17886.

O 74.7 Wed 13:30 P

High temperature reduction and reoxidation of cerium oxide on Cu(111) — •Linus Pleines[1], Lars Buss[1,2], Tevfik Onur Menteş[3], Francesca Genuzio[3], Andrea Locatelli[3], Jan Ingo Flege[2], and Jens Falta[1,4] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]ELLETRA Synchrotron Light Source, Basovizza, Italy — [4]MAPEX Center for Materials and Processes, Bremen, Germany

Cerium oxide is of great interest due to its technological importance in various electronic, optical and catalytic applications. The inverse model catalyst cerium oxide on Cu(111) shows a high activity for the production of methanol. Oxygen vacancies, e.g. in form of reduced ceria, are necessary for the production of methanol from CO_2 and H_2. The reduction of ceria may be achieved by exposure to H_2 at elevated temperatures. We studied the interaction of H_2 and CO_2 with cerium oxide islands on a Cu(111) substrate with low-energy electron microscopy (LEEM) and x-ray absorption spectroscopy (XAS). From earlier studies, the orientation of the cerium oxide is known to be decisive for the catalytic activity. In our experiments, the impact of both orientations are directly compared via growth of (100) and (111) cerium oxide islands side by side. At temperatures around 550 °C, exposure to H_2 leads to partial reduction and exposure to CO_2 leads to complete reoxidation of the cerium oxide. The (100) and (111) orientations show different reduction and reoxidation behaviors.

O 74.8 Wed 13:30 P

Low-temperature atomic layer deposition of indium oxide thin films using trimethylindium and oxygen plasma — •Ali Mahmoodinezhad[1], Carlos Morales[1], Franziska Naumann[2], Paul Plate[2], Robert Meyer[2], Christoph Janowitz[1], Karsten Henkel[1], Małgorzata Kot[1], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, K.-Zuse-Str. 1, 03046 Cottbus, Germany — [2]SENTECH Instruments GmbH, Schwarzschildstraße 2, 12489 Berlin, Germany

Indium oxide thin films were deposited on Si (100) by plasma-enhanced atomic layer deposition (PEALD) using trimethylindium (TMIn) and oxygen plasma (O2) in a low-temperature range of 80 to 200 °C. The In_2O_3 layers were characterized by in-situ spectroscopic ellipsometry (SE), ex-situ X-ray photoelectron spectroscopy (XPS) and electrical measurements. The SE data show a growth rate of 0.56 Å/cycle within the ALD window (100 to 150 °C) with a thickness inhomogeneity of $\leq$ 1.2%. In addition, the highest refractive index is 2.07 (at 632.8 nm) for the layer grown at 150 °C, and the films exhibit indirect and direct band gaps of 2.8±0.1 eV and 3.3±0.2 eV, respectively. XPS characterization indicates no carbon incorporation and a temperature-dependent off-stoichiometry of the layers. The chemical analysis of the In 3d and O 1s core levels confirms the formation of In-O bonds and suggests the additional presence of hydroxyl groups and defects. With increasing temperature, the contribution of OH groups and defects decreases whereas that of In-O bonds increases. Notably, higher growth temperatures result in an indium rich phase within the layers.

O 75: Poster Session VI: Organic molecules on inorganic substrates: electronic, optical and other properties II

Time: Wednesday 13:30–15:30 Location: P

O 75.1 Wed 13:30 P

Temperature induced conformational changes in phospholipid monolayers studied by sum-frequency spectroscopy — Damian Firla, •Tim Lämmerzahl, Matthias Linke, and Eckart Hasselbrink — Universität Duisburg-Essen, Germany

Phospholipids are a major component in cell membranes because they form bilayers due to their amphiphilic character. This was exploited to prepare monolayers on glass substrates using the Langmuir-Blodgett technique to study them by sum frequency spectroscopy (SFS). The main goal was to observe structural changes upon raising the temperature. SFS probes the local centrosymmetry of the methylene groups because of its inherent selection rules. Therefore, conformational disorder of the alkyl chains due to the increased temperature, and thus breaking of the local centrosymmetry, can be directly observed. Typically, *gauche* defects are observable by an increase of the intensities of CH_2 vibrational modes. Different types of phospholipids and mixtures of phospholipids with varying chain lengths were studied. Monolayers prepared using a single phospholipid species showed only changes of the intensity of CH_3 vibrational modes with rising temperatures. Furtheron, mixtures of phospholipids with different chain lengths were studied. In these cases CH_2 modes were observed as well, consistent with the larger space being available for conformational changes. The thermal stability of phopholipid monolayers was also examined. We found that monolayers of single phospholipid species were more stable than monolayers of phospholipid mixtures. Divalent cations also increased the thermal stability of these monolayers.

O 75.2 Wed 13:30 P

Rotation of Ethoxy and Ethyl Moieties on a Molecular Platform on Au(111) — Torben Jasper-Tönnies[1], Manuel Gruber[1], Sven Johannsen[1], Thomas Frederiksen[2], Aran Garcia-Lekue[2], Torben Jäkel[3], Fynn Roehricht[3], Rainer Herges[3], and •Richard Berndt[1] — [1]Institut fur Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel — [2]Donostia International Physics Center, E-20018 Donostia-San Sebastián; IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao — [3]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel

Molecular rotors have attracted considerable interest for their prospects in nanotechnology. However, their adsorption on supporting substrates, where they may be addressed individually, usually modifies their properties. Here, we investigate the switching of two closely-related three-states rotors mounted on platforms on Au(111) using low-temperature scanning tunneling microscopy and density functional theory calculations. Being physisorbed the platforms retain important gas-phase properties of the rotor. This simplifies a detailed analysis, and permits, for instance, the identification of the vibrational modes involved in the rotation process. The symmetry provided by the platform enables active control of the rotation direction through electrostatic interactions with the tip and charged neighboring adsorbates. The present investigation of two model systems may turn out useful for designing platforms that provide directional rotation and for transferring more sophisticated molecular machines to surfaces.

O 75.3 Wed 13:30 P

'Magnetic Coupling in Clusters of Rhombus-Shaped Nanographenes — •Nils Krane[1], Xuelin Yao[2], Qiang Chen[2], Kristjan Eimre[1], Carlo A. Pignedoli[1], Klaus Müllen[2], Pascal Ruffieux[1], Akimitsu Narita[2,3], and Roman Fasel[1,4] — [1]nanotech@surfaces Laboratory, Empa - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [2]Department of Synthetic Chemistry, Max Planck Institute for Polymer Research, Mainz, Germany — [3]Organic and Carbon Nanomaterials Unit, Okinawa Institute of Science and Technology Graduate University, Okinawa, Ja-pan — [4]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

The exact tailoring of open-shell nanographenes (NGs) with non-trivial magnetic ground states opens a pathway towards carbon-based molecular spintronics. The synthesis of these NGs remains challenging, due to their high reactivity. Embedding the NGs into a non-magnetic molecular network on the surface could allow for a passivation and more controlled growth.

In this work, we passivated 5-rhombenes [1] with p-terphenyl linkers, creating one-dimensional non-magnetic backbones in which the NGs are embedded. Scanning tunneling spectroscopy and inelastic electron tunneling spectroscopy reveal the antiferromagnetic ground state with a large magnetic coupling constant to be preserved upon passivation. Furthermore, magnetically coupled dimers of 5-rhombenes embedded in the phenyl backbone have been investigated.

[1]: Mishra et al.: https://arxiv.org/abs/2003.03577 (2020)

O 75.4 Wed 13:30 P

Decoupled or not decoupled? Investigation of charge transfer in organic/2D insulator/metal interfaces — •Maximilian Schaal[1], Iliyan Karadzhov[1], Takumi Aihara[2], Marco Gruenewald[1], Felix Otto[1], Jari Domke[1], Roman Forker[1], Hiroyuki Yoshida[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Graduate School of Engineering, Chiba University, 1-33, Yayoi-cho, Inage-ku, Chiba 263-8522, Japan

2D materials like hexagonal boron nitride (h-BN) are widely used as interlayer to decouple organic molecules from metallic surfaces. Nevertheless, there are also indications for a significant hybridization which results in a perturbation of the intrinsic molecular properties. This raises the question: what are the specific conditions under which an h-BN monolayer is sufficient to efficiently decouple organic molecules? In this work we deal with this question by comparing the electronic and optical properties as well as the lateral structure of about one monolayer 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) and tetraphenyldibenzoperiflanthene (DBP) on h-BN/Ni(111). Therefore, we combined *in situ* differential reflectance spectroscopy, ultraviolet photoelectron spectroscopy, low energy electron diffraction and low temperature scanning tunnelling spectroscopy. Our results reveal that an integer charge transfer happens for PTCDA on h-BN/Ni(111). In contrast, the DBP molecules on h-BN/Ni(111) are well decoupled from the metal substrate, and no charge transfer occurs.

O 75.5 Wed 13:30 P

Adsorption site dependent gating of C60 on h-BN/Rh(111) — •Max Bommert and Oliver Gröning — Empa Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Epitaxial, single layered hexagonal Boron Nitride (h-BN) on a metal substrate provides numerous interesting properties as it can be used as a template organizing the adsorption of organic molecules due to the substrate dependent Moirée pattern formation [1] as well as decoupling said molecules from the underlying metal preventing orbital hybridization [2]. In this project we use the topographic and electronic corrugation of the h-BN/Rh(111) Moirée pattern to form [3] and electrostatically gate specific C60 molecules in regular frameworks. Our experimental approach consists of two parts; in a first step, we use low-temperature scanning tunneling microscopy (STM) to analyze the C60 adsorption configuration. In a second step, we use scanning tunneling spectroscopy (STS), Kelvin probe force microscopy (KPFM) as well as non-contact atomic force microscopy (nc-AFM) to investigate the adsorption-site dependent gating effect of the on surface electric field on the C60 molecules. The combination of STS and KPFM grants insight into single molecular charging events. We can use the on surface electric field and the electric field of the STM tip to operate the C60 molecules as single molecular transistors. We will show how the molecular orbital level alignment and the site-dependent gating are related. [1]M. Iannuzzi et al., PCCP, 16 (2014), [2]L. Liu et al., ACS Nano, 9 (2015), [3]M. Corso et al., Science, 203 (2004)

O 75.6 Wed 13:30 P

Force Spectroscopy of Iron Tetraphenylporphyrin Molecules with Cl Tips — Katharina Scheil[1], •Manuel Gruber[1,2], Martin Ondrácek[3], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Faculty of Physics, University of Duisburg-Essen, D-47057 Duisburg, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, 182 21 Prague, Czech Republic

Cl ions are bidirectionally transferred between Fe tetraphenylporhyrin (FeTPP) molecules adsorbed on Au(111) and the tip of a low-temperature scanning probe microscope. This controlled transfer is used to switch between metal- and Cl-terminated tips. Both tips are employed to probe the forces and conductances upon contacting the Au(111) substrate, FeTPP and chlorinated FeTPP. The force spectroscopy of a Cl tip on Au(111) may be modeled by a point charge of -0.3 e at the Cl ion interacting with its image charge in the substrate. Such Cl tips, beside modifying electrostatic interactions and thereby the force spectra acquired over molecules, turned out useful for high-resolution imaging at small molecule-sample distances [1]. Density function theory calculations reproduce important aspects of the experimental data. [1] Scheil et al., J. Phys. Chem. C 124, 26889 (2020)

Financial support by the Deutsche Forschungsgemeinschaft through SFB 677 is acknowledged.

O 75.7 Wed 13:30 P

Uni-directional rotation of molecular motors on Cu(111) — •Monika Schied[1], Deborah Prezzi[2], Dongdong Liu[3], Peter Jacobson[1], Elisa Molinari[2], James M. Tour[3], and Leonhard Grill[1] — [1]Department of Physical Chemistry, University of Graz, Austria — [2]Nanoscience Institute of CNR, S3 Center, Modena, Italy — [3]Department of Chemistry, Rice University, USA

Artificial molecular motors that convert external energy into controlled motion have seen great developments in the last decades [1]. While many studies exist in solution, little is known how such functional molecules behave on a surface. However, such a solid support can be advantageous as it offers fixed points of reference as well as confinement in two dimensions, making it easier to study the directionality of their motion.

We have studied single molecules with a so-called Feringa motor [2,3] on a Cu(111) surface by low-temperature scanning tunnelling microscopy (STM). It was found that rotations of individual molecules can be induced over rather long distances by voltage pulses with the STM tip. Importantly, these rotations show high directionality (clockwise or anticlockwise), which will be discussed in view of their specific chemical structure and adsorption.

[1] W. R. Browne and B. L. Feringa, Nat. Nanotech. 1, 25 (2006)
[2] T. Kudernac et al., Nature 479, 208 (2011)
[3] A. Saywell et al., ACS Nano 10, 10945 (2016)

O 75.8 Wed 13:30 P

Light-assisted charge propagation in organic semiconductor networks on hexagonal boron nitride — Aleksandar Matkovic[1], Jakob Genser[2], •Markus Kratzer[1], Daniel Lüftner[3], Zhongrui Chen[4], Olivier Siri[4], Peter Puschnig[3], Conrad Becker[4], and Christian Teichert[1] — [1]Institute of Physics Montanuniversität Leoben Franz Josef Strasse 18, Leoben 8700, Austria — [2]Institute of Solid State Electronics, Technische Universität Wien, Gußhausstraße 25-25a, 1040 Vienna, Austria — [3]Institute of Physics Karl-Franzens-Universität Graz NAWI Graz Universitätsplatz 5, Graz 8010, Austria — [4]Aix Marseille University CNRS CINaM UMR 7325 Campus de Luminy 13288, Marseille cedex 09, France

Electrostatic force microscopy is utilized to track charge propagation in organic semiconductor nanoneedles. As model system, crystalline dihydrotetraazaheptacene needles epitaxially grown on ultrathin hexagonal boron nitride was investigated. Due to light exposure, the specific resistivity of the crystallites changed by two orders of magnitude. Exploiting the highly anisotropic optical properties of the organic nanoneedles, selective charge propagation along the crystallites was achieved by matching the incident light*s polarization direction with the direction of the molecular backbones in the crystals. Thus, it was possible to guide charge propagation along desired paths in self-assembled crystallite networks. This way, polarized light can be used as a ”light gate” to control charge propagation.

O 76: Poster Session VI: Supported nanoclusters: structure, reactions, catalysis

Time: Wednesday 13:30–15:30 Location: P

O 76.1 Wed 13:30 P

Cu nanoparticle morphology and growth behavior on the vicinal ZnO(10-14) surface — •Robert Gleissner[1,2], Heshmat Noei[1], Vedran Vonk[1], Simon Chung[1], Guilherme D. L. Semione[1], E. Erik Beck[1,2], Gökhan Gizer[3], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Universität Hamburg, Hamburg, Germany — [3]Helmholz Zentrum Geesthacht, Geesthacht, Germany

The ZnO(10-14) surface raised recent scientific interest for its outstanding stability despite its high indexed orientation, which results in a stepped mixed-terminated surface. In this study, copper nanoparticles were grown via physical vapor deposition onto a ZnO(10-14) single crystalline surface and the structure and morphology was investigated using low energy electron diffraction, high energy grazing incidence x-ray diffraction, scanning electron microscopy and scanning tunneling microscopy.

Caused by anisotropic diffusion, elongated Cu particles are formed parallel to the surface steps of the substrate. They show a unique tilt of their (111) planes parallel to the (0001) terraces of the vicinal surface. This causes the generation of large, high indexed Cu facets in which their atomic steps could act as reaction sites in catalytic reactions such as methanol synthesis and CO2 activation.

O 76.2 Wed 13:30 P

Metastability of Palladium Carbide Nanoparticles during Hydrogen Release from Liquid Organic Hydrogen Carriers — •Ralf Schuster[1], Manon Bertram[1], Henning Runge[2], Simon Chung[2], Vedran Vonk[2], Heshmat Noei[2], Yaroslava Lykhach[1], Andreas Stierle[2], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg

Surface carbon species can be formed by unselective decomposition during heterogeneously catalyzed dehydrogenation of liquid organic hydrogen carriers (LOHCs). These species may diffuse into the bulk of the catalyst, forming metal carbide phases and, thus, influence the activity and selectivity of the catalyst. For palladium, however, the carbide phase is metastable with respect to palladium and graphite. Therefore, we studied the formation and stability of palladium carbide phases on well-defined Pd/Al_2O_3 model catalysts. The phase composition of the nanoparticles was investigated as a function of particle size and gas flow rate under reaction conditions (500 K, 1 bar) by high-energy grazing incidence X-ray diffraction. We showed that the stability of palladium carbide critically depends on both nanoparticle size and gas flow rate. For small nanoparticles under low gas flow rate the Pd_6C phase is stable, while a high gas flow rate results in immediate decomposition of the carbide after formation. For bigger particles at a low gas flow rate, however, the carbide is stable for an incubation period, after which the growth of graphene triggers its decomposition.

O 76.3 Wed 13:30 P

Reactivity and Passivation of Fe Nanoclusters on h-BN/Rh(111) — •Natalie Jessica Waleska, Fabian Düll, Philipp Bachmann, Felix Hemauer, Johann Steinhauer, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität, Erlangen, Germany

Iron is a nontoxic and affordable element, which shows high catalytic activity. Iron containing catalysts are used in important industrial reactions, such as the Fischer-Tropsch synthesis and the Haber-Bosch process. Especially, iron nanoclusters are of interest because of their potential utilization in electrochemical devices or high-density data storage applications due to their magnetic properties.

To obtain monodisperse, ordered Fe nanocluster arrays, h-BN was used as a template on the Rh(111) surface. Due to the lattice mismatch, differences in the strength of interaction between the h-BN sheet and the Rh(111) surface occur, leading to corrugation of the nanosheet and the formation of pores and wires.

We studied Fe nanocluster arrays formed in the pores of h-BN/Rh(111) using in situ high-resolution X-ray photoelectron spectroscopy. CO was used as a probe molecule to investigate the morphology, such as the available adsorption sites and the reactivity of the nanoclusters. On the as prepared Fe clusters, CO was adsorbed at on-top and hollow/edge sites and dissociated at 300 K. For the C and O pre-covered Fe nanoclusters we found a passivation of the catalytic activity as a result of adsorption site blocking, allowing for the determination of the most active sites of the Fe clusters.

O 76.4 Wed 13:30 P

Systematic first-principles investigation of support effects for coinage metals on alkaline earth oxides — •Kyeonghyeon Nam[1], Julius Hornung[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Fritz Haber Institute of the Max Planck Society — [2]Technical University of Munich

Reaching an atomic-scale understanding of metal-support effects is a long-standing and still elusive goal of catalysis research. One avenue to disentangle the intricate interference of geometric and electronic effects is to engage in trend studies over structurally similar systems. To this end, we perform a systematic density-functional theory study of alkaline earth oxide (MgO, CaO, SrO, BaO) supported Cu and Ag thin films. Considering CO and hydroxyl adsorption at various surface sites, we compute adsorption energies with and without geometric optimization and correlate this data with electronic structure properties like Löwdin charges and interfacial energetics like adhesion energies. Metal doping of the oxide supports with Mo in varying positions was analyzed in an effort to expand our understanding of metal-support interactions and the critical parameters that determine catalyst activity and stability [1]. Our results indicate that oxide supports with heavier cations (SrO, BaO) favor the formation of Cu agglomerates in the presence of CO adsorbates, while such drastic rearrangements are not observed for oxides with lighter cations (MgO, CaO).

[1] X. Shao *et al.*, Angew. Chem. Int. Ed. **50**, 11525 (2011).

O 76.5 Wed 13:30 P

Structure and Chemical Properties of CeO_2 on a Curved Cu(111) Crystal — •Lorena Glatthaar[1,2], Khadiza Ali[2], J. Enrique Ortega[2], and Frederik Schiller[2] — [1]Physikalisch-Chemisches Institut, Justus Liebig University, D-35392 Giessen, Germany — [2]Centro de Física de Materiales, E-20018 San Sebastián, Spain

The system CeO_x/Cu has attracted interest as an inverse catalyst for CO oxidation, water-gas shift and CO_2 hydrogenation. While previous work focused on characterizing this system and the named reactions on Cu(111) or with powdered samples, we investigated this system on the vicinal surfaces of Cu(111), which are shown to be much closer to a nanostructured catalysts compared to the low index surfaces. We grew CeO_2 on a curved Cu(111) single crystal with well defined vicinal surfaces and a continuous variation of step density depending on the vicinal angle. We characterized the CeO_x/Cu system with LEED, STM and XPS. XPS analysis indicates only Ce(IV) oxide formed regardless of the position on the curved crystal. On the Cu(111) part of the curved sample, CeO_2 nanostructures seems to grown on Cu-oxide areas, leaving the remaining Cu(111) surface uncovered. On both A- and B-step vicinal surfaces of the curved crystal, facets build up after CeO_2 deposition. The stable facets of the B-step vicinals are (111) and (110). At the A-step side three stable facets have been observed, namely the (111), (223) and an additional one at 22° with respect to (111). STM measurements reveal that the CeO_2 structures mainly cover the Cu(111), leaving the (223) facet CeO_2 free.

O 77: Poster Session VI: Scanning probe techniques: Method development I

Time: Wednesday 13:30–15:30 Location: P

O 77.1 Wed 13:30 P

Identifying the atomic configuration of the tip apex using STM and frequency-modulation AFM with CO on Pt(111) — •Oliver Gretz, Alfred J. Weymouth, and Franz J. Giessibl — Institute of Experimental and Applied Physics, Department of Physics, University of Regensburg, 93053 Regensburg

We investigated the atomic structure of metal tips by scanning individual CO molecules adsorbed on Pt(111) using scanning tunneling microscopy (STM) and frequency-modulation atomic force microscopy (FM-AFM). When scanning very close over a CO molecule, the frontmost atoms of the tip can be individually resolved in both the FM-AFM image and in the STM image. This is in contrast to previous work where CO was adsorbed on a different substrate: Cu(111). In this previous study, individual atoms could not be observed in the raw STM image but only in FM-AFM. We discuss the mechanisms behind the higher spatial resolution in STM. On Cu(111), the occupied surface state plays a large role in STM images near the Fermi level, and as adsorbed CO repels the surface state, it appears as a wide trough in STM images. In contrast, Pt(111) lacks an occupied surface state and an adsorbed CO molecule appears as a peak. We investigate if CO bending strongly influences the STM images, concluding that the atomic resolution of the tip over Pt(111) is due to highly localized through-molecule tunneling and CO bending is insignificant for contrast formation. Modelling the current between the CO and front atoms of the tip supports our findings.

Gretz et al., Phys. Rev. Research 2, 33094 (2020).

O 77.2 Wed 13:30 P

Strumming a Single Chemical Bond — •Alfred J. Weymouth, Elisabeth Riegel, Oliver Gretz, and Franz J. Giessibl — Universität Regensburg

Atomic force microscopy and scanning tunneling microscopy can image the internal structure of molecules adsorbed on surfaces. One reliable method is to terminate the tip with a nonreactive adsorbate, often a single CO molecule, and to collect data at a close distance where Pauli repulsion plays a strong role. Lateral force microscopy, in which the tip oscillates laterally, probes similar interactions but has the unique ability to pull the CO over a chemical bond, load it as a torsional spring, and release it as it snaps over with each oscillation cycle. This produces measurable energy dissipation. The dissipation has a characteristic decay length in the vertical direction of 4 pm, which is 13 times smaller than the decay length in typical STM or AFM experiments.

Physical Review Letters, 124, 196101 (2020)

O 77.3 Wed 13:30 P

Bond-Level Imaging of Organic Molecules Using Q-Controlled Amplitude Modulation Atomic Force Microscopy — •Daniel Martin-Jimenez[1,3], Alexander Ihle[1,3], Sebastian Ahles[2,3], Hermann A. Wegner[2,3], André Schirmeisen[1,3], and Daniel Ebeling[1,3] — [1]Institute of Applied Physics (IAP), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [3]Center for Materials Research (LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The bond imaging atomic force microscopy (AFM) technique has become an invaluable tool for studying organic molecules on surfaces. The functionalization of the AFM-tip with a single CO molecule improves the lateral resolution and allows to visualize the chemical structure of adsorbed organic molecules. Such experiments are usually performed at low temperatures in UHV environment in the frequency modulation (FM) mode. Here, we use the Q-controlled amplitude modulation (AM) mode for imaging organic molecules with CO-functionalized tips in constant-height mode. By reducing the effective quality factor (Qeff) of the sensor from about 20000-30000 to 1500-4000, we are able to image molecules with atomic resolution. By using appropriate imaging parameters, an increased effective signal-to-noise ratio is achieved in the Q-controlled AM mode (on the order of 30-60 %). This advantage over the conventional FM mode might, e.g., be used for increasing the experimental throughput.

O 77.4 Wed 13:30 P

High-precision atomic force microscopy with atomically-characterized tips — •Alexander Liebig, Angelo Peronio, Daniel Meuer, Alfred J. Weymouth, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Germany

Traditionally, atomic force microscopy (AFM) experiments are conducted at tip-sample distances where the tip strongly interacts with the surface. This increases the signal-to-noise ratio, but poses the problem of relaxations in both tip and sample that hamper the theoretical description of experimental data. Here, we employ AFM at relatively large tip-sample distances where forces are only on the piconewton and subpiconewton scale to prevent tip and sample distortions. Acquiring data relatively far from the surface requires low noise measurements. We probed the $CaF_2(111)$ surface with an atomically-characterized metal tip and show that the experimental data can be reproduced with an electrostatic model. By experimentally characterizing the second layer of tip atoms, we were able to reproduce the data with 99.5 % accuracy. Our work links the capabilities of non-invasive imaging at large tip-sample distances and controlling the tip apex at the atomic scale [1].

[1] A. Liebig, A. Peronio, D. Meuer, A. J. Weymouth and F. J. Giessibl, New J. Phys. 22, 063040 (2020).

O 77.5 Wed 13:30 P

Charging single metal nanoparticles grown on thin alumina films by the AFM tip — Baptiste Chatelain, •Ali El Barraj, Clemence Badie, Lionel Santinacci, and Clemens Barth — Aix-Marseille University, CNRS, CINaM, 13288 Marseille, France

The characterization of charges inside a single metal island or nanoparticle (NP), which are supported on an insulating thin film, is of high interest in research fields like heterogeneous catalysis and microelectronics. The reason is that charges in a NP can have a large impact onto the NP*s catalytic activity and that they can interfere with the underlying insulating film, partially via defects of the film. Whereas the first aspect is certainly of importance in catalysis, the second phenomenon is of particular interest in micro-electronics because a detailed analysis of the charge-insulator interaction can explain phenomena that are related to leakage currents and device performance.

It has been already shown hat electrostatic force microscopy (EFM) and Kelvin probe force microscopyt (KPFM) are suitable techniques for charge manipulation experiments at nano-objects like NPs and that they can be used to monitor, in particular, the charge-insulator interaction. Here, we use KPFM to study injected charges inside PdNPs and AuNPs, which are grown on 15 to 80nm thin ALD grown aluminum oxide (alumina) films. We show that the alumina films have a high insulating character, which allows injecting charge into the surface or NP without loosing the charge into the film. Apart from the material specific results, we discuss the experimental procedures and related difficulties that may appear during charge manipulation experiments.

O 77.6 Wed 13:30 P

Ultra-Shallow Dopant Profiles in H:Si(001) as In-Situ Electrodes in Scanning Probe Microscopy — •Alexander Kölker, Takashi Kumagai, Martin Wolf, and Matthias Koch — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

To fully enable the potential of nano-devices a detailed understanding of the underlying physics is of importance linking the atomic structure to the electronic properties of the device. Although scanning probe microscopy (SPM), with its outstanding spatial resolution, is sensitive to both, the experimental capabilities are limited by the vertical arrangement of the tip-sample junction. Therefore it is often impossible to characterize an electrical nano-circuit in-operation with a conventional SPM. These restrictions can be addressed using multi-tip scanning tunneling microscopy (STM) [1]. However, upgrading an existing STM with additional electrodes requires severe and cost-intensive modifications of the experimental setup. Here, we demonstrate the applicability of ion-implanted electrodes as a feasible way to enhance a commercial Createc GmbH low-temperature SPM with additional electrodes. These electrodes are in close proximity to the surface and act as drain or gate and show ohmic behaviour [2], even after high temperature surface preparation needed to achieve an atomically flat surface. We used STM spectroscopy to probe the transition from metallic to insulating at the electrode interface. First gating experiments of dangling bonds on the H:Si(001) surface are presented. [1] B. Voigtländer et. Al, Rev. Sci. Instrum. 89, 101101 (2018) [2] A.N. Ramanayaka et. al Scientific Reports 8, 1 (2018)

O 78: Poster Session VI: 2D Materials: Electronic structure, excitations, etc. II

Time: Wednesday 13:30–15:30 Location: P

O 78.1 Wed 13:30 P

Transitional metal doped $Bi_{2-n}X_nO_2Se$ - novel 2D magnetic semiconductor — •Dominik Legut[1], Xiaopeng Liu[2], Ruifeng Zhang[2], Zhongheng Fu[2], Tinshuai Wang[2], Yanchen Fan[2], and Qianfan Zhang[2] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — [2]School of Mat. Sci. and Eng., Beihang University, Beijing, China

For the spintronic applications like large data storages (high capacity HDD) the industry searches for ferromagnetic insulators at nanoscale size. Recently the discovery of Bi_2O_2Se/Te phases that exist as 2D material and still are semiconducting attract attention. Here we investigate $Bi_{2-n}X_nO_2Se$ by transitional metal doping to introduce a magnetic spin order. We explore the electronic and magnetic properties of various ferromagnetic (e.g. Fe) or antiferromagnetic (e.g. Mn) transitional metals doped Bi_2O_2Se phases within the framework of density functional theory based electronic structure calculations. We start with the magnetic order of the bulk phase in which the magnetic atoms form interlayer coupling that vary with the type and concentration of doped atoms and go towards the nanoscale dimension, i.e. 2D materials. As a result of the competitions of magnetic interactions the magnetic anisotropy energy is a crucial quantity. In combinations with Monte Carlo simulations we are able to solve the exchange interaction constants for the Heisenberg model and therefore evaluate the Curie temperature to see if these types of materials are suitable to become novel dilute magnetic semiconductors for spintronic applications at room and above temperatures.

O 78.2 Wed 13:30 P

Analysis of interlayer excitons in the case of MoS_2 on GaSe. — •Christian Wagner, Mahfujur Rahaman, Dietrich R.T. Zahn, and Sibylle Gemming — Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

We study the formation of *interlayer* excitons in GaSe | MoS_2 heterostacks as a function of layer composition from first principles in order to specifically tailor photon absorption in layered heterostacks.

The electronic interaction in semiconducting 2D layered material heterostacks is often reasonably described by a perturbation of the physical effects of the isolated homostacks. But their optical properties go beyond this picture of weak layer interaction: moiré potentials influence exciton dynamics and bound *interlayer* excitons may emerge. Interlayer excitons are composed of electron and hole states from different layers. These mixed states are measured experimentally by photoluminescence and photocurrents and predicted by theory, e.g. in MoS_2 on GaSe [1].

The composition of all interlayer excitons are thoroughly analyzed by solving the Bethe-Salpeter equation for the heterobilayer of MoS_2 on GaSe. The exciton Hamiltonian is diagonalized and the exciton wave functions are projected onto layers as a function of k-space. By means of density functional theory and optical selection rules, these optical interlayer transitions are extrapolated for larger heterostacks and compared directly with experiments.

[1] M. Rahaman, C. Wagner et al., J. Phys.: Condens. Matter 31, 114001 (2019).

O 78.3 Wed 13:30 P

Spin-polarized VLEED from single-layer MoS_2/Au(111): Investigation of spin-orbit-induced effects — •Christoph Angrick[1], Annika Henriksen[1], Nicole Mutzke[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

The influence of spin-orbit interaction on low-energy electron reflection from single-layer MoS_2 on Au(111) was studied by VLEED (very-low-energy electron diffraction) [1,2]. The spin-dependent electron reflection was investigated for a wide range of electron incidence angles and kinetic energies. Since the adlayer coverage is about 30%, we studied the Au(111) substrate and a MoS_2 bulk sample for comparison. This approach enabled us to distinguish between adlayer and substrate signals.

For MoS_2/Au(111), we detected a spin asymmetry of the reflected intensities, which shows a characteristic feature with alternating sign in the energy region of a VLEED fine structure [1]. The Au(111) substrate, in contrast, shows qualitatively different spin-asymmetry features, partially with reversed sign compared with MoS_2/Au(111). The results of bulk MoS_2 confirm that the characteristic feature in the single-layer data originates from MoS_2. The influence of the adlayer-substrate interaction on the results will be discussed.

[1] Burgbacher *et al.*, Phys. Rev. B **87**, 195411 (2013)

[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020)

O 78.4 Wed 13:30 P

Four- and twelve-band low-energy symmetric Hamiltonians and Hubbard parameters for twisted bilayer graphene using ab-initio input — •Arkadiy Davydov, Kenny Choo, Mark H. Fischer, and Arkadiy Davydov — Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich (Switzerland)

A computationally efficient workflow for obtaining low-energy tight-binding Hamiltonians for twisted bilayer graphene, obeying both crystal and time-reversal symmetries, is presented in this work. The Hamiltonians at the first magic angle are generated using the Slater-Koster approach with parameters obtained by a fit to ab-initio data at larger angles. Low-energy symmetric four-band and twelve-band Hamiltonians are constructed using the Wannier90 software. The advantage of our scheme is that the low-energy Hamiltonians are purely real and are obtained with the maximum-localization procedure to reduce the spread of the basis functions. Finally, we compute extended Hubbard parameters for both models within the constrained random phase approximation (cRPA) for screening, which again respect the symmetries. The relevant data and results of this work are freely available via an online repository. The workflow is straightforwardly transferable to other twisted multi-layer materials.

O 78.5 Wed 13:30 P

Optoelectronic properties of point defects in hBN — •Alexander Kirchhoff, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

While pristine hexagonal boron nitride (hBN) is a wide-gap insulator, its point defects are discussed as light emitters in the visible optical spectrum. In this study, we examine two substitutional carbon impurities, C_N and C_B, the nitrogen vacancy V_N, the divacancy V_{NB} and a carbon substitution with a nitrogen vacancy adjacent to it, C_BV_N, in a hBN monolayer from an *ab initio* approach, via the GW/BSE approximation. Our results show deep defect states and defect-related excitations with energies in the visible regime. We present a detailed analysis of their spatial structure and energetic composition.

O 78.6 Wed 13:30 P

Proroper ab-initio dielectric function of 2D materials and their polarizable thickness — •Lorenzo Sponza and François Ducastelle — Université Paris-Saclay, ONERA, CNRS, Laboratoire d'étude des microstructures, 92322, Châtillon, France

We derive a formalism allowing us to separate inter-layer contributions to the polarizability of a periodic array of 2D materials from intra-layer ones. To this aim, effective profile functions are introduced. They constitute a tight-binding-like layer-localized basis involving two lengths, the effective thickness d characteristic of the 2D material and the inter-layer separation L. The method permits, within the same formalism, either to compute the single-layer dielectric function from an ab-initio periodic calculation (ab-initio exfoliation) or to stack several 2D materials to generate a finite-thickness van der Waals heterostructure (ab-initio stacking).

O 78.7 Wed 13:30 P

Electronic and vibrational properties of TMDs heterogeneous bilayers, non-twisted bilayers silicene/TMDs heterostructures and photovoltaic heterojunctions of fullerenes with TMDs monolayers — •Mohamed Barhoumi[1] and Moncef Said[2] — [1]Monastir university, Monastir, Tunisia — [2]Monastir university, Monastir, Tunisia

In the recent years, many studies have been showed that bilayer and heterobilayer transition metal dichalco- genides might offer properties superior to those of monolayer. Nevertheless, only very few have been synthe- sized. Using first-principles calculations, we study the structural, electronic and vibrational properties of new transition metal dichalcogenides heterogenous bilayers (i.e., MX2/MX2 with M, M = Pd, Pt, W; X, X = S, Se). Also, we investigate the structural, vibrational and electronic properties of silicene/TMDs and C60/TMDs. Our results show that the predicted geometry can well reproduce the structural parameters, where very well agreement was obtained between the calculated and previous studies for the monolayers. Our calculations show that all the heterobilayers are indirect band-gap semiconductors with the exception of the WS2/PdSe2 and WSe 2/PdSe2 heterobilayers, which are metallic systems. In the case of the heterostructures bilayers (silicene/MX2), the bandgap is decreased when Pd is changed to Pt, and when the atomic number of X increases, the band-gap increases. Also, by analyzing the electronic band structures and the electron density, it appeared that C60/MX2 is a promising system for photovoltaic applications.

O 78.8 Wed 13:30 P

Decoupled Strain Response of Ferroic Properties in Multiferroic VOCl$_2$ Monolayer — •Akshay Mahajan and Somnath Bhowmick — Department of Materials Science and Engineering, Indian Institute of Technology, Kanpur, Kanpur 208016, India

Two-dimensional (2D) magnetoelectric multiferroic materials are a special class of 2D materials that holds promising applications in the miniaturization of logic and memory devices, along with the possibility to realize new low-dimensional device architectures. In this work, we have reported a strain-engineering-based study for a 2D multiferroic material, VOCl$_2$ monolayer, that shows independent control of magnetic and ferroelectric properties via applying strain along the different in-plane crystallographic directions. An in-plane strain of around 4% along the non-polar axis was found to cause a transition from an antiferromagnetic (AFM) ground state with an out-of-plane magnetization to a ferromagnetic (FM) ground state with in-plane magnetization. Additionally, the tensile strain along the polar axis enhances the ferroelectric polarization. An increase in the ferroelectric switching energy barriers and the magnitude of the magnetic exchange coupling parameter suggest enhancing ferroelectric and ferromagnetic stability with tensile strain. The work reveals the VOCl$_2$ monolayer as a strain-tuneable multiferroic material holding great promises for future generation nanoelectronic devices.

O 78.9 Wed 13:30 P

Band structure and image potential states of hBN/Cu(111) — •Jan Beckord, Matthias Hengsberger, and Jürg Osterwalder — Physik-Institut, Universität Zürich, Schweiz

We present a study on the band structure and the image potential states of a hexagonal boron nitride (hBN) monolayer on the Cu(111) surface. The orientation of the bare copper surface was measured by XPD and ARPES. The hBN layer was then grown by chemical vapour deposition from borazine. XPS spectra confirm the presence of a full monolayer with the correct stoichiometry, and ARPES band structure measurements with He IIa radiation along the high symmetry directions $\overline{\Gamma K}$ and $\overline{\Gamma M}$ are in excellent agreement with literature values for other metal substrates. The work function is significantly reduced from 4.9 eV to 4.1 eV, which agrees with the reported work function in valleys of the corrugated surface measured by STM. We then measured the unoccupied electronic states with two-photon photoelectron spectroscopy on the bare copper as well as on the hBN covered surface. Varying the photon energy allowed us to separate the first two image potential states n=1 at 0.83 eV and n=2 at 0.16 eV below the vacuum level from the Shockley surface state at a binding energy of 0.27 eV. The valence band maximum in normal emission direction appeared at a binding energy of 2.21 eV.

O 78.10 Wed 13:30 P

Gate-Tunable Curvature-Induced Charge Localization in Two-Dimensional Semiconducting Monolayers — •bong gyu shin[1], jz-yuan juo[1], soon jung jung[1], and klaus kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, DE-70569Stuttgart, Germany — [2]Institut de Physique, École Polytechnique Fédérale deLausanne, CH-1015 Lausanne, Switzerland

The localized quantum states in two-dimensional (2D) materials are attractive for valley- and spin- related optoelectronics or other quantum applications. However, achieving these quantum states is still challenging due to technical difficulties. Here, we investigated strain-induced charge localization in monolayer MoS$_2$ on SiO$_2$/Si using a gate-tunable home-built scanning tunneling microscope at ~4.9K. A MoS$_2$ monolayer follows surface roughness of the substrate, exhibiting random distribution of bending strain with band gap reduction at a local region, acting like a potential well leading to charge localization. At higher electron doping levels, the tunneling-barrier-height over high curvature regions is reduced since localized electron charges lower the local work function. Moreover, we observed the spatial flattening of the conduction (valence) band edge over the band gap fluctuation at electron- (hole-) doping of ~10^{13} cm^{-2}. In our theoretical calculations, the trends of local work function and spatial flattening of band edges by doping levels were confirmed in various thin 2D semiconductors, providing the general mechanism of charge localization via curvature effects.

O 78.11 Wed 13:30 P

Spin and orbital nature of electronic structure in transition metal dichalcogenides — •Jakub Schusser[1,2,3], Mauro Fanciulli[1], Samuel Beaulieu[4], Maria C. Richter[2], Olivier Heckmann[2], Zakariae El Youbi[2,5], Cephise Cacho[5], Ralph Ernsthofer[4], Karol Hricovini[1], Jan Minar[2], and Friedel Reinert[3] — [1]LPMS, CY Cergy-Paris University, Neuville-sur-Oise, France — [2]NTC, University of West-Bohemia, Pilsen, Czech Republic — [3]EP VII and Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [4]DPC, Fritz-Haber-Institute, Berlin, Germany — [5]DLS, Harwell Campus, Didcot, UK

Our work is concerned with the polarization of electrons and orbital texture in non-magnetic materials. We studied stationary and dynamic electron states by photoemission and spin-polarized relativistic Korringa-Kohn-Rostoker calculations on three bulk transition metal dichalcogenide samples. On bulk WTe2, a Weyl type-II semimetal candidate, we performed spin-, time- and angle-resolved photoemission spectroscopy experiments at different pump-probe time delays to reveal the mechanism behind the relaxation process of spin-polarized electrons above the Fermi level in the supposed Weyl points region. On bulk 2H-WSe2, using different crystal orientations that are mathematically equivalent to time-reversal operation, we introduce a new observable called "time-reversal dichroism" which contains information about the hidden orbital texture of the electronic states. For 1T-HfTe2 as a model system with both inversion and time-reversal symmetries in the bulk, we performed an analysis of the spin-polarized photocurrent.

O 78.12 Wed 13:30 P

Strain control of the competition between metallic and semiconducting states in single-layers of TaSe$_3$ — •Jose Angel Silva-Guillen[1] and Enric Canadell[2] — [1]School of Physics and Technology, Wuhan University, Wuhan 430072, China — [2]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus Bellaterra, 08193 Bellaterra, Spain

Recently, layered group IV transition-metal trichalcogenides have been the object of much attention because they provide a convenient platform as single- or few-layers flakes for applications in devices. Interestingly, group V transition metal chalcogenides have not yet been thoroughly studied as single-layers or few-layer flakes. One of them, TaSe3, is a semi-metal and superconductor in the bulk and a charge density wave has been claimed to occur in mesowires. Since in the bulk there are noticeable interlayer Se–Se interactions it is challenging to see how suppression of interlayer interactions can modify the electronic structure and physical properties of this material. We report a DFT study of the electronic structure of TaSe$_3$ single-layers and its evolution under different types of strain. We find that the pristine TaSe3 single-layer exhibits a metallic state which can be modified in different ways under the application of biaxial strain or uniaxial strain along either the short or long directions of the layer. Electronic instabilities related to both electron and hole pockets as well as the stabilization of a semiconducting state are shown to be possible. These single-layers are thus predicted to be versatile materials where different states compete as a function of relatively small differences in strain.

O 78.13 Wed 13:30 P

Ab Initio study of the structural and electronic properties of Niobium Sulfide (NbS2) and Lithium Niobium Sulfide (LiNbS2) bulk and (001) surfaces — •Jorge D. Vega and Henry P. Pinto — Universidad Yachay Tech, Urcuqui, Ecuador

In the context of the discovery of new materials, intercalation of Lithium (Li) atoms among layers of NbS2 can be performed. However, few experimental works deal with this material. Recently, Voiry et al. performed some experiments with LiNbS2 providing some insights about the properties of this system. Hence, we describe this material with state of the art non-empirical density functionals in the framework of density-functional theory (DFT). Specifically, we describe various insights regarding the electronic and atomic structure, lattice parameters, scanning tunnelling microscopy images and phonons of the bulk and surfaces of LiNbS2. We perform the computations with the meta-GGA SCAN functional and some variations of the hybrid HSE as implemented in VASP. We found out that SCAN+rVV10 performs very well in the description of certain properties of LiNbS2 and NbS2. Besides, we tested the hybrid HSE12 and HSE12s and compared with the customary HSE06. The performance of the hybrids is discussed too. Interestingly, we found that the intercalation of Li on NbS2 produces a considerable band-gap, making the material a semiconductor and providing promising technological applications.

O 78.14 Wed 13:30 P

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistor — •Aleksandar Matković[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[3], Markus Kratzer[1], Esther Karner-Petritz[2], Alexander Fian[2], Herbert Gold[2], Michael Gärtner[4], Andreas Terfort[4], Christian Teichert[1], Egbert Zojer[3], Karin Zojer[3], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Joanneum Research MATERIALS, Weiz, Austria — [3]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Germany

This study aims at direct imaging of contact resistance in MoS$_2$-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS$_2$ have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both carrier injection and extraction points, we demonstrate asymmetry of contact resistances in MoS$_2$-based TFTs, as well as their non-linear and bias-dependent behavior [10.1002/aelm.202000110].

O 79: Poster Session VI: Ultrafast electron dynamics at surface and interfaces II

Time: Wednesday 13:30–15:30 Location: P

O 79.1 Wed 13:30 P

Momentum Microscope vs. Hemispherical analyzer - a quantitative comparison of electron analyzer performance for time-resolved ARPES experiments — Julian Maklar, Tommaso Pincelli, Samuel Beaulieu, Shuo Dong, Maciej Dendzik, Martin Wolf, Ralph Ernstorfer, and •Laurenz Rettig — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

For angle-resolved photoelectron spectroscopy (ARPES), an important element is the employed electron analyzer. While hemispherical analyzers with angle-dispersing electron lenses have been the working horse for decades, recently time-of-flight based momentum microscopes have shown a huge improvement in parallel detection efficiency, allowing for simultaneous detection of multiple Brillouin zones without the need to rearrange the sample geometry. However, one drawback of such instruments, in particular in time-resolved studies, arises from the large energy and momentum range covered simultaneously, which in combination with detection limitations of delay-line detectors can severely reduce the effective detection rate for selected energy-momentum regions compared to conventional hemispherical analyzers. Additionally, the high electron energies employed in the more complex electron lens system designs impose new constraints in terms of space charge. Using our XUV time-resolved ARPES system hosting both a hemispherical analyzer (SPECS Phoibos 150) and a momentum microscope (SPECS Metis 1000) in one experimental setup, we quantitatively compare the advantages and disadvantages of both types of analyzers for various kinds of trARPES experiments. Rev. Sci. Instr. 91, 123112 (2020)

O 79.2 Wed 13:30 P

Dynamic screening of quasiparticles in WS_2 monolayers — •Stefano Calati[1,2], Qiuyang Li[3], Xiaoyang Zhu[3], and Julia Stähler[1,2] — [1]Department of physical chemistry, Fritz-Haber-Institut der MPG, Berlin — [2]Institut für Chemie, Humboldt-Universität zu Berlin — [3]Department of Chemistry, Columbia University, New York

The low dimensional nature of TMDCs and the resulting reduced screening influence their non-equilibrium optical properties, as dynamic screening by photoexcited quasiparticles governs the transient response. Here, we investigate the respective roles of excitons and quasi-free carriers on the dynamic response of WS_2 monolayers on SiO_2. We find drastic changes in the reflectivity/transmittance contrast upon photoexcitation. The main observation is a pump photon energy-dependent blue/red shifts of the neutral exciton. Based on a phenomenological model, we disentangle the different impact of excitons and free carriers on the renormalization of the quasi-free-particle band gap and exciton binding energy. This work unravels and quantifies the competition and interplay of the multiple electronic and thermal processes contributing to the recovery of the system upon photoexcitation.

O 79.3 Wed 13:30 P

Transient band structure renormalizations and ultrafast exciton dynamics in fullerene thin films — •Sebastian Hedwig, Sebastian Emmerich, Benito Arnoldi, Johannes Stöckl, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany

Fullerenes have been subject to intense research in the past decades, with promising potential for their implementation in optoelectronic devices. Resonant optical excitation of a fullerene thin film leads to a transient renormalization of the polaronic valence band structure which follows the timescale of CT-exciton formation and decay, as recently shown for C_{60} [1,2]. Embedding metal atoms or clusters into the carbon cage can alter the cage symmetry and density of states leading to new relaxation channels, such as the cluster-cage electron transfer. Here, we present time resolved fs UV-pump XUV-probe photoemission studies carried out on thin films of C_{60} and the endohedral metallofullerene $Sc_3N@C_{80}$. Both fullerene complexes reveal almost identical band structure changes upon optical excitation evolving on similar timescales. For $Sc_3N@C_{80}$, we also show that the exciton and polaron dynamics are strongly altered upon K intercalation of the pristine film. This enables us to reveal the role of the cluster-cage charge transfer on the ultrafast carrier dynamics in fullerene thin films [3].

[1] B. Stadtmüller et al., Nat Commun 10, 1470 (2019)
[2] S. Emmerich et al., J. Phys. Chem. C 124, 23579-23587 (2020)
[3] S. Emmerich et al., arXiv:2002.04576 (2020)

O 79.4 Wed 13:30 P

Optical driven 4f-spin and orbital transitions in rare-earth metals — •N. Thielemann-Kühn[1], T. Amrhein[1], W. Bronsch[1], S. Jana[2], N. Pontius[2], R. Y. Engel[3], P. S. Miedema[3], M. Beye[3], B. E. van Kuiken[4], M. Teichmann[4], R. E. Carley[4], L. Mercadier[4], A. Yaroslavtsev[4], G. Mercurio[4], L. Le Guyader[4], N. Agarwal[4], A. Scherz[4], P. M. Oppeneer[5], M. G. Weinelt[1], and C. Schüssler-Langeheine[2] — [1]FU Berlin — [2]HZB — [3]DESY — [4]EuXFEL — [5]Uppsala University

4*f* rare earth (RE) metals exhibit strongly localized 4*f* states carrying the largest magnetic moment among the elements of the periodic table. Due to their energy-level scheme, 4*f* states are not directly accessible with optical wavelengths in contrast to the delocalized 5*d*6*s* valence electrons, that mediate the *inter*-atomic 4*f* exchange coupling. Despite the strong *intra*-atomic exchange coupling, local 5*d*-4*f* excitations have neither been observed upon optical excitation nor were considered to be relevant for non-equilibrium dynamics in RE metal based systems. In an X-ray absorption experiment at the EuXFEL we found that the 5*d* and 4*f* system interact directly via inelastic electron scattering and 4*f*-5*d* electron transfer, initiating transitions to higher energetic 4*f* configurations, which becomes pronouncedly visible in a change of the multiplet structure. The observed 4*f* electronic excitation are highly element-specific and strongly depend on pump pulse parameter. They directly cause changes in exchange and electron-phonon coupling and thus open a door for more fundamental understanding of non-equilibrium dynamics.

O 79.5 Wed 13:30 P

Extension of the two-temperature model capturing nonequilibrium electrons after ultrashort laser excitation — •Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

The understanding of materials' reaction on a laser excitation with pulse durations below one picosecond is of significant importance for industrial applications. The energy of ultrashort laser pulses in the visible range is absorbed by the electrons. This creates a non-equilibrium in the electron system that thermalizes typically in the following hundreds of femtoseconds [1]. On longer time scales, electrons and phonons relax to a joint temperature. The latter relaxation process is described by the well-known two-temperature model (TTM) [2]. However, this neglects the electronic non-equilibrium completely.

In this presentation, we investigate an extension of the TTM developed by Carpene [3] and Tsibidis [4]. This extension adds a system of nonthermal electrons to the TTM. We introduce several improvements and discuss selected results of the extended two-temperature model.

[1] B. Y. Mueller and B. Rethfeld, PRB **87**, 035139 (2013)
[2] S. I. Anisimov *et al.*, JETP **39**, 375 (1974)
[3] E. Carpene, PRB **74**, 024301 (2006)
[4] G. D. Tsibidis, Appl. Phys. A **124**, 311 (2018)

O 79.6 Wed 13:30 P

Carrier dynamics in a laser-excited Fe/MgO(001) heterostructure from real-time TDDFT — •elaheh shomali, Markus Ernst Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

The interaction of a femtosecond optical pulse with a metal/oxide interface has been addressed based on time-dependent density functional theory (TDDFT) in the real-time domain using the Elk code. We systematically studied electronic excitations of a $Fe_1/(MgO)_3(001)$ heterostructure as a function of laser frequency, peak power density and polarization direction. We find a marked anisotropy in the response to in-plane and out-of-plane polarized light, which changes its character for frequencies lower and higher than the MgO band gap. For laser frequencies between the MgO band gap and the charge transfer gap, interface states resulting from the hybridization of the $d_{3z^2-r^2}$ orbitals of Fe and the p_z orbitals of O at the interface may foster the propagation of excitations into the central layer of MgO. Spin-orbit coupling (SOC) is found to result in a small time-dependent reduction of magnetization only. Finally, we extend our investigation to examine the effect of spin-orbit coupling.

Financial support from the DFG within SFB 1242 (project C02) is gratefully acknowledged.

O 79.7 Wed 13:30 P

Tracing magnetization dynamics in Fe at the BZ edge by TR-ARPES — •Christian Strüber, Xinwei Zheng, Shabnam Haque, and Martin Weinelt — Freie Universität Berlin, Berlin, Germany

Time- and angle-resolved photoemission spectrocopy (TR-ARPES) allows for the investigation of magnetization dynamics by observing shifts in the electronic band structures and transient changes of the electronic population [1]. The focus of previous experiments often lay on the centre of the Brillouin zone (BZ). However, large parts of the electrons contributing to magnetism are distributed over the whole BZ.

We prepare single-crystalline layers of Fe on W(110) at 300 K and measure TR-ARPES signals at cryogenic temperatures (<100 K). In a pump-probe experiment photoelectrons are excited by ultrashort monochromatic XUV pulses (27.2 eV, 10 kHz, <100 fs) generated via HHG in an argon target. Demagnetization dynamics in the thin-film samples are pumped by intense NIR (770 nm) pulses. We measure the electronic excitation and energy shifts of majority and minority spin bands at the centre of the BZ and for high lateral momentum. We observe different dynamics of bulk and surface resonance states.

Additionally, we observe kinetic energy modulations before the temporal overlap resulting from an interaction with the ponderomotive potential of the pump pulse in front of the Fe sample. We investigate these modulations as a function of kinetic energy, emission angle and pump incidence angle and compare to results in Gd [2].

[1] B.Frietsch et al., *Science Advances* **6**,39(2020)

[2] U. Bovensiepen et al. *Physical Review B* **79**, 045415 (2009)

O 80: Poster Session VI: Poster to Mini-Symposium: Electrified solid-liquid interfaces I

Time: Wednesday 13:30–15:30 Location: P

O 80.1 Wed 13:30 P

Vibrational Sum Frequency Generation Studies of Carbon Dioxide Reduction on Gold: Effects of Electric Fields and Electrolyte Cations. — •Spencer Wallentine[1], Quansong Zhu[1], Savini Bandaranyake[1], Somnath Biswas[2], and Robert Baker[1] — [1]Ohio State University, Columbus Ohio, USA. — [2]Princeton University, Princeton New Jersey, USA

The electrochemical interface is complex in function yet elegant in its ability perform redox processes. These processes are sensitive to the electrolyte cation during carbon dioxide reduction, however the reason for this remains the subject of debate. Using vibrational sum frequency generation we measure in-situ spectra of adsorbed carbon monoxide on polycrystalline gold during carbon dioxide reduction. The surface bound carbon monoxide redshifts with applied potential due to the Stark effect. From this Stark shift we measure the interfacial electric field, which reaches a maximum of 35 MV/cm. We find that the interfacial electric field begins to saturate at -0.9 V vs SHE, and is indicative of the formation of a dense cation layer in the interfacial region. Interestingly, -0.9 V is coincident with the onset of high efficiency carbon monoxide production, which suggest that interfacial cations or the associated electric field enhance this faradaic process. These results are further corroborated by an increase in the Tafel slope, which is predicted to occur as the active site density decreases due to site blocking by ions. Taken together we obtain a atomistic picture of the electrode electrolyte interface where ions block some of the active sites, but the remaining sites are more active due to electric field stabilization.

O 80.2 Wed 13:30 P

Dodecanethiol on gold nanoparticles promotes catalytic performance by preventing trace ion deposition — •Hongyu Shang[1], Spencer Wallentine[1], Daniel Hofmann[2], Quansong Zhu[1], Catherine Murphy[2], and Robert Baker[1] — [1]The Ohio State University, Columbus, Ohio, USA — [2]University of Illinois: Urbana, IL, US

Nanoparticles are very efficient heterogeneous catalysts due to their inherent surface to volume ratio and tunability. Small organic molecules are usually used as capping agents to stabilize and control the size of the nanoparticles, which significantly affect the catalytic performance. To study the influence of capping agents in catalyzing carbon dioxide (CO2) to carbon monoxide (CO), we have performed carbon dioxide reduction (CDR) reaction on ultra-small (d=2nm) gold nanoparticles capped with different capping agents. We find that dodecanethiol on gold nanoparticles promotes catalytic selectivity and stability by inhibiting trace ion deposition that are responsible for rapid deactivation. Both the geometric structure and the microscopic ordering of the stabilization agent are found to influence the inhibition ability of the catalyst toward ion deposition. In addition, dodecanethiol capped gold nanoparticles exhibit a CO yield that is 100 times greater than polycrystalline gold when using ambient water source to prepare electrolyte. These findings give a better understanding in improving catalytic performance and provide a good opportunity to address the overlooked challenge of electrolyte purity.

O 80.3 Wed 13:30 P

Turn on the power - a theoretical adsorption study of electrified low- and high-index platinum/electrolyte interfaces — •Simeon D. Beinlich[1,2], Nicolas G. Hörmann[1,2], and Karsten Reuter[1,2] — [1]Technical University of Munich, Munich, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Simulating properties of electrified solid-liquid interfaces critically depends on the ability of modeling the energetics of such a system in a sensitive way. For over a decade now, the computational hydrogen electrode (CHE) was very successful in approximating the energetic influence of an applied electrode potential. By construction, however, it lacks the ability to model important electric-field and double-layer induced effects such as electrode potential or pH-dependent shifts in the relative stability of adsorption sites.

By describing the solid-liquid interface in a more detailed, grand canonical (GC) manner [1], that explicitly accounts for capacitive charging, we are able to simulate such shifts for various adsorption sites and adsorbate species on a high- and a low-index platinum surface. We compare classical CHE simulations with the GC approach and with a second-order approximation of it – the latter, in essence, consisting of the classical CHE expression and additional double-layer contributions (CHE+DL, [1]). It turns out that the CHE+DL approach – at computational costs comparable to the classical CHE approach – very accurately reproduces the GC results, offering a powerful tool for modeling electrified solid-liquid interfaces.

[1] N.G. Hörmann *et al.*, npj Comp. Mat. **6**, 136 (2020).

O 80.4 Wed 13:30 P

***Ab initio* Study of NiOOH (0001) Surfaces: Deprotonation and Alkali Metal Cation Adsorption** — •Mohammad J. Eslamibidgoli[1], Piotr Kowalski[1], Axel Gross[2], and Michael H. Eikerling[1] — [1]Institute of Energy and Climate Research, Modeling and Simulation of Materials for Energy Technology (IEK-13), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Nickel-based oxides are highly active, cost effective materials for the oxygen evolution reaction (OER) in alkaline conditions. Recent experimental studies have revealed the importance of surface deprotonation and alkali metal cation adsorption on the OER activity of Ni oxide surfaces, in contact with aqueous alkaline electrolyte [1,2]. In this study, we employ the DFT+U method within the grand-canonical scheme based on the computational hydrogen electrode [3,4] to determine the stable interface structure of β-NiOOH (0001) under varying electrochemical conditions (pH and electrode potential). We will discuss the effect of surface water layer and the potential-dependent shift in Gibbs free energy of adsorption arising from the interaction of surface dipoles with the interfacial electric field on the computed surface Pourbaix diagrams. [1] Diaz-Morales, O. et al. Chem. Sci. **2016**, 7, 2639-2645. [2] Garcia, A. C. et al. Angew. Chem. Int. Ed., **2019**, 58, 12999-13003. [3] Nørskov, J. K. et al. J. Phys. Chem. B, **2004**, 108, 17886-17892. [4] Groß, A. **2021**, Curr. Opin. Electrochem., accepted for publication.

O 80.5 Wed 13:30 P

Parameterization of ESM-RISM for the Pt(111)-Electrolyte Interface — •Rebekka Tesch[1,2,3], Michael H. Eikerling[1,2,3], and Piotr M. Kowalski[1,2] — [1]Theory and Computation of Energy Materials (IEK-13), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance, JARA-CSD and JARA-ENERGY, 52425 Jülich, Germany — [3]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Modeling of electrode/electrolyte interfaces at the atomic scale under applied potential is essential for understanding electrocatalytic reactions. A promising approach to treat the coupled interface phenomena is the Effective Screening Medium Reference Interaction Site Method (ESM-RISM) [1] that combines Density Functional Theory with the integral theory of liquids. However, ESM-RISM implements Lennard-Jones (LJ) interaction potentials for electrolyte-electrolyte and electrode-electrolyte interactions. The choice of LJ parameters is thus crucial for obtaining a realistic description, but these parameters are rarely transferable. To address this issue we fit the LJ parameters to reproduce ab initio electrolyte density profiles for the Pt(111)-aqueous electrolyte interface. We also scrutinize the choices of further input parameters in the ESM-RISM implementation [2]. These steps yield a more accurate description of the Pt(111)-electrolyte interface.

[1] Nishihara and Otani, Phys. Rev. B 96, 115429, 2017.

[2] Fernandez-Alvarez and Eikerling, ACS Appl. Mater. Interfaces 11, 46, 43774, 2019.

O 80.6 Wed 13:30 P

Recent advancements in the development of screening approaches and descriptors for electrocatalytic processes — •Kai Exner — University Duisburg-Essen, Faculty of Chemistry, Theoretical Chemistry, Universitätsstraße 5, 45141 Essen, Germany — Cluster of Excellence RESOLV, Bochum, Germany

For the identification of electrocatalysts from databases, heuristic screening approaches have been established to categorize materials into active and inactive [1]. Most of these studies rely on the initial idea of Nørskov, Rossmeisl, and coworkers in that only the binding energies (thermodynamics) of potential reaction intermediates (RIs) within the electrocatalytic cycle are assessed. Recently, this thermodynamic picture was challenged, reporting that the optimum binding energy shifts from thermoneutral to weak bonding with increasing driving force [2]. This result, explained by an extension of the Sabatier principle for electrocatalytic reactions [3], has direct implications on the energetics of multiple-electron processes, such as the four-electron oxygen evolution reaction. There, the thermodynamic overpotential, commonly used as activity descriptor, has been replaced by a universal descriptor, Gmax(η), factoring overpotential and kinetic effects into the analysis [4]. The present contribution aims to provide an overview of the recent advancements in the application of heuristic screening approaches and descriptors for the hydrogen and oxygen evolution reactions.

[1] KSE, Adv. Funct. Mater. 2020, 30, 2005060. [2] KSE, Angew. Chem. Int. Ed. 2020, 59, 10236. [3] K.S. Exner, Curr. Opin. Electrochem. 2021, 26, 100673. [4] KSE, ACS Catal. 2020, 10, 12607.

O 80.7 Wed 13:30 P

We hold these truths to be self-evident, that all halide CVs are created equal. — •Nicolas G. Hörmann[1,2] and Karsten Reuter[2] — [1]Technische Universität München, Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Consistent with chemical intuition, the cyclic voltammograms (CVs) of Ag(111) in halide containing solutions are essentially identical for Cl, Br, and I, when simulated based on DFT calculations and the computational hydrogen electrode (CHE) approximation. Quite in contrast, experiments reveal significant differences in CV peak heights and shapes.

Here we show that the DFT results can be reconciled with experiment, when using a fully grand canonical description in an implicit solvent model that allows for capacitive charging [1]. It is thus only the latter and not the adsorption energetics at the potential of zero charge, that leads to the experimental variation in the CVs across the halide series. This finding is supported by a general analysis of the relation between grand canonical and CHE energetics, which in addition provides new insights into non-Nernstian behavior and the relevance of classical electrochemical concepts such as the electrosorption valency[2].

[1] N.G. Hörmann *et al.*, J. Chem. Phys. **150**, 041730 (2019). [2] N.G. Hörmann *et al.*, npj Comput. Mater. **6**, 136 (2020).

O 81: Poster Session VI: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces II

Time: Wednesday 13:30–15:30 Location: P

O 81.1 Wed 13:30 P

Spin polarization of quantum confined surfaces states of 2D metal-organic network structures — •Lu Lyu, Tobias Eul, Wei Yao, Benito Arnoldi, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics, TU Kaiserslautern, Germany

Controlling the quantum confinement of spin-dependent electronic states by design of two-dimensional (2D) metal-organic networks (MON) opens a unique avenue to accelerate the implementation of quantum technology into the next generation of spintronic applications. In our work, we focus on the quantum confinement of occupied Shockley surface states (SS) and unoccupied image potential states (IPS) of noble metal (111) surfaces by the formation of 2D metal-organic networks. Both surface states are well-known quasi-free 2D electron gases (2DEGs) with a Rashba spin-orbit splitting. For the exemplary case of the Cu-T4PT network on Cu(111) surface, we investigate the trapping of the 2DEG into a 2D quantum dot system using spin- and momentum-resolved photoemission. We reveal that the dispersion free electron-like surface states transform into periodic bands in momentum space. The details of the band structure depend critically on the intercoupling between electrons trapped in neighboring pores. In addition, we demonstrate that the mixing of molecular and metallic states reduces the magnitude of the spin-splitting of confined SS and IPS due to the strongly reduced spin-orbit coupling strength of the molecular materials. Our works open up a new avenue towards manipulating the spin-dependent trapping of electrons in metal-organic network structures.

O 81.2 Wed 13:30 P

A scanning tunneling microscope capable of electron spin resonance and pump-probe spectroscopy at mK temperature and in vector magnetic field — •Werner M.J. van Weerdenburg[1], Manuel Steinbrecher[1], Niels P.E. van Mullekom[1], Jan W. Gerritsen[1], Henning von Allwörden[1], Fabian D. Natterer[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Department of Physics, University of Zürich, Switzerland

Recent advances in detecting atomic spin dynamics have combined techniques like electron spin resonance (ESR) and pump-probe spectroscopy with scanning tunneling microscopy (STM). Such methods have been employed to detect small magnetic interactions, and spin relaxation and coherence times in the nanosecond regime.

Here, we demonstrate the implementation of ESR and all-electrical pump-probe spectroscopy in a dilution-refridgerator (DR) STM, equipped with a vector magnetic field [1]. The efficient cooling of the DR permits the use of appreciable RF amplitudes at the STM junction while remaining at mK base temperature. We measure ESR resonances of a single TiH molecule on MgO/Ag(100) in an unprecedented low frequency band [2], enabled by the mK temperature, and use pump-probe spectroscopy to study the spin relaxation time of single Fe atoms on MgO/Ag(100) in a vector magnetic field.

[1] W. van Weerdenburg et al., arXiv:2007.01835v2;

[2] M. Steinbrecher et al., arXiv:2007.01928

O 81.3 Wed 13:30 P

Experimental connection between Yu-Shiba-Rusinov states and the Kondo effect using numerical renormalization group theory — •Haonan Huang[1], Sujoy Karan[1], Robert Drost[1], Ciprian Padurariu[2], Alfredo Levy Yeyati[3], Juan Carlos Cuevas[3], Björn Kubala[2], Joachim Ankerhold[2], Klaus Kern[1,4], and Christian R. Ast[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, Ulm, Germany — [3]IFIMAC, Universidad Autónoma de Madrid, Madrid, Spain — [4]EPFL, Lausanne, Switzerland

Magnetic impurities on superconductors give rise to Yu-Shiba-Rusinov (YSR) states in the gap. When the superconductivity is quenched, the Kondo effect manifests itself as a spectral anomaly at the Fermi energy. Both phenomena can be understood quantitatively with the single impurity Anderson model (SIAM) using numerical renormalization group (NRG) theory. One prediction of this theory is that the YSR energy depends universally on the ratio between the Kondo temperature T_{K} and the superconducting order parameter Δ. Nevertheless, deviations from this universal behavior have been observed in different experiments. Using a scanning tunneling miscroscope, we show that for a spin 1/2 impurity on the apex of a superconducting vanadium tip, both the YSR state and the Kondo peak can be quantitatively reproduced by the NRG theory using the Ljubljana code. Intriguingly, the asymmetry of the experimental spectra is also contained within the SIAM for both cases, indicating the essential role of the particle-hole asymmetry which is absent in the conventional Kondo impurity model.

O 81.4 Wed 13:30 P

Engineering atomic-scale magnetic fields by dysprosium single atom magnets — •Aparajita Singha[1,2,3], Philip Willke[1,2,4], Tobias Bilgeri[5], Xue Zhang[1,2], Harald Brune[5], Fabio Donati[1,2], Andreas Heinrich[1,2], and Taeyoung Choi[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Republic of Korea — [2]Ewha Womans University, Republic of Korea — [3]Max-Planck-Institut für Festkörperforschung, Germany — [4]Physikalisches Institut, KIT, Germany — [5]Institute of Physics, EPFL, Switzerland

Atomic-scale engineering of magnetic fields is a key ingredient for miniaturizing quantum devices and precision control of quantum systems. This requires a unique combination of magnetic stability and spin-manipulation capabilities. Surface-supported single atom magnets [1,2] offer such possibilities, where long temporal and thermal stability of the magnetic states can be achieved by maximizing the magnetic anisotropy and by minimizing quantum tunnelling of the magnetization. Here, we show that dysprosium atoms adsorbed on magnesium oxide have a giant anisotropy of 250 meV, currently the highest among all surface spins. Using a variety of STM techniques including single atom electron spin resonance [3], we confirm no spontaneous spin-switching in these atoms over days at ≈ 1 K under low and even at vanishing magnetic fields. We utilize these robust single atom magnets to engineer magnetic nanostructures, demonstrating unique control of magnetic fields with atomic-scale tunability. [1] Science 352, 318 (2016); [2] Nature 543, 226 (2017); [3] Science 350, 417 (2015).

O 81.5 Wed 13:30 P

An ultra-high vacuum electron spin resonance spectrometer for investigation of magnetic atoms and molecules at surfaces — •Jisoo Yu[1,2], Franklin Cho[1,2], Luciano Colazzo[1,2], Yejin Jeong[1,2], Junjie Liu[3], Arzhang Ardavan[3], Giovanni Boero[4], Andreas Heinrich[1,2], and Fabio Donati[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul, Republic of Korea — [2]Department of Physics, Ewha Womans Universitiy, Seoul, Republic of Korea — [3]The Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, UK — [4]Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratory for Microsystems, Lausanne, Switzerland

Magnetic atoms and molecules on surfaces are model systems to control and manipulate quantum coherence properties at the smallest scale of matter. Their performances as qubits can be investigated through electron spin resonance (ESR) spectroscopy [Nat. Chem. 11, 301(2019)]. However, commercial spectrometers do not meet the requirements of ultra-high vacuum (UHV) and surface-sensitivity to measure a single layer of surface-adsorbed spin centers. We present an UHV ESR spectrometer that enables us to measure thin molecular films in a wide range of temperature (2.5-300 K) and magnetic field (0-3.2 T). This spectrometer operates in the X-band (10 GHz) both in continuous wave (CW) and pulsed mode. To maximize the microwave field on a 2D spin system we deposited the molecular layer directly on the resonator surface. We demonstrate sensitivity of 10^{12} spins/G*Hz in CW, which allows ESR measurements down to a single layer of molecular spins.

O 81.6 Wed 13:30 P

Quantifying the interplay between fine structure and geometry of an individual molecule on a surface — •Manuel Steinbrecher[1], Werner M.J. v. Weerdenburg[1], Etienne F. Walraven[1], Niels P.E. v. Mullekom[1], Jan W. Gerritsen[1], Fabian D. Natterer[2], Danis I. Badrtdinov[3,1], Alexander N. Rudenko[4,3,1], Vladimir V. Mazurenko[3], Mikhail I. Katsnelson[1,3], Ad v.d. Avoird[1], Gerrit C. Groenenboom[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics, University of Zurich, Zurich, Switzerland — [3]Theoretical Physics and Applied Mathematics Department, Ural Federal University, Ekaterinburg, Russia — [4]School of Physics and Technology, Wuhan University, Wuhan, China

With spin-resolved scanning tunneling microscopy (SP-STM) and electron spin resonance (ESR) we have probed single TiH molecules deposited on a thin insulating MgO layer in a vector magnetic field at mK temperatures down to MHz frequencies. We find that the molecule retains a non-trivial orbital angular momentum. This results in a strongly renormalized and anisotropic g-tensor. As we prove, the latter does not stem from Kondo or Jahn-Teller effects. From quantum chemistry embedded cluster calculations we find an analytical expression for the g-tensor, which solely depends on the splitting of the ground states and the spin-orbit coupling. In a dynamic expansion of the model, the position of the H atom and rotational dynamics of the molecule were investigated. [1] Steinbrecher *et al.*, arXiv 2007.01928 (2020)

O 81.7 Wed 13:30 P

Inducing and Controlling Molecular Magnetism through Supramolecular Manipulation — •Jan Homberg, Alexander Weismann, Richard Berndt, and Manuel Gruber — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24118 Kiel, Germany

Diamagnetic H_2 phthalocyanine molecules are probed on superconducting Pb(100) using a low-temperature scanning tunneling micoscope (STM). In supramolecular arrays made with the STM, the molecules acquire a spin as detected *via* the emergence of Yu-Shiba-Rusinov resonances. The spin moments vary among the molecules and are determined by the electrostatic field that results from polar bonds in the surrounding Pc molecules. The moments are further finely tuned by repositioning the hydrogen atoms of the inner macrocycle of the surrounding molecules.

O 82: Poster Session VI: Poster to Mini-Symposium: Frontiers of electronic-structure theory III

Time: Wednesday 13:30–15:30 Location: P

O 82.1 Wed 13:30 P

Diagrammatic Monte Carlo study of the acoustic lattice polaron — •Thomas Hahn[1], Andrey Mishchenko[2,3], Naoto Nagaosa[2], and Cesare Franchini[1,4] — [1]Faculty of Physics, Center for Computational Materials Science, University of Vienna, A-1090 Vienna, Austria — [2]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan — [3]National Research Center Kurchatov Institute, 123182 Moscow, Russia — [4]Dipartimento di Fisica e Astronomia, Università di Bologna, 40127 Bologna, Italy

The Diagrammatic Monte Carlo (DMC) method is used to study an electron interacting with acoustic phonons via the deformation potential. For the first time, we obtain unbiased results for the acoustic polaron in a realistic condensed matter discrete lattice model and resolve self-contradictory conclusions from previous studies based on the continuum approximation. We present accurate numerical results for the ground state energy, effective mass, quasiparticle weight and the structure of the phonon cloud of the polaron. The most interesting data is obtained for excited states in the parameter range of the transient region between the weak and strong coupling regime. The unique structureless shape of the incoherent part of the spectral function and the flat background of the optical conductivity allows us to follow the behavior of excited states, whose studies are hindered in optical polaron models. We show that the behavior of the excited states in the spectral function is different from what is seen in the optical conductivity. This confirms the different nature of the excited states observed in these different probes of the excited spectra of the polaron.

O 82.2 Wed 13:30 P

First principles study of spin spirals in the multiferroic $BiFeO_3$ — •Sebastian Meyer[1], Bin Xu[2,3], Matthieu Verstraete[1], Laurent Bellaiche[2], and Bertrand Dupé[1,4] — [1]Nanomat/Q-mat/CESAM, University of Liège, Belgium — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, USA — [3]Jiangsu Key Laboratory of Thin Films, School of Physical Science and Technology, Soochow University, China — [4]Fonds de la Recherche Scientifique (FNRS), Bruxelles, Belgium

We carry out density functional theory (DFT) calculations to explore the antiferromagnetic (AFM) spin spiral in multiferroic $BiFeO_3$. We calculate the spin spiral energy dispersion $E(\mathbf{q})$ along the high symmetry directions of the pseudocubic unit cell, for four different structural phases: *cubic*, $R\bar{3}c$, $R3m$ and $R3c$. In all cases, we find a large exchange frustration. The comparison provides detailed insight into how polarization and octahedral anti-phase tilting affect the different magnetic interactions and the magnetic ground state in $BiFeO_3$. For the $R3c$ structural ground state, we find an AFM spin spiral ground state with a periodicity of ~80 nm in good agreement with experiments and previous findings. This spin spiral is driven by a Dzyaloshinskii-Moriya interaction stemming from the Fe–Bi ferroelectric displacement. The spiral appears to be stable because the anisotropy energy in $R3c$ $BiFeO_3$ is too small to enforce the collinear order. For all the four phases, we discuss the magnetic ground state and identify its stabilization mechanisms.

O 82.3 Wed 13:30 P

Influence of electronic excitations on defect formation on GaAs — •Daniel Muñoz-Santiburcio[1], Natalia Koval[1], Fabiana Da Pieve[2], and Emilio Artacho[1,3] — [1]CIC Nanogune, Tolosa Hiribidea 76, 20018 San Sebastián, Spain — [2]Royal Belgian Institute for Space Aeronomy, Av Circulaire 3, 1180 Brussels, Belgium — [3]Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom

Solar cells in spacecrafts are subject to high energy ions of solar and cosmic radiation, which promote the formation of defects in their different layers, notably affecting their performance.

The formation of defects in such materials has been abundantly studied, but usually assuming that the system stays in its electronic ground state during the whole process. On the other hand, when the target is irradiated with high energy particles, its electronic subsystem is significantly excited as a consequence of the projectile' passing. These electronic excitations may greatly alter the process of defect formation in the material in comparison to the ground-state conditions.

Here we present a study via first-principles Molecular Dynamics of the influence of the electronic excitations on the formation of defects on GaAs. We simulate the formation of different types of defects in the material for excitations of varying extent. We will show that the electronic excitations have a significant impact on the defect formation, changing the threshold displacement energy and causing different types of defects, even promoting local phase changes in the target material.

O 82.4 Wed 13:30 P

Optimized effective potentials to increase the accuracy of approximate proton transfer energy calculations in the excited state — •Pouya Partovi-Azar and Daniel Sebastiani — Institute of Chemistry, MLU Halle-Wittenberg, Halle (Saale), Germany

In various systems, acidic properties emerge when the system is electronically excited. Although the time scale attributed to the dynamics of the electrons is usually on the order of femtoseconds, the electronic excitations can in general trigger much slower processes.

Here, we propose and benchmark a novel approximate first-principles molecular dynamics simulation idea for increasing the computational efficiency of density functional theory-based calculations of the excite states. We focus on obtaining proton transfer energy at the S_1 excited state through actual density functional theory calculations at the T_1 state with additional optimized effective potentials. The potentials are optimized such as to reproduce the time-dependent density functional theory energy surface, but can be generalized to other more accurate quantum chemical methods. We demonstrate the applicability of this method for two prototypical photoacids, namely phenol and 7-hydroxyquinoline. We show that after optimizing the additional effective potentials for carbon, nitrogen, oxygen, and the acidic hydrogens, both thermodynamics and kinetics of proton dissociation reaction can be well reproduced as compared to reference excited-state calculations. It is found that a good agreement can be reached by only optimizing two effective potential parameters per each species in the photoacids.

O 82.5 Wed 13:30 P

Assessment of the Ab Initio Bethe-Salpeter Equation Approach for the Low-Lying Excitation Energies of Bacteriochlorophylls and Chlorophylls — •Zohreh Hashemi[1] and Linn Leppert[1,2] — [1]Institute of Physics, University of Bayreuth, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

Bacteriochlorophyll and Chlorophyll molecules are crucial building blocks of the photosynthetic apparatus in bacteria, algae and plants. In this contribution we assess the accuracy of ab initio many body perturbation theory within the GW approximation and Bethe-Salpeter equation (BSE) approach for calculating the electronic structure and optical excitations of seven members of this important family of light harvesting pigments. We compare our calculations with results from time-dependent density functional theory, multireference RASPT2 and experimental literature results. We find that optical excitations calculated with GW+BSE are in excellent agreement with experimental data, with an average deviation of less than 100 meV for the first three bright excitations of the entire family of (Bacterio)chlorophylls. Contrary to state-of-the-art TDDFT with an optimally-tuned range-separated hybrid functional, this accuracy is achieved in a parameter-free approach. Moreover, GW+BSE predicts the energy differences between the low-energy excitations correctly, and eliminates spurious charge transfer states that TDDFT with (semi)local approximations is known to produce.

O 82.6 Wed 13:30 P

microscopic modeling of rare-earth perovskite properties — •alireza sasani[1], jorge iniguez[2,3], and eric bousquet[1] — [1]Physique Théorique des Matériaux, QMAT, CESAM, Université de Liège, B-4000 Sart-Tilman, Belgium — [2]MaterialsResearch and Technology Department, Luxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362, Esch/Alzette, Luxemburg — [3]Department of Physics and Materials Science, University of Luxembourg, Rue du Brill 41, L-4422 Belvaux, Luxembourg

Rare earth perovskites(RFeO_3,RCrO_3 and R a rare earth element) have been studied for a long time due to having interesting magnetic behaviors,i.e magnetization reversal(Mr) and spin reorientation(SR). In this work, we shed some more light onto the magnetic properties of the rare earth perovskites(RFeO's) by using density functional theory (DFT) to fit a microscopic Heisenberg model that includes the superexchange and the DMI between both Fe-Fe and Fe-*R* interactions. This model is used to do classical spin dynamics and it is employed as a global general model where the different parameters are tuned to understand their specific role in the (MR) and (SR) transitions. The results are also compared with analytical solutions to confirm the consistency of the spin dynamics solutions. Our works allow to explain the origin of the SR by determining the important parameters for the SR temperature interval and how the *R* magnetism is affected while it is in its paramagnetic regime. Our study also allows to fully understand the exact microscopic origin of the MR.

O 82.7 Wed 13:30 P

***Ab initio* phonon self-energies and fluctuation diagnostics of phonon anomalies: Lattice instabilities from Dirac pseudospin physics in transition metal dichalcogenides** — •Jan Berges[1], Erik van Loon[1], Arne Schobert[1], Malte Rösner[2], and Tim Wehling[1] — [1]Universität Bremen, Germany — [2]Radboud Universiteit Nijmegen, The Netherlands

We present an *ab initio* approach for the calculation of phonon self-energies and their fluctuation diagnostics, which allows us to identify the electronic processes behind phonon anomalies. Application to the transition-metal-dichalcogenide monolayer TaS_2 reveals that coupling between the longitudinal–acoustic phonons and the electrons from an isolated low-energy metallic band is entirely responsible for phonon anomalies such as the mode softening and associated charge-density waves observed in this material. Our analysis allows us to distinguish between different mode-softening mechanisms including matrix-element effects, Fermi-surface nesting, and Van Hove scenarios. We find that matrix-element effects originating from a peculiar type of Dirac pseudospin textures control the charge-density-wave physics in TaS_2 and similar transition metal dichalcogenides.

O 83: Poster Session VI: Poster to Mini-Symposium: Infrared nano-optics IV

Time: Wednesday 13:30–15:30 Location: P

O 83.1 Wed 13:30 P

Dipole model for far-field thermal emission of a nanoparticle above a planar substrate — •Florian Herz and Svend-Age Biehs — Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany

I will present our latest efforts in developing a dipole model describing the thermal far-field radiation of a nanoparticle close to a substrate. The nanoparticle serves as a first approximation for the cantilever tip usually used in infrared near-field thermal imaging experiments [1-3].

We generalized existing approaches by including the possibility to have different temperatures for substrate, nanoparticle, and background to cover setups like the thermal radiation scanning tunnelling microscope (TRSTM) [1], the thermal infrared near-field spectroscopy (TINS) [2], and the scanning noise microscope (SNoiM) [3]. Apart from the induced electric dipole moment, we also considered eddy currents being particularly important for metallic particles. Furthermore, instead of neglecting divergent terms of the Green's function appearing in the dipole model, we carry out a renormalization procedure.

I will explain how we methodically incorporated these generalizations and discuss how they affect the numerical simulations. Additionally, I will discuss the impact of parameters like particle size and emission angle as well as the distance dependence for all four combinations of the materials gold and SiC for nanoparticle and substrate.

1 Y. De Wilde et al., Nature 444, 740 (2006)
2 A. C. Jones and M. B. Raschke, Nano. Lett. 12, 1475 (2012)
3 Q. Weng et al., Science 360, 775 (2018)

O 83.2 Wed 13:30 P

Nanoimaging of vibrational strong coupling between propagating phonon polaritons and organic molecules — •A Bylinkin[1,2], M Schnell[1], M Autore[1], F Calavalle[1], P Li[1], J Taboada-Gutierrez[3], S Liu[4], J Edgar[4], F Casanova[1], L Hueso[1], P Gonzalez[3], A Nikitin[2], and R Hillenbrand[1] — [1]CIC nanoGUNE BRTA, Spain — [2]DIPC, Spain — [3]Universidad de Oviedo, Spain — [4]Kansas State University Manhattan, USA

Enhanced light-matter interaction in polar crystals attracts considerable attention since the latter support phonon polaritons (PPs) - hybrid electromagnetic modes involving atomic vibrations. PPs in the thin slab of van de Waals materials (vdW) demonstrate long lifetime and ultra-high field confinement which can lead to intriguing vibrational strong coupling (VSC) phenomena and potential sensing applications. Recently VSC between h-BN nano-resonators and molecular vibration has been demonstrated. However, the basic interaction between molecular vibrations and propagating PPs in unstructured slabs of the vdW materials has not yet studied. In this work, we use nanoimaging techniques to study the interaction between propagating h-BN PPs and organic molecular vibrations. We performed near-field polariton interferometry, showing that VSC leads to the formation of a hybrid mode with a pronounced anti-crossing region in its dispersion. Our work shows the fundamental study of the strong-coupling between molecular vibration and propagating PPs.

O 83.3 Wed 13:30 P

Nonlocal response of polar dielectric systems — Christopher Gubbin and •Simone De Liberato — School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom

Surface phonon polaritons hosted in polar nanostructures are fast becoming a leading platform for mid-infrared nanophotonics, permitting deep subdiffraction energy localisation in comparatively low-loss modes. Recent experiments have demonstrated that as polar resonators approach the nanoscale their optical response diverges from that predicted using a local dielectric model [1, 2]. Although this divergence can be explained by microscopic ab-initio methods it is impractical to apply these intensive calculations to optical systems. To solve this issue we develop a nonlocal dielectric theory which captures the essence of the material response by accounting for propagating phonon modes in the dielectric. Unlike in plasmonic nonlocality these modes can propagate into the host medium, yielding a discrete spectrum and unique phenomenology. In this talk I outline our theory [3], its applications to nanoscale polar resonators [4] and superlattices [5], and finally discuss some of the predicted features, including the impact on the resonator spectral response and quality factor.

[1] D. C. Ratchford et al., ACS Nano 13, 6730 (2019).
[2] C. R. Gubbin et al., Nat. Comm. 10, 1682 (2019).
[3] C. R. Gubbin et al., Phys. Rev. X 10, 021027 (2020).
[4] C. R. Gubbin et al., Phys. Rev. B 102, 201302(R) (2020)
[5] C. R. Gubbin et al., Phys. Rev. B 102, 235301 (2020)

O 84: Key Note VI

Time: Wednesday 15:30–16:00 Location: R1

Plenary Talk O 84.1 Wed 15:30 R1

Surface structure by way of machine learning — •Bjørk Hammer — Aarhus University, Denmark

Atomistic simulations of the physico-chemical processes at inorganic surfaces often require knowledge of the energetically most optimal state of the surfaces. In this talk, examples are given of intricate surface reconstructions and surprising shapes assumed by metal nano-particles supported on oxide surfaces. The focus of the talk will be on how to identify such optimal structure given a costly total energy method as implemented in an electronic structure program, typically a density functional theory program (DFT). A number of approaches will be presented. i) A purely **evolutionary approach**[1] in which new structural candidates are created by random cross-over and mutation operations, ii) a **machine learned-enhanced evolutionary approach**[2,3] in which an on-the-fly learned surrogate energy landscape directs the candidate production, and finally iii) a **reinforcement learning approach**[4] in which image recognition via a convolutional neural network is used to build up rational knowledge about the energy landscape, that eventually leads to the construction of globally optimal structure.

[1] Phys. Rev. Lett. **108**, 126101 (2012).

[2] Phys. Rev. Lett. **124**, 086102 (2020).

[3] **https://gofee.au.dk**

[4] Phys. Rev. B, **102**, 075427 (2020).

O 85: Key Note VII

Time: Thursday 10:00–10:30 Location: R1

Plenary Talk O 85.1 Thu 10:00 R1

On-surface reactions and molecular charge-state transitions by atom manipulation — Katharina Kaiser, Shadi Fatayer, Florian Albrecht, and •Leo Gross — IBM Research - Zurich

Molecules can be created using atom manipulation to break and to form covalent bonds. High-resolution atomic force microscopy (AFM) with functionalized tips provides insights into the structure, geometry, aromaticity, charge states and bond-order relations of the molecules created and into the reactions performed [1]. Recently, we generated the elusive molecular carbon allotrope cyclo[18]carbon and resolved its long debated structure [2].

On insulating substrates, we control the charge state of molecules by deliberately attaching and detaching single electrons and measured the reorganization energy of a molecule [3] and recently probed molecular excited states [4]. Moreover, we resolved changes of molecular geometry, adsorption and aromaticity related to its oxidation state [5].

References [1] L. Gross et al. Angew. Chem Int. Ed 57, 3888 (2018). [2] K. Kaiser et al. Science 365, 1299 (2019). [3] S. Fatayer et al. Nature Nanotechnol. 13, 376 (2018). [4] S. Fatayer et al. arXiv:2011.09870 (2020). [5] S. Fatayer et al. Science 365, 142 (2019).

O 86: Mini-Symposium: Machine learning applications in surface science II

Time: Thursday 10:30–12:30 Location: R1

Invited Talk O 86.1 Thu 10:30 R1

Machine learning for robotic nanofabrication with molecules — •Christian Wagner — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — JARA Fundamentals of Future Information Technology, Jülich, Germany

The ability to handle single molecules as effectively as macroscopic building-blocks would enable the construction of complex supramolecular structures that are not accessible by self-assembly. A central difficulty on the way towards this technology is the uncontrolled variability and poor observability of atomic-scale conformations, especially during the manipulation process. We present a generic strategy to overcome both obstacles, and demonstrate autonomous robotic nanofabrication with single molecules using reinforcement learning (RL). Quite generally, RL is able to learn strategies even in the face of large uncertainty and with sparse feedback. Indeed, RL based prediction models recently exceeded human performance in several games. However, to be useful for nanorobotics, standard RL algorithms must be adapted to also cope with the limited training opportunities that are available there. We demonstrate our correspondingly enhanced RL approach by applying it to an exemplary task of subtractive manufacturing with a scanning probe microscope (SPM). Complementary to that we outline how machine learning and control theory methods in combination with molecular simulations can be utilized to recover atomic-scale conformations from the sparse experimental SPM data available during manipulation.

Invited Talk O 86.2 Thu 11:00 R1

Chemisorbed or Physisorbed? Resolving surface adsorption with Bayesian inference and atomic force microscopy — •Milica Todorović — Department of Applied Physics, Aalto University, P.O. Box 11100, Aalto 00076, Finland

The knowledge on structure, bonding and properties of organic adsorbates to inorganic substrates underpins key technologies from catalysis through coatings to optoelectronics. Atomic force microscopy (AFM) and ab initio simulations are powerful tools for characterising molecular adsorption, but both struggle with complex bulky adsorbates where lack of chemical intuition and inconclusive imaging render the structure identification problematic. We address this challenge with Bayesian Optimization Structure Search (BOSS), a computational tool for global configurational structure search at surfaces and interfaces.

We employed BOSS to study the adsorption of (1S)-camphor on the Cu(111) surface, where AFM experiments recorded an unusual variety of images. From a single configurational search we retrieved 8 unique stable adsorbates. We discovered that camphor undergoes both covalent and dispersive binding to this substrate. Matching our findings to experimental data allowed us to categorise the AFM images into those associated with chemisorbed and physisorbed molecules. By simulating AFM images of the chemisorbed model structures, we identified three distinct adsorbates in the experimental images, further clarifying AFM image interpretation. This study illustrates how machine learning applications advance understanding in surface science by complementing both computation and experiment.

O 86.3 Thu 11:30 R1

Ab initio structure search of flexible molecules at interfaces — •Dmitrii Maksimov[1,2] and Mariana Rossi[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

We investigate how the accessible conformational space of two flexible amino acids, Arg and Arg-H$^+$, changes upon adsorption, by building and analyzing a database of thousands of structures optimized at Cu(111), Ag(111) and Au(111) surfaces with the PBE functional including screened pairwise (vdW) interactions. We employ an unsupervised dimensionality reduction procedure that enables us to understand the alteration of the high-dimensional conformational space [1]. The creation of this database, which is paramount to train further diverse machine-learning models, suffers from well-known bottleneck related to the efficiency of the geometry optimizer. We introduce a flexible way of preconditioning approximate Hessian matrices in the BFGS algorithm that is tailored to accelerate the relaxation of vdW bonded structures that can handle large structural changes. An automated sampling of these systems is implemented within a random structure search package [2] that can take explicitly into account the flexibility of molecules, their position and orientation with respect to fixed surroundings and interfaces.

[1] Maksimov et. al., Int. J. Quantum Chem., e26369 (2020)

[2] https://github.com/sabia-group/gensec

O 86.4 Thu 11:45 R1

Configurational polaron energies using machine learning — •Viktor Birschitzky, Michele Reticcioli, and Cesare Franchini — University of Vienna, Faculty of Physics

Polarons are quasiparticles formed by the coupling of excess charge carriers with the phonon field. Polarons form preferentially at surfaces and have a wide range of effects on the chemical and physical properties of the hosting material.[1] First principles calculations of polarons conformational energies typically require large supercells and long molecular dynamics (MD) simulations, making the modeling of multipolaron system within reasonable timescales very challenging. Here, we propose a supervised machine learning scheme based on kernel-regression to solve this problem by learning single polaron energies for the prototypical oxygen-defective rutile $TiO_{2-x}(110)$ surface, where each oxygen vacancy provides two excess electrons. To achieve accurate predictions on an ab initio MD database of polaronic energies[2] a descriptor has been developed, which embodies the interactions between polarons with defects and other localized charge carriers. Our results show that the proposed ML method is able to expand the DFT database with energetically more favorable polaron configurations – improving the convex hull construction – and that generalization at arbitrary polaron concentration and defect types is possible.

[1] C. Franchini et al., Polarons in Material, Nature Review Materials, (2021)

[2] M. Reticcioli et al., Formation and dynamics of small polarons on the rutile TiO_2 surface, Physical Review B, (2018)

O 86.5 Thu 12:00 R1

Neural Network Analysis of Neutron and X-Ray Reflectivity Data: Pathological Cases, Performance and Perspectives — •Alessandro Greco[1], Vladimir Starostin[1], Alexander Hinderhofer[1], Alexander Gerlach[1], Maximilian Skoda[2], Stefan Kowarik[3], and Frank Schreiber[1] — [1]Institute of Applied Physics, University of Tübingen, Germany — [2]Rutherford Appleton Lab, ISIS Neutron and Muon Source, UK — [3]Department of Physical Chemistry, University of Graz, Austria

Neutron and X-ray reflectometry (NR and XRR) are powerful techniques to investigate the structural, morphological and even magnetic properties of solid and liquid thin films. Having demonstrated the general applicability of neural networks to analyze XRR and NR data before [1], this work discusses challenges arising from certain pathological cases as well as performance issues and perspectives. These cases include a low signal to noise ratio, a high background signal (e.g. from incoherent scattering), as well as a potential lack of a total reflection edge (TRE). We show that noise and background intensity pose no significant problem as long as they do not affect the TRE. However, for curves without strong features the prediction accuracy is diminished. Furthermore, we discuss the effect of different scattering length density combinations on the prediction accuracy. The results are demonstrated using simulated data of a single-layer system.

[1] Greco et al., *J. Appl. Cryst.*, **52**, 1342 (2019)

O 86.6 Thu 12:15 R1

Materials genes of heterogeneous catalysis from clean experiments and AI — •Lucas Foppa[1,2], Luca M. Ghiringhelli[1,2], Frank Rosowski[3], Robert Schloegl[1,4], Annette Trunschke[1], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft — [2]Humboldt-Universität zu Berlin — [3]BASF SE — [4]Max-Planck-Institut für Chemische Energiekonversion

Heterogeneous catalysis is an example of a complex materials function, governed by an intricate interplay of several processes, e.g. the dynamic re-structuring of the catalyst material at reaction conditions and different surface chemical reactions. Modelling the full catalytic progression via first-principles statistical mechanics is impractical, if not impossible. Instead, we show here how an artificial-intelligence approach can be applied, even to an extremely small number of materials, to model catalysis and determine the key descriptive parameters (materials genes) reflecting the processes that trigger, facilitate, or hinder the catalyst performance. We start from a consistent, unparalleled experimental set of "clean data", containing nine vanadium-based oxidation catalysts which were carefully synthesized, fully characterized, and tested according to standardized protocols.[1] By applying the symbolic-regression SISSO approach,[2,3] we identify correlations between the few most relevant materials properties and their reactivity. This approach highlights the underlying physico-chemical processes, and accelerates catalyst design. [1] A. Trunschke, et al., Top. Catal. 63, 1683 (2020). [2] R. Ouyang et al., Phys. Rev. Mater. 2, 083802 (2018). [3] R. Ouyang et al., J. Phys. Mater. 2, 024002 (2019).

O 87: Mini-Symposium: Infrared nano-optics I

Time: Thursday 10:30–12:30 Location: R2

Opening remarks

Paper discussion O 87.1 Thu 10:35 R2

In-Situ Thin Film Nanoscale Hydrogenography in Magnesium Plasmonics — •Harald Giessen, Julian Karst, Florian Sterl, Heiko Linnenbank, and Mario Hentschel — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Magnesium is an active plasmonic material that can switch from metallic to dielectric optical properties when undergoing hydrogenation. We perform s-SNOM phase contrast measurements to image the phase transition from Mg to MgH2 on the nanometer scale. This reveals the diffusion mechanism of hydrogen in free-standing Mg thin films in nanoscopic detail.

Paper discussion with expert panel members

Prof. S.A. Maier (LMU München), Prof. P. Klarskov Pedersen (U Aarhus), Prof. O. Mitrofanov (UCL London, UK) and Prof. J. Karst (U Stuttgart)

O 87.2 Thu 11:30 R2

The Role of Polarization in Resonant s-SNOM — •Felix G. Kaps[1], Hamed Aminpour[1], Susanne C. Kehr[1], and Lukas M. Eng[1,2] — [1]Technische Universität Dresden, Germany — [2]ct.qmat, Dresden-Würzburg Cluster of Excellence - EXC 2147, Technische Uni- versität Dresden, Germany

Scattering scanning near-field optical microscopy (s-SNOM) is known to be highly polarization-dependent. Most commonly, p-polarized light is employed to excite the tip-sample system with an electric field standing perpendicular to the sample surface, with only a few works commenting on polarization control to e.g. suppress unwanted far-field contributions [1] or local 3D vector field steering [2].

Here, we explore the fundamental role of polarization in s-SNOM by theoretically and experimentally controlling and analyzing the polarization of both incident and scattered light. Particularly, we compare our experimental findings obtained at mid-infrared wavelengths to polarization-dependent simulations that include the full near-field measuring setup [3]. One eye-catching outcome is, that resonant sample excitation using s-polarized light (E-field parallel to the sample surface) may achieve significant signal strengths and a polarization-specific signature, enabling a novel route for nanoscale polarization-sensitive surface characterization.

[1] M. Esslinger et al., Rev. Sci. Instrum. 83, 033704 (2012).

[2] K.-D. Park and M.B. Raschke, Nano Lett. 18, 2912 (2018).

[3] H. Aminpour et al., Opt. Express 28, 32329 (2020).

O 87.3 Thu 11:45 R2

Vector Microscopy - Nonlinear Photoemission Microscopy Reveals Plasmonic Fields — •David Janoschka[1], Pascal Dreher[1], Yannik Paul[1], Timothy Davis[1,2,3], Bettina Frank[2], Michael Horn- von Hoegen[1], Harald Giessen[2], and Frank-J. Meyer zu Heringdorf[1] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany. — [2]4th Physics Institute, University of Stuttgart, 70569 Stuttgart, Germany. — [3]School of Physics, University of Melbourne, Parkville, Victoria 3010 Australia

Exploring the topology of electromagnetic near-fields is one of the central topics in nano-optics. To investigate spatiotemporal details of the topology on a local scale intrinsically requires knowledge of the time-dependent local electric field vectors. While time-resolved photoemission microscopy (TR-PEEM) has been established as an excellent tool to study the dynamics of nano-optical fields at surfaces, the vectorial nature of the fields was not accessible so far.

Here, we present the new method of 'vector microscopy' as a local field vector sensitive development of TR-PEEM. We use femtosecond laser pulses to excite and probe surface plasmon polaritons (SPPs) in tailored nanostructures. Using two different probe laser pulses of orthogonal polarization at the same pump-probe delay enables us to extract the in-plane component of the SPP's near-field. The out-of-plane field component is reconstructed using Maxwell's equations. We apply the new vector microscopy method to complex topological SPP fields. We demonstrate reconstruction of the electric and the magnetic field, and extract the topological properties in time and space.

O 87.4 Thu 12:00 R2

Amplitude- and phase-resolved infrared nanoimaging and nanospectroscopy of polaritons in liquid environment — •Divya Virmani[1], Andrei Bylinkin[1], Irene Dolado[1], Eli Janzen[2], James H. Edgar[2], and Rainer Hillenbrand[3,4] — [1]CIC nanoGUNE BRTA, Donostia, Spain. — [2]Kansas State University, Tim Taylor Department of Chemical Engineering, Durland Hall, Manhattan,USA — [3]CIC nanoGUNE BRTA and Department of Electricity and Electronics, UPV/EHU, Donostia, Spain. — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain.

Polaritons are well known for their ability to focus light to deep subwavelength sized spot allowing for highly sensitive analysis of bio(chemical) substances and processes. Nanoimaging of the polaritons evanescent fields is critically important for experimental mode identification and field confinement studies. In this work, we describe two setups for scattering-type scanning near-field optical microscopy (s-SNOM) based polariton nanoimaging and spectroscopy in liquid. We first demonstrate the mapping of near-field distribution of plasmonic metal antennas in liquid with a normal-incidence mid-infrared s-SNOM setup. We then demonstrate our total internal reflection (TIR) setup for infrared nanoimaging and nanospectroscopy of ultra-confined propagating phonon polaritons (PhPs) on h-BN flakes. Our work lays the foundation for s-SNOM based polariton interferometry in liquid for future exploitation, for example, in-situ studies of strong coupling between polaritons and molecular vibrations or chemical reactions at the bare or functionalized surfaces of polaritonic materials.

O 87.5 Thu 12:15 R2

Tunable s-SNOM for nanoscale infrared optical measurement of electronic properties of bilayer graphene — •Konstantin G. Wirth[1], Heiko Linnenbank[2,3], Tobias Steinle[2,3], Luca Banszerus[4], Eike Icking[4], Christoph Stampfer[4], Harald Giessen[2,3], and Thomas Taubner[1] — [1]Institute of Physics (IA), RWTH Aachen — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart — [3]SI Stuttgart Instruments GmbH, 70771 Leinfelden-Echterdingen — [4]2nd Institute of Physics (IIA), RWTH Aachen University, 52074 Aachen

The stacking and rotation of individual graphene layers changes its band structure, opening up new physical properties. Local probing of their electronic properties at the nanoscale is usually done by scanning tunneling microscopy, which requires electrical contact. Optical measurements such as infrared absorption or Raman spectroscopy, work for non-contacted and encapsulated samples, but are limited in lateral resolution by diffraction to a few micrometer. Here we directly probe the electronic properties of bilayer graphene (BLG) using s-SNOM measurements with a broadly tunable laser source over the energy range from 0.3 to 0.54 eV. We tune an OPO/OPA system around the interband resonance of Bernal stacked BLG and extract amplitude and phase of the scattered light. This enables us to retrieve and reconstruct the complex optical conductivity resonance in BLG around 0.39 eV with nanoscale resolution. Our technique opens the door towards nanoscopic noncontact measurements of the electronic properties in complex hybrid 2D and van der Waals material systems.

O 88: Poster Session VII: Oxides and insulators: Adsorption and reaction of small molecules I

Time: Thursday 10:30–12:30 Location: P

O 88.1 Thu 10:30 P

Electron Stimulated Desorption of Vanadyl-Groups from Vanadium Oxide Thin Films on Ru(0001) probed with STM — •Piotr Igor Wemhoff, Ying Wang, and Niklas Nilius — Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg,

Low-temperature STM is employed to study electron-stimulated desorption of V=O groups from a vanadium oxide film grown on Ru(0001). The film is built of an ordered network of three, six and twelve membered V-O rings, the former ones capped by upright vanadyls. These V=O groups can be reproducibly desorbed by electron injection from the STM tip. From hundreds of experiments, desorption rates are determined as a function of bias voltage and tunneling current. The rates show a threshold behavior with +3.3 V and -2.6 V bias onsets, and depend quadratically (cubically) on current for positive (negative) polarity. Apparently, V=O desorption is a multi-electron process that proceeds via resonant tunneling into bonding (anti-bonding) resonances of the V=O system followed by vibrational ladder climbing in the binding potential. The involved electronic states are identified in STM conductance spectra of the oxide surface.

O 88.2 Thu 10:30 P

Heterogeneous Adsorption and Local Ordering of Formic Acid on Magnetite (111) — •Marcus Creutzburg[1,2], Kai Sellschopp[3], Steffen Tober[1,2], Vedran Vonk[1], Heshmat Noei[1], Gregor B. Vonbun-Feldbauer[3], and Andreas Stierle[1,2] — [1]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [2]Fachbereich Physik, Universität Hamburg — [3]Institut für Keramische Hochleistungswerkstoffe, Technische Universität Hamburg

Magnetite (Fe_3O_4) is an important and diverse transition metal oxide with applications as a catalyst in various industrial processes such as the water-gas shift reaction [1]. Formic acid (HCOOH), as the elementary carboxylic acid, is proposed to occur as an intermediate during this reaction. In material science magnetite nanoparticles are linked by larger carboxylic acids to form supercrystals with exceptional mechanical properties [2]. Thus, a detailed atomic understanding of the interaction at the magnetite surface/carboxylic acid interface is vital. In this contribution the adsorption of formic acid on the magnetite (111) single crystal surface is studied under UHV conditions at room temperature. Our FT-IRRA spectroscopy results and DFT calculations show dissociative adsorption of formic acid in quasi-bidentate and chelating geometries, the latter being stabilized by the presence of tetrahedral iron vacancies at the surface. The locally observed $(\sqrt{3} \times \sqrt{3})\,R\,30^\circ$ superstructure by STM consists of formate in a triangular arrangement, adsorbed predominantly in chelating geometry.

[1] M. Zhu *et al.*, ACS Catal. **6**, 722-732 (2016)
[2] A. Dreyer *et al.*, Nat. Mater. **15**, 522-528 (2016)

O 88.3 Thu 10:30 P

Atomic-Scale Studies of Hydroformylation on $Rh_1/Fe_3O_4(001)$ — •Manuel Ulreich[1], Zdeněk Jakub[1], Florian Kraushofer[1], Matthias Meier[1,2], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria — [2]Center for Computational Materials Science, University of Vienna, 1090 Vienna, Austria

Hydroformylation (alkene + CO + H_2 → aldehyde) is an important industrial reaction typically performed in solution using highly-selective mononuclear complexes. Recently, Rh-based “single-atom” catalysts (SACs) have been shown to catalyze this reaction heterogeneously with similar levels of selectivity, suggesting SAC can be a strategy to heterogenize problematic reactions. The main advantage of heterogeneous catalysis is easy separation of the catalyst from the products. SAC is intended to unify this advantage with the high selectivity and activity of homogeneous catalysis. In this talk, TPD and XPS are used to study the coadsorption of ethylene and carbon monoxide on isolated Rh_1 adatoms on $Fe_3O_4(001)$, a critical first step in the hydroformylation reaction. Our results show that 2-fold coordinated Rh_1 adatoms on $Fe_3O_4(001)$ are able to coadsorb C_2H_4 and CO, but 5-fold coordinated Rh_1 adatoms cannot. We conclude that gaining control of the active site geometry is key to the development of highly-selective single-atom catalysis.

O 88.4 Thu 10:30 P

Comparison of single Rh adatoms on α-$Fe_2O_3(1\bar{1}02)$ and $TiO_2(110)$ stabilized by adsorbed water — •Lena Haager[1], Florian Kraushofer[1], Moritz Eder[2], Ali Rafsanjani-Abbasi[1], Giada Franceschi[1], Michele Riva[1], Panukorn Sombut[1], Marlene Atzmueller[1], Michael Schmid[1], Cesare Franchini[3,4], Ulrike Diebold[1], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Chair of Physical Chemistry, TU München, Germany — [3]University of Vienna, Vienna, Austria — [4]Universitá di Bologna, Bologna, Italy

Despite its high cost, rhodium is a widely applied catalyst primarily used in nanoparticle form for converting toxic gases in automobiles. It is also utilized in organometallic complexes, such as the Wilkinson catalyst, for the hydrogenation of olefins and for converting alkenes to aldehydes through a process known as hydroformylation. So-called “single-atom“ catalysis offers an opportunity to reduce the amount of Rh required for traditional heterogeneous catalysis, and a path to heterogenize homogeneous reactions, with the advantage of easy separation of catalyst and product.

Using STM, nc-AFM and XPS we compare the stability of Rh adatoms on two different model supports: α-$Fe_2O_3(1\bar{1}02)$ and $TiO_2(110)$, both in UHV and $2 * 10^{-8}$ mbar of water. We show that the Rh adatoms on α-$Fe_2O_3(1\bar{1}02)$ sinter in UHV, but are stabilized by water up to 150 °C through coordination to 2–3 OH ligands. In contrast, Rh adatoms on $TiO_2(110)$ could not be stabilized above room temperature in either environment.

O 88.5 Thu 10:30 P

Unravelling CO Adsorption on Model Single-Atom Catalysts (SAC) — Jan Hulva[1], •Matthias Meier[1,2], Roland Bliem[1], Zdenek Jakub[1], Florian Kraushofer[1], Michael Schmid[1], Ulrike Diebold[1], Cesare Franchini[2,3], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Computational Materials Physics, University of Vienna, Vienna, Austria — [3]Alma Mater Studiorum, Universitá di Bologna, Bologna, Italy

The electronic structure of a surface atom is crucial when it comes to predicting and understanding its binding to adsorbates. This has been demonstrated in depth on metal surfaces, where the d-band center of mass and d-band filling are two of the main descriptors when its comes to defining the adsorption of small molecules. We propose an extension of this model towards oxide surfaces and SACs, based on a combination of density functional theory (DFT) and surface sensitive techniques (Hulva et al, Science (in press)). The same rules regarding the electronic structure of the binding atom apply and govern the adsorption energies. But additionally, the exact local environment, affecting the electronic states, also leads to two particular deviations. Firstly, if the surface atom is saturated in ligands, no matter the electronic structure, the atom will bind CO poorly, and therefore the metal will be almost inert. On the other hand, if the coordination of the metal atom at the surface is low and the CO adsorption geometry is not ideal, CO-induced relaxations occur. This can lead to strong offsets with respect to the adsorption energy estimated by the electronic structure alone.

O 88.6 Thu 10:30 P

Rapid surface oxygen exchange at the hematite-water interface — Zdenek Jakub[1], Matthias Meier[1], Florian Kraushofer[1,2], Jan Balajka[1], Jiri Pavelec[1], Michael Schmid[1], Cesare Franchini[2,3], Ulrike Diebold[1], and •Gareth S. Parkinson[1] — [1]TU Wien, Vienna, Austria — [2]University of Vienna, Vienna, Austria — [3]Universitá di Bologna, Bologna, Italy

It seems natural to assume that low-index surfaces of insoluble minerals do not exchange atoms with their surroundings. Here, we will show using surface science techniques that all oxygen atoms on the *r-cut* (1-102) surface are exchanged with oxygen from surrounding water vapour within minutes at temperatures below 70°C, even though the structure remains intact. Density functional theory computations suggest the oxygen exchange occurs during on-surface diffusion, and that cooperative stabilization of an HO-HOH-OH complex compensates the cost of the lattice oxygen extraction. Such a rapid oxygen exchange mechanism affects the isotope composition in the near-surface region, and the knowledge of the mineral-liquid interface dynamics is relevant for many fields ranging from hydrogen production to paleoclimatology.

O 88.7 Thu 10:30 P

Real-time Dynamics During TiO_2 Photocatalysis — •Michael Wagstaffe[1], Lukas Wenthaus[1,2], Adrian Dominguez-Castro[3], Thomas Frauenheim[3,4,5], Adriel Dominguez[3], Angel Rubio[2,6], Wilfried Wurth[1,2,7], Andreas Stierle[1,7], and Heshmat Noei[1] — [1]DESY, 22607, Hamburg, Germany — [2]CFEL, 22761, Hamburg, Germany — [3]BCCMS, 28359, Bremen, Germany — [4]CSAR, 518110, Shenzhen, China — [5]CSRC, 100193, Beijing, China — [6]MPI for the Structure and Dynamics of Matter, 22761, Hamburg, Germany — [7]Fachbereich Physik Universität Hamburg, 20355, Hamburg, Germany

Studies of photocatalytic reactions on TiO_2 are instrumental to the development of technology used for self-cleaning surfaces and for air and water purification. We utilize femtosecond X-ray laser pulses synchronized with an optical laser to directly follow the reaction dynamics of the photooxidation of CO on the anatase TiO_2(101) surface. Our time-resolved soft X-ray photoemission spectroscopy results, combined with theoretical calculations, allow us to elucidate the mechanism of oxygen activation and provides evidence of ultrafast timescales. The reaction takes place between 1.2 - 2.8 (± 0.2) ps after irradiation with an ultrashort laser pulse, resulting in CO_2. No intermediate species were observed on a picosecond time scale. Theoretical calculations predict that the reaction can be initiated following the formation an O_2-TiO_2 charge-transfer complex. This allows the reaction to take place following laser illumination at a photon energy of 1.6 eV (770 nm), following the direct transfer of electrons from TiO_2 to physisorbed O_2.

O 88.8 Thu 10:30 P

Interaction of formic acid with magnetite surfaces – the DFT perspective — •Kai Sellschopp[1], Marcus Creutzburg[2,3], Björn Arndt[2,3], Heshmat Noei[2], Andreas Stierle[2,3], Stefan Müller[1], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology — [2]DESY NanoLab, Deutsches Elektronen-Synchrotron, Hamburg — [3]Fachbereich Physik, Universität Hamburg

Formic acid (HCOOH) molecules are present in atmospheric conditions and furthermore, can be seen as the smallest representative of the carboxylic acid family. Magnetite (Fe_3O_4) nanoparticles are utilized in various applications, such as waste water treatment, single-atom catalysis or hybrid materials. Therefore, studying the interaction of formic acid with the major facets of magnetite nanoparticles, namely the {111} and {001} facets, is highly interesting for improving their performance. Here, we present results on the adsorption of formic acid on both magnetite (111) and (001) studied through Density Functional Theory (DFT) calculations. In agreement with surface science experiments, the formation of a $(\sqrt{3} \times \sqrt{3})R30^\circ$ superstructure and two different binding modes, a quasi-bidentate and a chelating mode, are found on the (111) surface, and the observed restructuring of the (001) surface is explained. In all studied cases, the dissociation of formic acid into formate and hydrogen is energetically favourable. Calculated surface phase diagrams give further insights in the processes involved under experimental conditions and indicate a stabilisation of iron vacancies on the (111) surface upon formic acid dissociation.

O 89: Poster Session VII: Organic molecules on inorganic substrates: electronic, optical and other properties III

Time: Thursday 10:30–12:30 Location: P

O 89.1 Thu 10:30 P

Single-molecule rotation and translation — •Grant J. Simpson[1], Samuel Hajek[1], Víctor García-López[2], A. Daniel Boese[1], James Tour[2], and Leonhard Grill[1] — [1]University of Graz, Graz, Austria — [2]Rice University, Houston, TX, USA

Control of the orientation and the rotation direction of a single molecule is crucial to the understanding of molecular machines. In turn, the rotational orientation of a molecule can affect the efficiency of translation in a particular direction. Here, we report how single dipolar nanocar-type molecules adsorbed on a Ag(111) surface can be rotated with 100% directionality using the electric field of a scanning tunnelling microscope [1]. This high control relies on a specific interaction of the molecule with a silver surface atom and can be disrupted either by introducing a further adatom or by changing the chemical structure of the molecule. The influence of chemical modification on the nanocar-surface interaction is also explored on different noble metal surfaces in view of the upcoming nanocar race in early 2022.

[1] Simpson, G.J., García-López, V., Boese, A.D., Tour, J., Grill, L., Nat. Commun., 10, 4631 (2019)

O 89.2 Thu 10:30 P

Molecular orientation and phase transitions of DHTAP on Cu(110) — •Claudia López-Posadas[1], Michael Györök[1], Antony Thomas[2], Thomas Leoni[2], Olivier Siri[2], Conrad Becker[2], and Peter Zeppenfeld[1] — [1]Institute of Experimental Physics, Johannes Kepler University Linz, Altenberger Str. 69, A-4040 Linz, Austria — [2]Aix-Marseille University, CNRS, CINaM, UMR 7325, F-13288 Marseille, France

The structure and orientation of 5,14-dihydro-5,7,12,14-tetraazapentacene (DHTAP) layers deposited on Cu(110) was studied using reflectance difference spectroscopy (RDS), Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). The evolution of the RDS signal allows to identify the sequential formation of up to three monolayers as well as a phase transition upon completion of the first one. DHTAP molecules in the first monolayer are always lying flat with their long molecular axis aligned parallel to the [-110]-direction of the Cu(110) surface. However, for subsequent layers the orientation critically depends on the deposition temperature T. At T=240K the DHTAP molecules are mostly aligned parallel to the ones in the first layer, whereas at room temperature and above their preferential orientation is along the [001]-direction, i.e.,orthogonal to the molecules in the first layer. Finally, the main optical transitions and the orientation of the transition dipole moments of the DHTAP layers were extracted from the RDS spectra and compared with recent theoretical investigations on individual DHTAP molecules.

O 89.3 Thu 10:30 P

Exciton-trion dynamics of a single molecule probed by Radio-frequency STM-induced luminescence — Jiří Doležal[1,2], Sofia Canola[1], •Pablo Merino[3,4], and Martin Švec[1,5] — [1]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10/112, CZ16200 Praha 6, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, CZ12116 Praha 2, Czech Republic — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz 3, E28049 Madrid, Spain — [4]Instituto de Física Fundamental, CSIC, Serrano 121, E28006 Madrid, Spain — [5]Regional Centre of Advanced Technologies and Materials, Šlechtitelů 27, CZ78371 Olomouc, Czech Republic

Combination of radio-frequency (RF) modulated bias and photon detection overcomes the microsecond time resolution limit of transimpedance amplifiers in conventional STM. Here, we report two novel tip-enhanced optical methods: for calibration of RF transmission by detecting the energy of the plasmon edge and for measuring time evolution of fluorescent systems by phase shift of the RF signal. The RF phase-shift method corrected for amplitude transmission is applied to Zinc Phthalocyanine (ZnPc) molecules on NaCl/Ag(111). We generate excitons and trions in ZnPc, determine their dynamics and trace the evolution of the system in the picosecond range. In addition, we explore dependence of effective lifetimes on bias voltage, propose a conversion mechanism from neutral excitons to trions via charge capture and perform a stochastic simulation to corroborate the experimental results.

O 89.4 Thu 10:30 P

Excited state dynamics of terrylene — •Boubacar Tanda Bonkano[1,2], Samuel Palato[1,2], Sergey Kovalenko[1], Lukas Gierster[1,2], Bjoern Kobin[1], Stefan Hecht[1,3], and Julia Staehler[1,2] — [1]Institut für Chemie, Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG, Berlin — [3]Leibniz-Institut für Interaktive Materialien, RWTH Aachen

In hybrid solar cells, the separation of the electron-hole pairs after photogeneration is a key aspect of the light harvesting functionality. This requires, in hybrid inorganic/organic systems, the use of molecules that have excited states with sufficiently long lifetime to allow charge separation. In order to investigate terrylene molecules, we performed two types of time-resolved spectroscopy, time-correlated single photon counting (TCSPC) and broadband transient absorption (TA) using a white light continuum probe. The steady state absorption and emission spectra of terrylene monomers in solution show mirrored lineshapes. Both the TCSPC and TA consistently show a decay of 3.7 ns for the excited state S_1. Thin terrylene film shows absorption bands strongly (> 0.5 eV) blue-shifted due to H-aggregation. Photoexcitation of the H-aggregate leads to the formation of an induced absorption band at 2.3 eV, indicating the presence of transient terrylene monomers. A phenomenological fit model allows for the disentanglement of the participating elementary processes. The determination of the relaxation pathways is challenging but yet necessary for a better understanding and control of terrylene-based systems, beneficial for applications.

O 89.5 Thu 10:30 P

On-surface synthesis of porphyrin tetramers — •Eduardo Corral-Rascon[1], Alexander Riss[1], Pingo Mutombo[2], Adam Matej[2], Yang Bao[1], Pavel Jelinek[2], and Willi Auwärter[1] — [1]Physics Department E20, Technical University Munich, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Covalently coupled porphyrins [1,2,3] hold great promise for molecular electronics, optoelectronics, gas sensing and light-harvesting. Furthermore, the electronic conjugation [4] might lead to antiaromatic behavior [3] and additionally offers ways to fabricate spin-coupled nanoarchitectures via introduction of metal centers into the porphyrin cores. Here we present the synthesis of Ag(100)-supported porphyrin tetramers that possess a cyclooctatetraene (COT) moiety at their center. Bond-resolved atomic force microscopy (AFM) and scanning tunneling microscopy (STM) supported by density functional theory (DFT) calculations were used to characterize the coupling and the emerging electronic properties. In particular we compared the apparent bond lengths and electronic states of Zn-metalated and different tautomers of base-free tetramers.

[1] Wiengarten, A. et al. J. Am. Chem. Soc. 2014, 136, 26, 934.
[2] Bischoff, A. et al. Angew. Chem. 2018, 130, 16262.
[3] Nakamura, Y. et al. J. Am. Chem. Soc. 2006, 128, 4119.
[4] Fatayer, S. et al. Science 2019, 6449, 365, 142.

O 89.6 Thu 10:30 P

Nuts and bolts of core-hole constraint based ab-initio simulations for K-shell x-ray photoemission and absorption spectra — •Benedikt P. Klein[1,2], Samuel J. Hall[1], and Reinhard J. Maurer[1] — [1]Department of Chemistry, University of Warwick, Coventry, United Kingdom — [2]Diamond Light Source, Didcot, United Kingdom

X-ray Photoemission (XPS) and Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy are important tools used to study the electronic structure of materials and surfaces. Here, ab-initio simulations can help with the interpretation of complex spectra consisting of overlapping signatures. Approximate core-hole constraint based simulation methods using Density Functional Theory (DFT) such as the Delta-Self-Consistent-Field (ΔSCF) method or the transition potential (TP) method are widely employed to predict the K-shell XPS and NEXAFS spectra for a wide range of systems at reliable accuracy and affordable computational cost. We present our variants of both the ΔSCF and the TP method (coined ΔIP-TP) by applying them to exemplary molecules in the gas-phase, in molecular crystals, and at metal-organic interfaces. Thereby we systematically assess how practical simulation choices affect the stability and accuracy of the calculated transitions, which we compare to experimental data. The investigated choices include the exchange-correlation functional, the basis set, the method of core-hole localization, and the use of periodic boundary conditions. For the benefit of practitioners in the field, we discuss sensible default choices and limitations of the methods.

O 89.7 Thu 10:30 P

Atomic band structure of occupied and unoccupied states of C_{60} multilayer films — •Ralf Hemm, Florian Haag, Norman Haag, Martin Mitkov, Sebastian Emmerich, Martin Aeschlimann, and Benjamin Stadtmüller — University of Kaiserslautern (TUK) and research center OPTIMAS, Erwin-Schroedinger-Str. 46, 67663 Kaiserslautern, Germany

The implementation of molecular materials in everyday technology is hindered by their poor charge carrier mobility that is rooted in the strong localization of the molecular valence states on single molecular sites. Only in rare cases, strongly dispersive bands have been observed in these materials. Here, we focus on such an exceptional case and study the band structure of C_{60} multilayers on Ag(111) and Cu(111). Using momentum microscopy, we find strongly dispersive valence bands with complex momentum-dependent photoemission patterns that point to the formation of an atomic crystal-like band structure in C_{60} thin films [1]. Interestingly, these strongly dispersing states in C_{60} are not limited to the valence band structure, but also extend to the unoccupied band structure above the vacuum level [2]. These states above the vacuum energy are of particular interest since they are typical final states of the photoemission processes. Hence, their momentum distribution has to be taken into account when extracting the band dispersion of occupied and excited states in a (inverse) photoemission experiment of molecular films on surfaces.

[1] N. Haag et al. Phys. Rev. B 101, 165422 (2020)
[2] J. H. Weaver et al., Phys. Rev. Lett. 66, 1741 (1991)

O 90: Poster Session VII: Surface reactions I

Time: Thursday 10:30–12:30 Location: P

O 90.1 Thu 10:30 P

Hierarchically Structured Janus Membrane Surfaces for Enhanced Membrane Distillation Performance — •Nick Chew[1,2], Yujun Zhang[2], Kunli Goh[2], Jia Shin Ho[2], Rong Xu[2], and Rong Wang[2] — [1]University of North Carolina at Chapel Hill, Chapel Hill, USA — [2]Nanyang Technological University, Singapore, Singapore

Commercial hydrophobic poly(vinylidene fluoride) (PVDF) membranes are vulnerable to membrane fouling and pore wetting, hampering the use of membrane distillation (MD) for the treatment of surfactant- and oil-containing feed streams. To address these challenges, we designed novel Janus membranes with multilevel roughness. Specifically, fouling- and wetting-resistant Janus MD membranes with hierarchically structured surfaces were tailored via oxidant-induced dopamine polymerization followed by in-situ immobilization of silver nanoparticles (AgNPs) on commercial PVDF hollow fiber substrates. These membranes demonstrated outstanding anti-fouling properties and salt-rejection performances in comparison to membranes with single-level structures. We ascribed their excellent performance to the coupled effects of improved surface hydrophilicity and self-healing mechanism brought about by AgNPs. Furthermore, the newly engineered membranes exhibited antibacterial properties in Bacillus acidicola solutions as evidenced by clear inhibition zones observed on a confocal laser scanning microscope. The development of hierarchically structured Janus MD membranes with multilevel roughness paves a way to mitigating membrane fouling and pore wetting caused by low-surface-tension feed streams in the MD process.

O 90.2 Thu 10:30 P

Dehydrogenation Reactions of O-Heterocyclic LOHC Molecules — •Felix Hemauer, Philipp Bachmann, Fabian Düll, Johann Steinhauer, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität, Erlangen, Germany

With the dwindling of fossil fuels and the alarming progression of global warming, the ecological and social demand for cleaner and more sustainable energy sources has never been as high. As renewable sources, such as wind and solar power, give no continuous and constant power output, hydrogen is a promising candidate for the chemical storage of energy. The concept of Liquid Organic Hydrogen Carriers (LOHCs) avoids unfavorable handling of elemental hydrogen.

Heterocyclic LOHC molecules display advantageous thermodynamic properties regarding their heat of dehydrogenation. Consequently, several N-heterocycles have been successfully investigated, e.g. the indole-based systems and their derivatives.

In order to investigate the feasibility of O-heterocyclic compounds as possible LOHCs, synchrotron radiation-based high resolution X-ray photoelectron spectroscopy and temperature-programmed desorption measurements of furan and benzofuran were performed on Pt(111) under UHV conditions. By applying heating ramps after the adsorption experiment, the respective dehydrogenation and decomposition reactions are monitored via evaluation of the characteristic spectra. This allows for fundamental insights into the reactivity and stability and helps assessing the viability of the compound class as LOHC.

O 90.3 Thu 10:30 P

Intramolecular Coupling of Terminal Alkynes by Atom Manipulation — •Florian Albrecht[1], Dulce Rey[2], Shadi Fatayer[1], Fabian Schulz[1], Dolorez Perez[2], Diego Pena[2], and Leo Gross[1] — [1]IBM Research - Zurich, Switzerland — [2]CiQUS and Departamento de Quimica Organica Universidade de Santiago de Compostela, Spain

Performing chemical reactions in a scanning probe microscope offers ultimate control over the reaction. The characterization of both, reactant and product, can be performed. Functionalizing the tip of an AFM enables elucidation of molecular geometries down to the atomic level [1] and performing the reaction on ultra-thin insulating films decouples the molecules sufficiently to characterize their electronic structure [2].

Here, we show a Glaser-like coupling reaction of terminal alkynes within individual molecules. Voltage pulses from the tip initiate the reaction and geometric as well as electronic structure of reactant and product are characterized on bilayer NaCl on Cu(111). The observation of partially dehydrogenated reaction intermediates provides insight into the reaction pathway [3].

References: [1] L. Gross, et al. Science 325, 1110 (2009) [2] J. Repp, et al. Phys. Rev. Lett. 94, 026803 (2005) [3] F. Albrecht, et al. Angew. Chem. Int. Ed. 59, 22989 (2020)

O 90.4 Thu 10:30 P

Temperature-dependent decomposition reactions of oxygen-containing LOHC contaminants on Pt(111) — •Valentin Schwaab, Johann Steinhauer, Felix Hemauer, Eva Marie Freiberger, Natalie Waleska, Christian Papp, and Hans-Peter Steinrück — Friedrich-Alexander-Universität, Erlangen, Germany

Liquid organic hydrogen carriers (LOHCs) represent an attractive way for energy storage and transportation utilizing reversible hydrogenation of an organic compound. The system of dibenzyltoluene (H0-DBT) and perhydro dibenzyltoluene (H18-DBT) has been reported as promising candidate featuring suitable physicochemical properties and a favorable toxicology. Technical H0-DBT, however, contains up to 1% of oxygenate impurities, which might negatively affect the quality of the released H_2 gas from the hydrogenated molecule.

To gain insight in the surface reaction of these oxygenates, we investigated several model compounds on Pt(111) using high-resolution temperature-programmed X-ray photoelectron spectroscopy (HR-TPXPS). Diphenylmethanol, benzophenone and dicyclohexylmethanol are found to undergo C-O bond cleavage at the methylene bridge around 350 K, leading to an oxygen-free carbon fragment and adsorbed atomic oxygen. By contrast, dicyclohexylketone shows C-C bond cleavage and the formation of carbon monoxide above 220 K.

CO represents a catalyst poison and is problematic for further applications of the released H_2 gas. A possible solution might be pre-purification of industrially produced H0-DBT.

O 90.5 Thu 10:30 P

On-surface synthesis of graphene nanoribbons on the superconducting Ag/Nb(110) substrate — •Jung-Ching Liu[1], Philipp D'astolfo[1], Carl Drechsel[1], Xunshan Liu[2], Silvio Decurtins[2], Shi-Xia Liu[2], Rémy Pawlak[1], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056 — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, Bern, CH 3012

Previously, Majorana bound states (MBS) realized in condensed matter systems were based on the interaction between 1D magnetism and s-wave superconductivity[1-3]. To improve the structural diversity for studying MBS braiding, we propose realizing MBSs in graphene sheets or nanoribbons (GNR) through on-surface synthesis[4,5] on a superconducting substrate. Using DBBA as monomers[4], GNR on-surface synthesis is completed via Ullmann polymerization in ultra-high vacuum environment. As the surface reaction is limited on noble metal surfaces, we grow Ag films on the superconducting Nb(110), and introduce superconductivity to Ag by proximity[6]. Measuring with STM and AFM at 4.7K, we confirm proximity-induced superconductivity on Ag with thicknesses up to 5 ML, as well as successful GNR synthesis on the Ag/Nb substrate. We believe our work paves the way to a new research field in graphene topology. References: [1]S. Nadj-Perge et al. Science 2014, 346, 602-607 [2]M. Ruby et al. Nano Lett. 2017, 17, 4473-4477 [3]R. Pawlak et al. Npj Quantum Inf. 2016, 2, 16035 [4]J. Cai et al. Nature 2010, 466, 470-473 [5]K. A. Simonov et al. Nature 2018, 8, 3506 [6]T. Tomanic et al. Phys. Rev. B 2016, 94, 20503

O 90.6 Thu 10:30 P

Impact of atomic hydrogen on decomposition reactions of SiO_2 layers on Si(100): a LEEM study — •Jonas Darius Fortmann[1,2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany — [2]Department for Physics, Experimental Physics, Universität Duisburg-Essen, Lotharstr. 1-21, 47057 Duisburg, Germany

Clean and well-ordered Si surfaces can be obtained by annealing Si wafers covered with a thin, protective layer of SiO_2 in UHV. Tromp et al. first showed that the decomposition of thermally grown SiO_2 layers on Si(100) upon annealing occurs in form of square-like voids appearing spontaneously or at defects [1]. Accordingly, diffusion of Si monomers from the voids to the reaction fronts and their reaction with SiO_2 at the interface are crucial elements of the decomposition process. In this study, we used LEEM to investigate the impact of atomic hydrogen on decomposition reactions of thermally grown and native surface films of SiO_2 on Si(100). For 10 nm thermal oxide, the presence of atomic hydrogen leads to voids of highly irregular shape with crack-like extensions of the reaction fronts into the surface oxide. Moreover, the growth rates of these voids at 900°C are much higher than those found in comparative experiments without hydrogen. In contrast, atomic hydrogen reduces the growth rates of more circular voids in 2 nm native SiO_2 layers on Si(100) at 790°C. The different impact of atomic hydrogen for native and thermal surface oxides will be discussed. [1] R. Tromp et al., Phys. Rev. Lett. **55**, 2332 (1985).

O 90.7 Thu 10:30 P

Surface-controlled intramolecular radical addition versus C-H insertion toward cyclodehydrogenation under mild conditions — •Qigang Zhong[1], Daniel Kohrs[2], Jannis Jung[3], Daniel Ebeling[1], Doreen Mollenhauer[3], Hermann A. Wegner[2], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus-Liebig University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany

Despite the ubiquitous existence of aryl radicals in surface reactions, the reactivity of surface-stabilized aryl radicals and its influence on the reaction pathways to C-C coupling remain elusive. Here, we studied the debromination and cyclodehydrogenation of 1-bromo-8-phenylnaphthalene (BPN) on Cu(111) and Ag(111) using bond-resolved scanning probe microscopy. Debromination of BPN at room temperature generated a radical at the naphthyl group which enabled the subsequent cyclodehydrogenation to proceed at mild temperatures (about 350 K on Cu and 420 K on Ag). The reaction temperature is lower on Cu than Ag due to the higher activity of Cu. High-resolution imaging of the cyclized intermediates revealed that radical addition to the phenyl ring transformed the connected C(sp2)-H bond into an out-of-plane C(sp3)-H bond on Cu(111), while the protruding hydrogen atom was shifted to the naphthyl group on Ag(111), reminiscent of C-H insertion in solution. In combination with DFT calculations, we rationalized the different routes to radical C-H activation by the varied reactivity of the aryl radicals depending on the substrate materials.

O 90.8 Thu 10:30 P

On-surface synthesis of diradical organic one-dimensional polymers — •Ana Sánchez-Grande[1], José I. Urgel[1], Ales Cahlík[2], José Santos[1,3], Shayan Edalatmanesh[2], Koen Lauwaet[1], Pingo Mutombo[2], Bruno de la Torre[2], Rodolfo Miranda[1,4], Oliver Gröning[5], Nazario Martín[1,3], Pavel Jelínek[2], and David Écija[1] — [1]C/ Faraday 9, Campus de Cantoblanco. 28049 Madrid (Spain) — [2]Institute of Physics of the Czech Academy of Science, 6253 Praha (Czech Republic) — [3]ltad de Ciencias Químicas, Universidad Complutense de Madrid. 28040 Madrid (Spain) — [4]Departamento de Física de la Materia Condensada, UniversidadAutónoma de Madrid, 28049 Madrid (Spain) — [5]Empa, Swiss Federal Laboratories for Materials Science and Technology 8600 Dübendorf (Switzerland)

In this work, we present the on-surface synthesis of one-dimensional polymers based on cumulene-bridged peripentacene units on a bare Au(111) surface under ultra-high-vacuum (UHV) conditions. The structural characterization of the polymers has been realized via scanning tunneling microscopy (STM) and confirmed by non-contact atomic force microscopy (nc-AFM). The electronic characterization of polymers has been performed via scanning tunneling spectroscopy (STS) which, complemented by theoretical calculations, reveals that the polymers present an experimental band gap of 0.8 eV and pure diradical character, exhibiting one unpaired spin at each end. We observe a transition from an antiferromagnetic ground state for peripentacene dimers to a paramagnetic ground state for trimers or longer polymers.

O 91: Poster Session VII: Scanning probe techniques: Method development II

Time: Thursday 10:30–12:30 Location: P

O 91.1 Thu 10:30 P

Fast low-noise transimpedance amplifier for scanning tunneling microscopy — Martin Štubian[1], Juraj Bobek[1,2], Martin Setvin[1,3], Ulrike Diebold[1], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Brno University of Technology, Brno, CZ — [3]Charles University, Praha, CZ

Scanning tunneling microscopy is one of the most versatile techniques in surface physics. One of the factors limiting its performance is the bandwidth and noise of the preamplifier. Higher bandwidth enables faster scanning, and also implies low phase shifts, which reduces the susceptibility to feedback loop oscillations. STM preamplifiers are transimpedance amplifiers (TIAs), usually with a high feedback resistor. Increasing its resistance leads to lower current noise (Johnson noise of the resistor), but at the same time usually results in lower bandwidth. Using a multi-stage amplifier design, we could achieve an input noise of $\approx 5\,\mathrm{fA}/\sqrt{\mathrm{Hz}}$ at room temperature and low frequencies, but nevertheless a large bandwidth of up to 200 kHz and large dynamic range (<0.1 pA to 50 nA). For low noise, it is important to minimize the input capacitance. Connecting the STM tip to the preamplifier via a long coaxial cable should be avoided, and the performance can be substantially improved by placing the first amplifier stage into vacuum. Additionally, for low-temperature STMs, the Johnson noise is reduced by placing the feedback resistor in thermal contact with the cryostat. We also discuss a source of noise in operational amplifiers usually not considered, but important for TIAs.

[1] M. Štubian et al., Rev. Sci. Instrum. 91, 074701 (2020).

O 91.2 Thu 10:30 P

Theoretical models for KPFM with flexible tip apexes — •Ondrej Krejci[1] and Adam S. Foster[1,2,3] — [1]Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany — [3]WPI-NanoLSI, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Kelvin Probe Force Microscopy (KPFM) started as a technique with the possibility to determine areas of a sample with different work functions [1], but as lateral resolution moved towards (sub)angstrom precision, it found its place also in identifying differently charged parts of molecules (e.g. [2]). This ability was in specific cases used in KPFM to obtain chemical resolution using SPM [3,4,5]. On the other hand, the exact interpretation of KPFM data with flexible tip apices (e.g. CO-tip) remains unknown. In this work, we will summarise up-to-date knowledge about KPFM [1,4,6] focusing mainly on measurements with FM-AFM/STM. Based upon this, we will present a new model for electrostatic field, which is describing the experiments with CO-metal tips [5] and metal substrates. This new electrostatic model is applied in a DFT calculations simulating the full tip-sample system. These calculations will be compared with simple mechanistic models capturing various sources of achieved signal. With this, we aim to recover the physics behind KPFM with flexible tip apices.

Ref: [1] APL 58, 2921 (1991). [2] Nat. Nanotechnol. 7, 227-231 (2012). [3] Nano Lett. 14, 3342-3346 (2014) [4] PRB, 90, 155455 (2014). [5] ACS Nano 12, 5274-5283 (2018) [6] PRB 86, 075407 (2012).

O 91.3 Thu 10:30 P

Radio-frequency transmission to the junction of a scanning tunneling microscope — •Nafise Kalantari, Thomas Jürgens, Rene Woltmann, Manuel Gruber, Alexander Weismann, and Richard Berndt — Institut fur Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Electron spin resonance scanning tunneling microscopy (ESR-STM), as implemented by Baumann et al. [1], requires the application of a constant-amplitude radio frequency (RF) voltage at the tunnel junction over a wide range of frequencies. To achieve constant amplitude the RF input power is adjusted to compensate for frequency dependent variations of the cable transmission. This approach relies on a precise determination of the RF transmission function. Here, we discuss the upgrade of a low-temperature STM with high-frequency cables and a superconducting magnet. In particular, we present the RF transmission achieved with 40 dB attenuation at maximum.

[1] S. Baumann, W. Paul, T. Choi, C. P. Lutz, A. Ardavan, A. J. Heinrich, Science 350, 417-420 (2015).

O 91.4 Thu 10:30 P

Single Asperity Sliding Friction across the Superconducting Phase Transition — •Wen Wang[1,2], Dirk Dietzel[1], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, University of Giessen, 35392 Giessen, Germany — [2]School of Mechanical Engineering, Southwest Jiaotong University, 610031 Chengdu, China

In sliding friction, different energy dissipation channels have been proposed, including phonon and electron systems, plastic deformation, and crack formation. However, the details of how energy is coupled into these channels is heavily debated, and especially the relevance of the electron system for energy dissipation often remains elusive. Here, we present contact mode AFM friction experiments of a single asperity sliding on a high-T_C BSCCO-superconductor in a wide temperature range from 40 K to 300 K [1]. Overall, friction decreases with temperature as expected based on thermally activated friction models, but we find an unexpected large peak around T_C of 95 K. We model these results by a superposition of different energy dissipation channels, where the influence of electronic contributions vanishes when cooling below the superconducting phase transition temperature. Our experiments thereby unambiguously link electronic friction effects to the number of normal state electrons in the superconducting phase below T_C, allowing us to quantify the relative importance of the electron system to overall friction.

[1] W. Wang, D. Dietzel, A. Schirmeisen, Science Advances, eaay0165 (2020)

O 91.5 Thu 10:30 P

Microwave-assisted tunnelling and interference effects in superconducting junctions under fast driving signals — •Robert Drost[1], Pitor Kot[1], Maximilian Uhl[1], Juan Carlos Cuevas[2], Joachim Ankerhold[3], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

As scanning tunnelling microscopy is pushed towards fast local dynamics, a quantitative understanding of tunnel junctions under the influence of a fast AC driving signal is required, especially at the ultra-low temperatures relevant to spin dynamics and correlated electron states. We subject a superconductor-insulator-superconductor junction to a microwave signal from an antenna mounted in situ and examine the DC response of the contact to this driving signal. Basic quasi-particle tunnelling can be interpreted using a modified density of states in the electrodes. The situation is more complex when it comes to higher order effects such as multiple Andreev reflections. Microwave assisted tunnelling unravel these complex processes, providing deeper insights into tunnelling than are available in a pure DC measurement.

O 91.6 Thu 10:30 P

Development of a Variable-Temperature High-Speed Scanning Tunneling Microscope — •Zechao Yang, Leonard Gura, Jens Hartmann, Heinz Junkes, Florian Kalass, Matthias Brinker, William Kirstaedter, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

To understand the crystalline to vitreous transition in oxide films as a function of temperature in real space and at real time, we developed a variable-temperature high-speed scanning tunneling microscope.

The scanner consists of two independent tube piezos for slow and fast scanning, respectively. For fast scans, we use spiral geometries to avoid image distortions. The spiral geometry and the tip velocity are adjustable.

The STM tip scans in quasi-constant height mode with a predefined tilt correction. The surface topography can then be deduced from the logarithm of the tunneling current. We implemented the scan control into the EPICS framework [1] and developed highly customizable, purely python based software for the image analysis.

With these tools, we atomically resolved diffusion processes within an O(2x2) structure on Ru(0001) with a time resolution of 25 milliseconds per frame. The measurements prove the vibrational stability and low thermal drift characteristics of our microscope.

For future high temperature measurements we will use a continuous flow cryostat to counter-cool the piezo material of the scanner.

[1] Junkes, H. et al. (2018). ICALEPCS2017, pp. 1762-1766.

O 91.7 Thu 10:30 P

Combined AFM and STM with high optical access achieving atomic resolution in ambient conditions — •Korbinian Pürckhauer, Simon Maier, Anja Merkel, Dominik Kirpal, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

Performing atomic force microscopy (AFM) and scanning tunneling microscopy (STM) with atomic resolution under ambient conditions is challenging due to enhanced noise and thermal drift. We show the design of a compact combined atomic force and scanning tunneling microscope that uses qPlus sensors and discuss the stability and thermal drift. By using a material with a low thermal expansion coefficient, we can perform constant height measurements and achieve atomic resolution in both AFM and STM on various samples. Moreover, the design allows a wide angle optical access to the sensor and the sample that is of interest for combining with optical microscopes or focusing optics with a high numerical aperture.

[1] Pürckhauer et al., Rev. Sci. Instrum. 91, 083701 (2020)

O 92: Poster Session VII: Ultrafast electron dynamics at surface and interfaces III

Time: Thursday 10:30–12:30 Location: P

O 92.1 Thu 10:30 P

FEL based tr-ARPES of ultrafast electron dynamics in quantum materials — •M. Heber[1], K. Kühlmann[2], D. Kutnyakhov[1], F. Pressacco[1], N. Wind[3], D. Curcio[4], K. Volckaert[4], V. Shokeen[5], A. Yaroslavsev[5], H. Noei[1], M. Wagstaffe[1], Ch. Sanders[6], S. Y. Agustsson[7], H. Redlin[1], S. Dziarzhytski[1], G. Brenner[1], L. Wenthaus[1], K. Medjanik[7], H.J. Elmers[7], G. Schönhense[7], Y. Acremann[2], Ph. Hofmann[4], H. Dürr[5], W. Wurth[1,3], and K. Rosnagel[1,8] — [1]DESY, Hamburg, D — [2]Department of Physics, ETH

Zürich, CH — [3]Physics Department, University of Hamburg, D — [4]Aarhus University, DK — [5]Uppsala University, S — [6]Rutherford Appleton Laboratory, Harwell, GB — [7]University of Mainz, D — [8]IEAP, CAU Kiel, D

We investigated the ultrafast electronic structure dynamics of various quantum materials by time- and angle-resolved photoelectron spectroscopy. To this end, a time-of-flight momentum microscope enabling the parallel detection of the photoelectrons two surface-parallel momentum components plus their kinetic energy was combined with the short-pulsed monochromatized XUV radiation from the PG2 beamline of FLASH at DESY. The use of XUV pulses specifically provides the possibility to study the combined temporal response of valence and core electrons. Here, the results of three different experiments will be presented, focusing on the Dirac cone of graphene on Ir(111), the surface and bulk valence bands and core levels of Bi_2Se_3, as well as the hot electrons in a thin ferromagnetic nickel film on W(110). Pump fluence- and momentum-dependent dynamical effects will be discussed.

O 92.2 Thu 10:30 P

Dynamics of charge transfer processes at nanoparticle/oxide interface studied by free electron laser — •Eleonora Spurio[1,2], Jacopo Stefano Pelli Cresi[3], Emiliano Principi[3], Daniele Catone[4], Patrick O'Keeffe[4], Stefano Turchini[4], Stefania Benedetti[2], Avinash Vikatakavi[1,2], Sergio D'Addato[1,2], Claudio Masciovecchio[3], Jagadesh Kopula Kesavan[5], Federico Boscherini[5], and Paola Luches[2] — [1]Università degli Studi di Modena e Reggio Emilia — [2]CNR-NANO, Modena — [3]Elettra-Sincrotrone Trieste — [4]ISM-CNR, Rome — [5]Università di Bologna, Italy

In order to make wide band gap semiconductors suitable for a widespread use as green solar photocatalysts, it is fundamental to expand their photoactivity in the visible range. This is possible for example combining these materials with plasmonic nanoparticles(NP). In our work, we have studied a system based on Ag NP embedded in a film of CeO2. Here, we have exploited the chemical sensitivity of free electron laser time-resolved soft X-ray absorption spectroscopy to obtain information on the ultrafast energy transfer process at the NP/film interface, following photoexcitation of the plasmon resonance of Ag NP. We have observed ultrafast changes (< 200 fs) of the Ce N4,5 absorption edge, revealing a highly efficient charge transfer from Ag NP to the Ce atoms of the CeO2 film[1]. These results also demonstrate the power of this technique for the characterization of energy transfer in these novel hybrid plasmonic/semiconductor materials. [1] J. S. Pelli Cresi et al., submitted for publication (2021).

O 92.3 Thu 10:30 P

Density-dependent electron-phonon coupling in multiband systems. — •Tobias Held, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

When a solid is irradiated with a short-pulsed visible light laser, the energy is almost entirely absorbed by the electrons while the lattice remains cold. The subsequent energy flow between electrons and phonons is commonly described by the electron-phonon coupling parameter, a central parameter in the Two-Temperature Model and most other temperature-based models.

This coupling parameter depends on a multitude of variables as reinforced by recent results. The most commonly considered dependence is the one on the electron temperature.

In this work we aim to see how the density distribution between different electronic subsystems affects the coupling parameter in combination with the electronic temperature. For the different electron subsystems we distinguish between orbital types in gold and spins in magnetic nickel. The results show that the total coupling strongly depends on the density distribution for gold, while for nickel the influence is compensated within both bands.

O 92.4 Thu 10:30 P

Electron-phonon coupling for different stages of relaxation dynamics after ultra-short laser-excitation — •Sebastian T. Weber and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

For the excitation of metals with ultra-short laser pulses of visible light, the energy is absorbed by the electrons. Later, the energy is transferred to the phonons.

The strength of this energy transfer is determined by the electron-phonon coupling parameter. It in turn depends on a multitude of parameters, like the electronic temperature, the different stages of electronic nonequilibrium [1] and phononic properties [2].

We study the electron-phonon coupling in dependence on different states of ultra-fast dynamics after laser-excitation. First, the coupling strength is mostly determined by the electron temperature. It is also influenced by the laser-induced nonequilibrium electron distribution. With the heating of the phonons, the lattice temperature comes into play. The decreasing Debye Temperature [2] leads to a strong drop of the electron-phonon coupling strength. Moreover, the cooling of electrons by phonons induces a long-lasting nonequilibrium of the electronic system, which influences the coupling strength as well [1].

[1] S. T. Weber and B. Rethfeld, PRB **99**, 174313 (2019)
[2] M. Z. Mo *et al.*, Science **360**, 1451 (2018)

O 92.5 Thu 10:30 P

Electron Thermalization in laser-excited Graphite — •Katharina Hilgert, Sebastian T Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schroedinger- Strasse 46, 67663 Kaiserslautern, Germany

In this contribution we present a theoretical calculation of electron thermalization in a laser-excited graphite sample. Our calculations are motivated by an experimental paper applying trARPES, which concludes that the electron gas has reached a Fermi-Dirac distributed state only 50 fs after the excitation [1]. We have recreated these observations using a simulation based on full Boltzmann collision integrals [2] and were able to achieve comparable results. We then extended our examination by using two alternative analyzation methods utilizing the energy density of non-equilibrium electrons and the temporal evolution of the entropy, respectively. We have found that the method proposed in the experimental paper slightly underestimates the relaxation time but overall predicts results in an accurate order of magnitude.

[1] G. Rohde *et al.*, PRL **121**, 256401 (2018)
[2] B.Y. Mueller and B. Rethfeld, PRB **87**, 035139 (2013)

O 92.6 Thu 10:30 P

Ultrafast dynamics of direct and indirect excitation pathways of the topologically protected surface state on Sb2Te3 — •Jan Böhnke[1], Haydar Altug Yildirim[1], Cornelius Gahl[1], Jaime Sánchez-Barriga[2], Oliver Rader[2], and Martin Weinelt[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Dirac cone like topologically protected surface states (TSS) have attracted high interest for spintronic applications due to their specific spin texture in momentum space and the long electron mean free path because of reduced scattering phase space. Optical control of electric currents at the surface of topological insulators has been discussed controversially. We investigated the role of direct and indirect population channels for the TSS on Sb_2Te_3 in 2D momentum space by time- and angle-resolved two-photon photoemission spectroscopy. Excitation with 1.55 eV photons leads to an initially anisotropic population of the Dirac cone depending on the helicity of the excitation pulse. This circular dichroism however predominantly exhibits a 3-fold symmetry, which reflects the symmetry group of the bulk material but does not correspond to a macroscopic current in the TSS. Since the photon energy exceeds the bulk band gap, the optical excitation creates also a significant electron population in the conduction band, which relaxes towards the band minimum on the timescale of few 100 fs. On the same timescale electrons scattered from the conduction band dominate the population in the TSS so that the anisotropy decays rapidly.

O 93: Poster Session VII: Graphene and beyond I

Time: Thursday 10:30–12:30 Location: P

O 93.1 Thu 10:30 P

Electric-field control of a single-atom polar bond — •Maryam Omidian[1], Susanne Leitherer[2], Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center of Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The polar chemical bond between a single Au atom terminating the apex of an atomic force microscope tip and a C atom of graphene on SiC(0001) is exposed to an external electric field. For one field orientation the Au-C bond is strong enough to sustain the mechanical load of partially detached graphene, whilst for the opposite orientation the bond breaks easily. Calculations based on density functional theory and nonequilibrium Green's function methods support the experimental observations by unveiling bond forces that reflect the polar character of the bond. Field-induced charge transfer between the atomic orbitals modifies the polarity of the different electronegative reaction partners and the Au-C bond strength.

O 93.2 Thu 10:30 P

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •Sebastian Wille[1,2,3], Hongyan Jiang[2], Oliver Bünermann[2], Alec M. Wodtke[1,2], Jörg Behler[3], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

Understanding the formation of covalent bonds due to atomic-scale motions and energy dissipation pathways involved is an ongoing challenge in the field of chemistry. Measurements performed in our group show a bimodal pattern of the translational energy loss distribution of hydrogen atoms scattered from graphene. The second generation reactive empirical bond order potential was fitted to ab initio electronic structure data obtained from embedded mean-field theory to generate a potential energy surface (PES). First-principles dynamics simulations using the provided PES were able to reproduce the bimodal feature of the energy loss spectrum and were in qualitative agreement with experimental results. But these investigations could not fully provide a detailed description of the scattering and sticking mechanisms. Therefore, we developed a full-dimensional neural network PES by fitting to the density functional data in order to further reduce the remaining errors by the fitting procedure of the PES underlying molecular dynamics simulations performed, which better fits the experiment.

O 93.3 Thu 10:30 P

Intercalation of silver between graphene and silicon carbide studied by PEEM and AFM — •Philipp Weinert[1,2], Richard Hönig[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer Straße 2, 44227 Dortmund, Germany

Due to its outstanding electronic, magnetic, and mechanical properties graphene is of particular interest multiple fields.

In this study the intercalation of silver between one layer of graphene, the so-called buffer layer, and a silicon carbide substrate is investigated. Other studies have shown that covalent bounds between the silicon carbide and the buffer layer are released by intercalation, which leads to quasi free standing graphene.

To achieve the intercalation, samples have been coated with thin silver-films of different and defined thicknesses. Subsequently, the samples have been annealed to initiate the intercalation. In different steps of the annealing process, photoemission electron microscopy (PEEM) has been carried out to investigate the work function of the surface. This investigation has proven that silver intercalated underneath the buffer layer during the annealing. Moreover, in the case of thick silver layers a contrast inversion was visible. Furthermore, atomic force microscopy (AFM) has been carried out to investigate the topography of the samples after the intercalation. This study has shown that a small part of the silver does not intercalate, but forms islands on the surface.

O 93.4 Thu 10:30 P

Modeling the self-assembly of graphene flakes on liquid Cu — •Juan Santiago Cingolani, Mie Andersen, and Karsten Reuter — Chair of Theoretical Chemistry, Technical University of Munich, Germany

The use of liquid Cu as a catalyst for the production of graphene during chemical vapor deposition has been shown to lead to high-quality single layer millimeter-scale graphene flakes. In-situ optical microscopy revealed that the flakes are mobile on the liquid surface and interact with each other leading to the formation of self-assembled structures. We carry out a series of molecular dynamics simulations of graphene flakes on liquid Cu employing the third-generation charge optimized many body potential (COMB3) to shed some light on the origin of such inter-flake interactions.

From our simulations we extract information regarding the interaction of the flakes with the liquid substrate; namely the adsorption height, interaction energy, and charge transfer into the adsorbate. We extrapolate these properties to the limit of large flakes and use them as input for a mesoscopic model which accounts for electrostatic repulsion and capillary attraction assuming charged spherical particles. The resulting interaction potential predicts interflake distances within an assembly that lie within an order of magnitude of the experimental observations. While quantitative agreement is out of the scope for such a simple model, we show that the experimental observations are compatible, under the proposed mesoscopic model, with the microscopic properties derived from atomistic simulations.

O 93.5 Thu 10:30 P

Reduced step bunching during growth of epitaxial graphene on silicon carbide (0001) — •Robert Appel, Philipp Weinert, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany

Epitaxial graphene (EG) has attracted significant interest in the recent years due to the simple preparation method by heating silicon carbide (0001). The major drawback of this approach is step bunching (SB) that leads to large terraces and tall step heights. These disconnect the EG layers from step to step resulting in anisotropic electronic and magnetic properties. To prevent this, samples with shallow steps are desired. The $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$-reconstruction (so-called buffer layer (BL)) of the SiC(0001) constrains the SB and forms while heating. Therefore, a fast formation of the BL while heating without mono layer or bilayer patches is of utmost importance.

We use the confinement controlled sublimation (CCS) method in argon atmosphere because it is known for reproducibility and tunability. Thus, it is a promising method to find the ideal parameters for fast BL formation. Kruskopf et al. demonstrated the preparation of EG with shallow steps and less SB by using a high heating rate, a short heating time and a high preparation temperature.

In this study, we explore the applicability of the CCS method in order to obtain similar results with shallow steps and less SB. For this purpose, we systematically modify the preparation parameters and characterize the obtained samples with atomic force microscopy.

O 93.6 Thu 10:30 P

Influence of Chemical Interactions on Low Energy Ion bombardment of 2D Materials: Insights from ab-initio Molecular Dynamics — •Silvan Kretschmer[1], Sadegh Ghaderzadeh[1], and Arkady V. Krasheninnikov[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Department of Applied Physics, Aalto University, Finland

Low energy ion implantation (LEII) provides a valuable tool to tune the mechanical, electronic and catalytic properties of 2D materials by the targeted implantation of impurities. In contrast to ion irradiation at higher energies the commonly applied binary collision formula fails to describe the outcome of the irradiation process for ions close to the displacement energy, that is the minimum ion energy needed to displace the target atom. The dominating influence of the chemical interaction of projectile and target atoms and its effect on the displacement energy are addressed in this work. For that, we carried out ab-initio molecular dynamics (MD) simulations for a broad range of projectiles (elements Hydrogen to Argon) impacting on graphene and h-BN, and determined the energies needed to displace C, N and B atoms, respectively. We further present and validate a scheme to incorporate the effect of spin-polarization on the displacement process - as spin-polarized ab-initio MD runs tend to fail at bond-breaking.

O 93.7 Thu 10:30 P

hBN/Pt(111) and hBN/Ir(111): distinctive templates for Cs adsorption — •Jiaqi Cai, Robin Ohmann, and Carsten Busse — Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen

High-quality two-dimensional materials (2DM) can be grown by epitaxial methods on the high-symmetry surfaces of transition metal crystals. This epitaxy leads to the interaction between 2DMs with the underlying substrate, which periodically modulates their geometric and electronic structure. This spatial periodicity constitutes a moiré pattern.

The periodic electronic modulation of the moiré pattern provides a template for adsorbates. To study this templating effect, we deposit Cs onto hBN/Pt(111) and hBN/Ir(111). Our scanning tunneling microscopy measurements reveal, hBN/Pt(111) and hBN/Ir(111) are very different templates: the preferred adsorption sites on hBN/Pt(111) are the strongly bonded regions (valleys) of the moiré unit cell, and on hBN/Ir(111) the weakly bonded regions (hills). Furthermore, one valley region on hBN/Pt(111) can accommodate multiple alkali metal atoms, while only one single Cs atom can adsorb on the hill of the hBN/Ir(111) moiré unit cell. An additional feature of Cs adsorption on hBN/Ir(111) is that there are two hill regions in one moiré unit cell. With the proper preparation procedure, the adsorbed Cs atoms form an unusual honeycomb lattice.

O 93.8 Thu 10:30 P

Preparation of antimony monolayers on Ag(111) — •Stefanie Hilgers[1], Julian A. Hochhaus[1,2], Anneke Reinold[1], Malte G. H. Schulte[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227, Dortmund, Germany

In the here presented research, we prepare and investigate antimony monolayers on Ag(111). Similar to graphene, the elements of the 5th main group such as phosphorus, arsenic, and antimony are predicted to have extraordinary electronic properties.

Due to the small lattice mismatch between silver and free-standing antimonene, Ag(111) is a suitable substrate for the preparation of antimony monolayers. The substrate was cleaned by argon sputtering and heating in UHV, while the antimony monolayers were prepared by molecular beam epitaxy (MBE). Auger electron spectroscopy (AES) was used to investigate the chemical surface composition, while structural investigations were carried out using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at room temperature.

O 93.9 Thu 10:30 P

Preparation and characterization of lead monolayers on Pd(111) — •Anneke Reinold[1], Julian Hochhaus[1,2], Ismail Baltaci[1], Stefanie Hilgers[1], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

The research presented here focuses on the preparation of lead monolayers on Pd(111). With the experimental realization of two-dimensional lead by Yuhara et al. in 2019, the field of 2D materials was recently expanded. According to theoretical predictions, the so-called plumbene has the largest band gap and the highest spin-orbit coupling from all group 14 elements due to its high mass. Additionally, plumbene was predicted to show the quantum spin Hall effect (QSHE) even at room temperature. Therefore, plumbene is an ideal candidate for topological insulators and future electronic applications.

We want to achieve a more detailed knowledge of the behavior of different layer thicknesses of lead on palladium. We prepared Pd(111) by repeated cycles of argon sputtering and heating. The monolayers were deposited by thermal vapor deposition. Low-Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) were used to characterize the Pb/Pd(111) system.

O 93.10 Thu 10:30 P

Ultrathin oxide/graphene heterostructures — •Andrea Picone — Department of Physics, Politecnico di Milano, Milano, Italy

Graphene interfaced with oxide ultrathin films is a particularly appealing system for the development of new devices, since the dielectric layer can be used to modulate the physical properties of the carbon monolayer. Furthermore, graphene can be used as a template to synthesize novel two-dimensional oxide materials.[1] Despite such an extreme technological and scientific interest, only few successful examples of sharp graphene/oxide interfaces have been reported so far, since the growth of atomically flat ultrathin oxide films on the honeycomb monolayer is hampered by the extremely low surface free energy of graphene, which promotes the nucleation of three-dimensional clusters. Here, by using standard surface science techniques, I will analyze the structural, chemical and electronic properties of transition metals oxide (CrxOy and FexOy) and rare earths oxide (ErxOy)ultrathin films grown on the graphene/Ni(111) substrate.[2,3] The experimental results reveal a rich variety of graphene heterostructures, depending on the element used and the synthesis procedure.

[1] Netzer, F. P.; Surnev, S. Oxide Materials at the Two-Dimensional Limit; Springer, (2016)

[2] Lodesani, A. ; Picone, A.; Brambilla, A.; Giannotti, D.; Jagadeesh, M.S.; Calloni, A.; Bussetti, G.; Berti, G.; Zani, M.; Finazzi, M.; Duò, L.; Ciccacci, F. ACS Nano 13, 4361-4367 (2019)

[3] Lodesani, A.; Picone, A.; Brambilla, A.; Finazzi, M.; Duò, L.; Ciccacci, F. J. Chem. Phys. 152, 054706 (2020)

O 93.11 Thu 10:30 P

Kinetic nanoscale friction and intermittent hybridization in graphene stacks on SiC — •Bartosz Szczefanowicz[1], Leonhard Mayrhofer[2], Andreas Klemenz[2], Michael Moseler[2], and Roland Bennewitz[1] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]IWM Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany

Graphene is an excellent lubricant on micro- and nanoscale due to its weak normal-to-plane interactions. Friction Force Microscopy (FFM) demonstrated ultralow friction for graphene on many different substrates. However, the friction force for epitaxial graphene on SiC(0001) increases dramatically above a normal load threshold [1]. We suggest that the observation can be explained by a pressure-induced temporal and local orbital rehybridization from sp^2 to sp^3 and a corresponding change of interlayer van der Waals interaction into metastable covalent bonds [2].

We report friction force measurements for graphene/SiC(0001) in ultrahigh vacuum as function of normal load and sliding rate and compare the results to atomistic simulations based on density functional theory (DFT). An excellent agreement of the load-dependence reveals friction mechanisms involving pressure-induced intermittent bonds.

[1] T. Filleter, R. Bennewitz, Physical Review B, 81 (2010), 155412

[2] Y. Gao, et al, Nature Nanotechnology, 13 (2018), 133-+.

O 93.12 Thu 10:30 P

Hetero-Stacking of 2D Materials by Sequential Chemical Vapour Deposition — •Nicolas Néel, Alexander Mehler, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

A multi-step method that enables the growth of graphene on hexagonal boron nitride (h-BN) on Pt(111) is presented. Using borazane (BNH6) as a molecular precursor, h-BN is grown on the surface in the first step. In a next step, a sufficiently thick Pt film is adsorbed and buries the h-BN mesh. It acts as a catalyst for the subsequent growth of graphene via the chemical vapour deposition of ethylene (C2H4). The last step involves the thermally induced entire intercalation of the Pt film beneath h-BN giving rise to large surface regions of a graphene/h-BN stacking. A unique moiré superstructure results from the h-BN-Pt interface. Upon reducing the tip-sample separation an additional $\sqrt{3} \times \sqrt{3}\,\mathrm{R}\,30^\circ$ superlattice gradually appears.

O 93.13 Thu 10:30 P

In-plane heterostructures of transition metal dichalcogenide monolayers — •Kai Mehlich[1,2], Daniela Dombrowski[1,2], Thais Chagas[1], Daniel Kurz[1], Thomas Michely[3], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — [2]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]II. Physikalisches Institut , Universität zu Köln, Zülpicher Str. 77, 50937 Köln

Modern electronics and optoelectronics utilise complex materials to maximize efficiency and reduce size, while requiring specific electronic properties. 2D-materials can fulfill these desires excellently. With epitaxial growth of monolayer transition metal dichalcogenides like TaS_2, WS_2 and MoS_2 already an established line of research, we increased the range of possibilities by successfully growing in-plane heterostructures of these materials. The heterostructures are realised by sequential epitaxial growth of monolayers on Au(111), thereby forming the thinnest possible heterostructures. The material combination was chosen because of the difference in lattice parameters and electronic structure (as monolayer MoS_2 and WS_2 are semiconductors and monolayer TaS_2 is metallic). The difference in lattice parameters induces stress, which has to be compensated. We categorised the relieve mechanisms into three groups, being: Defects, compression or stretching of the materials, and deformation in the z-plane. The mechanisms are observed by STM-imaging and analysed quantitatively on their appearance depending on the hetero-boundary, mostly showing an uninterrupted boundary.

O 93.14 Thu 10:30 P

Catalytically assisted growth of molybdenum disulfide monolayers on silicon dioxide substrates — Ana Burgos[1], Valeria Del Campo[1], and •Patricio Häberle[1,2] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso 2390123, Chile — [2]Institute of Applied Physics, Vienna University of Technology, 1040 Vienna, Austria

MoS2 monolayers grown by chemical vapor deposition (CVD), starting from MoO3 and S precursors, occurs mostly in form of patches over the substrates, leaving some sections nearly clean. There is a large heterogeneity of the resulting products, regarding size and shape of the structures, obtained. We have explored, the formation of MoS2 layers grown by CVD on silicon dioxide substrates, while exposed to HOPG (Highly Oriented Pyrolytic Graphite). HOPG provides a catalytic surface that promotes the chemical reactions involved in the formation of MoS2. We have proposed a detailed model of the chemical reactions involved in this monolayer growth. It proceeds via the formation of MoO2 on the HOPG surface, followed by the gas phase synthesis of MoS2, which is subsequently collected over the substrate. Our analysis, using optical microscopy and Raman spectroscopy of the resulting products, indicate that the ratio between MoO2 and S is a crucial variable in the formation of monolayers. A set of optimal experimental conditions were established in order to promote homogeneous growth of MoS2 monolayers.

O 94: Poster Session VII: Poster to Mini-Symposium: Electrified solid-liquid interfaces II

Time: Thursday 10:30–12:30 Location: P

O 94.1 Thu 10:30 P

Peeling graphite layer by layer to study the charge exchange dynamics of ions inside a solid on the fs time scale — •Anna Niggas[1], Sascha Creutzburg[2], Janine Schwestka[1], Benjamin Wöckinger[1], Pedro L Grande[3], Bernhard C Bayer[4,5], José P Marques[6], Friedrich Aumayr[1], Robert Bennett[7], and Richard A Wilhelm[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute of Ion Beams and Materials Research, HZDR, Dresden, Germany — [3]Instituto de Fisica, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil — [4]Institute of Materials Chemistry, TU Wien, Vienna, Austria — [5]Faculty of Physics, University of Vienna, Vienna, Austria — [6]BioISI - Biosystems & Integrative Sciences Institute, Faculdade de Ciências da Universidade de Lisboa, Lisbon, Portugal — [7]Department of Physics and Astronomy, University of Glasgow, Glasgow, UK

Charge exchange is one of the many effects taking place when particles penetrate through matter. For a long time experiments were limited to studying secondary particles because observation of the ion inside a solid is not possible. We perform highly charged ion transmission through single-, bi- and trilayer graphene to study the ions' exit charge state after intaction. Thereby we adress the charge state changes in graphite with monolayer precision. Following our results of two independent approaches, accompanied by a first-principles model on interparticle de-excitation, we find that the ultra-fast neutralisation dynamics depend only on the time the ion interacts with material layers and neutralisation happens primarily in the topmost surface layers.

O 94.2 Thu 10:30 P

Electrooxidation of Isopropanol on Pt and Ru Single Crystals: an An in situ X-Ray Diffraction Study — •Xin Deng[1,2], Ralf Schuster[1], Leon Jacobse[2], Vedran Vonk[2], Yaroslava Lykhach[1], Olaf Brummel[1], Andreas Stierle[2], and Jörg Libuda[1] — [1]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg

By combining isopropanol fuel cells with liquid organic hydrogen carriers, it is possible to convert chemically bound hydrogen into electricity without generation of gaseous gas. Platinum is the best catalyst for alcohol oxidation, however, partial poisoning by the product acetone impacts the activity. The addition of ruthenium increases the reaction rates, however, the origin of the beneficial effect is not clear so far. In this work, we investigated the electrochemical oxidation of isopropanol on Pt(111) and Ru(0001) single crystals by employing high-energy grazing incidence X-ray diffraction. The existence of isopropanol does not influence the oxidation of Pt(111) as the crystal truncation rods (CTRs) show similar shapes in the electrolyte with and without isopropanol. Platinum is severely roughened by potential cycling with an upper potential limit higher than 1.35 V, while Ruthenium is much stable. Further analysing the XRD data of Ru(0001) by fitting the CTRs will help us understand its behavior.

O 94.3 Thu 10:30 P

Resolving the structure of oxidized Cu surfaces with machine-learned Gaussian Approximation Potentials — •Nicolas Bergmann[1], Nicolas G. Hörmann[1,2], and Karsten Reuter[2] — [1]Technische Universität München, Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Copper was recently shown to exhibit promising capabilities toward electrochemical CO oxidation [1], yet only after undergoing activating surface morphological changes. The detailed structure and composition of the formed surface oxidic layer is hitherto unknown, preventing further mechanistic analyses. Here we use the high computational efficiency of machine-learned Gaussian Approximation Potentials (GAPs [2]) to systematically investigate the Cu(111) surface structure with varying concentrations of adsorbed oxygen. The potentials are trained with density-functional theory data of bulk CuO_x and molecular dynamics generated slab structures.

While low oxygen coverages do not alter the Cu substrate significantly, we find dramatic morphological changes above a critical coverage of ~ 25% monolayer: Surface copper atoms are extruded from the top layer, forming CuO_x islands, while at the same time the amount of subsurface oxygen increases. A detailed analysis of local atomic environments reveals predominant local structural motives resembling those in well known bulk copper oxides.

[1] A. Auer *et al.*, Nature Catal. **3**, 10, (2020). [2] A.P. Bartok and G. Csanyi, Int. J. of Quantum Chem. **115**, 16 (2015).

O 94.4 Thu 10:30 P

Under potential deposited Hydrogen on Pt(111) is both terminal and bridge-bonded — Gregor Zwaschka[1,2], Yujin Tong[1,2], and •R. Kramer Campen[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]University of Duisburg-Essen, Duisburg, Germany

Despite decades of effort, finding catalysts for either half reaction of electrolytic water splitting that are reactive, stable and inexpensive has proven remarkably challenging. For the hydrogen evolution half reaction (HER) in acidic solution platinum meets the first and second of these goals remarkably well but understnading why it does so, *i.e.* understanding the mechanism of the HER on Pt, has proven challenging.

H adsorbs on Pt at potentials positive of those at which H_2 appears. Understanding the potential-dependent structure of this under-potential-deposited (UPD) H, how it differs from H adsorbed on Pt in UHV, and its relationship to H_2 generation is a necessary step in understanding the HER mechanism. Here we perform vibrational sum frequency spectroelectrochemistry to collect the potential dependent Pt-H spectral response on single crystal Pt(111) electrodes in acidic solution. In contrast to suggestions from UHV and previous infrared spectroelectrochemical studies, we find that both terminal and bridge-bonded H appear throughout the UPD region and that, depending on the defect density, distinct types of terminal-bonded hydrogen can be observed. Intriguingly, for pristine Pt(111) surfaces we also observe an interfacial hydronium species heretofore only predicted in calculation.

O 94.5 Thu 10:30 P

Characterization of excitonic behaviour of MoS_2 on gold electrode by final state resonant sum frequency spectroscopy — •Tao Yang, Erik Pollmann, Marika Schleberger, Yujin Tong, and Richard Kramer Campen — University of Duisburg-Essen, Faculty of Physics, 47057 Duisburg, Germany

Two dimensional (2D) materials are promising candidate electrocatalysts for the hydrogen evolution reaction (HER) because of their large surface area and tunable electronic properties. Particularly MoS_2, a transition metal dichalcogenide, has been intensively studied in this context showing comparable efficiency for the HER as Pt. While continuous breakthroughs in HER activity of MoS_2 have been achieved, less attention has been devoted to the mechanistic investigation, e.g., charge transfer between a metal electrode and the MoS_2. Here we use final state resonant sum frequency spectroscopy to study the optical response of MoS_2 exfoliated on a gold electrode in aqueous solution as a function of applied bias. The results show the evolution of the A and B excitons with electron doping. Together with Raman and electrochemical characterization, the current study provides important insights into understanding the relationship between electronic structure, atomic configuration and electron transfer at metal/MoS_2/aqueous electrolyte interface.

O 94.6 Thu 10:30 P

Effect of water co-adsorption on the electrochemical stability of H-covered Pt(111)-water interfaces — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck_institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

Using density functional theory based molecular dynamics simulations we study the relation between H-coverage and electrode potential at the Pt(111)/water interfaces. We find that chemisorbed water molecules strongly interact with the H-adatoms and strongly impact the electrode potential. Above a critical H adsorbate coverage, chemisorbed water becomes unstable at these interfaces. The loss of co-adsorbed water molecules results in a steep increase in the electrode potential, making the interface thermodynamically unstable. The presence of a critical upper H concentration well below 1 ML has been observed experimentally but is absent in surface science modeling. This allows for the first time to understand the mechanisms that limit H adsorption on these surfaces and that lead to the onset of the hydrogen evolution reaction (HER).

S.Surendralal, M. Todorova, and J. Neugebauer, (under review).

O 94.7 Thu 10:30 P

Implicit solvation limitations and beyond for potential-dependent electrochemical interfaces modelling — •Arthur Hagopian[1,2] and Jean-Sébastien Filhol[1,2] — [1]ICGM, University of Montpellier, CNRS, ENSCM, Montpellier, France — [2]RS2E French network on Electrochemical Energy Storage, FR5439, Amiens, France

In recent years, processes at solid/liquid interfaces have attracted considerable attention due to their major role in scientific and engineering applications. In the battery domain, solid/liquid interfaces are critical for the development of high energy density batteries such as lithium-metal batteries (LMB), which are the current missing key to a large-scale vehicle electrification and renewable energy generation. In LMB, the interface of interest corresponds to the interface between a lithium metal anode and an organic electrolyte, where in this particular case, the solid electrolyte interphase (SEI) layer is formed between the solid and liquid phases. Despite decades of research, our knowledge on the atomistic structure and chemical evolution of the SEI is still rather limited. In this work, we investigate the particular case of LiF, one of the most commonly found SEI phases in lithium-based batteries. A polarizable continuum model (PCM) is used to described the solvent dielectric response and a grand canonical DFT approach is used to simulate potential variation. We show that in the case of LiF, which is a highly polar surface, PCM suffers limitations due to its inability to simulate chemical reactivity. We highlight that these limitations are also found while investigating charged interfaces. We finally propose a hybrid implicit/explicit model to overcome PCM limitations.

O 94.8 Thu 10:30 P

Doping of Free-standing Graphene Measured with Kelvin Probe Force Microscopy under Electrochemical Reaction Conditions — •Salma Khatun, Sidney Cohen, Irit Goldian, and Baran Eren — Weizmann Institute of Science, Rehovot, Israel

Solid-liquid interfaces play a central role in electrochemistry, electrolysis, and catalysis. The electrical double layer (EDL) which forms at the solid-electrolyte interface, plays a key role in moderating these processes. Due to the difficulty in probing this thin layer, very few experimental mechanistic studies under realistic reaction conditions have been reported. We know, free-standing single layer graphene (SLG) is transparent to both electrons and photons. When used as the solid interface in an electrochemical environment, a variety of microscopic and surface-sensitive spectroscopic techniques can be used to probe that interface from the upper side. Our study examines some of the fundamental issues in such a set-up. We have built an electrochemical micro-reactor cell enclosed by a SLG membrane. The double layer thickness is varied controllably by changing the pH of the aqueous NaOH solution. Since our SLG is not doped via any support or contaminants, the changes occur only due to doping from applied electric field. KPFM measurements are used to monitor the shift of Fermi-energy. Due to cleanliness of our technique, the result can be described fairly well by a model considering the applied electrochemical potential, modified by the capacitative drop in the EDL. Differences between experimental values and those predicted by the model can be explained by electrochemical doping during the evolution of O2 and H2.

O 95: Poster Session VII: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces III

Time: Thursday 10:30–12:30 Location: P

O 95.1 Thu 10:30 P

Single-atom electron paramagnetic resonance in a scanning tunneling microscope driven by a radiofrequency antenna at 4 K — •Stepan Kovarik[1], Tom S. Seifert[1], Dominik Juraschek[2], Nicola A. Spaldin[1], Sebastian Stepanow[1], and Pietro Gambardella[1] — [1]Department of Materials, ETH Zürich, Switzerland — [2]Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA

Combining electron paramagnetic resonance (EPR) with scanning tunneling microscopy (STM) enables detailed insight into the interactions and magnetic properties of single atoms on surfaces [1]. A requirement for EPR-STM is the efficient coupling of a microwave excitation to the tunnel junction. Here, we present a coupling efficiency of the order of unity by using a radiofrequency (RF) antenna placed parallel to the STM tip [2]. This highly efficient coupling allows us to observe the EPR of individual atoms on an MgO surface routinely at 4 K. Using this technique, we perform a systematic study of the EPR of Fe and hydrogenated Ti atoms on MgO, comparing different tunneling parameters, frequency, and magnetic field sweeps as well as amplitude and frequency modulation in order to maximize the EPR signal. We interpret the data based on density functional theory and charge transfer multiplet calculations, revealing the important role of the tip magnetic field in EPR-STM [3].

[1] S. Baumann, et al., Science 350, 417 (2015).
[2] T. S. Seifert, et al., Phys. Rev. Research 2, 013032 (2020).
[3] T. S. Seifert, et al., Sci. Adv. 6, eabc5511 (2020).

O 95.2 Thu 10:30 P

Exploring inelastic electron tunneling with functionalized STM tip using cluster Hubbard model — •Daria Medvedeva and Jindřich Kolorenč — Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Prague 8, Czech Republic

Inelastic electron tunneling spectroscopy (IETS) is a widely used experimental technique to explore vibrations and magnetic excitations of atoms and molecules adsorbed on metal surfaces [1]. Functionalization of the STM tip, for instance by attaching a magnetic molecule to it, introduces spin sensitivity and expands the possibilities of the scanning-probe technique [2]. We use a co-tunneling theory of STM-IETS [3] to investigate how a nickelocene-terminated tip (Nc-tip) senses excitations in a magnetic system (atom, molecule, cluster of atoms) adsorbed on a surface. In our approximation, the Nc molecule on the tip and the object on the surface are modeled by a cluster Hubbard model (one site for each magnetic atomic shell). We reproduce the spectra measured in STM experiments where the object on the surface was Nc molecule [4] or Fe atom (spin 3/2 with an out-of plane easy axis) [3], and predict spectra for several more complex magnetic systems. In particular, we compare cases with in-plane and out-of-plane easy axis.

[1] J.D.Langan, P.K.Hansma. Surf. Science **52**, Issue 1, pp. 211-216, Sept. (1975).
[2] K.W. Hipps, U. Mazur. *Inelastic Electron Tunneling Spectroscopy* (2006).
[3] B. Verlhac et al. Science **366**, 6465, pp. 623-627 (2019).
[4] F. Delgado and J. Fernández-Rossier. PRB **84**, 045439 (2011).

O 95.3 Thu 10:30 P

Engineering of Fe Spin Excitation on NaCl — •Shinjae Nam[1,2], Jinoh Jung[1,4], Christoph Wolf[1,3], Andreas Heinrich[1,2,3], and Jungseok Chae[1,3] — [1]center for Quantum Nano Science — [2]Physics department, Ewha Womans University — [3]Ewha Womans University — [4]Physics of department, KAIST

For scanning tunneling microscopy (STM) study of single magnetic atoms, a decoupling thin layer of Cu2N and MgO have been widely used to isolate magnetic atoms from the conducting substrate. However, NaCl wasn't commonly used for single magnetic atom even though it has been widely used for decoupling layer of single organic molecules.

Here, we investigated the electronic and magnetic properties of single Fe atoms absorbed on NaCl thin film on the Au (111) substrate depending on its absorption sites using STM. Notably, the Fe atoms are adsorbed on the interstitial bridge site of NaCl after deposition, while density functional theory (DFT) calculations indicate the Cl-top site as a preference absorption site. We confirmed the dynamic absorption process by atomic manipulation and simulation using DFT calculations. Moreover, Fe on the interstitial bridge shows an apparent stepwise increase at 23 meV, as expected for a spin-excitation. The DFT+multiplet calculation reproduces the spin excitation energy of Fe at the interstitial bridge of 3d7 electronic configuration with spin 3/2. Interestingly, the Fe at interstitial bridge has in-plane magnetic anisotropy due to the large transverse crystal field and its ground spin 1/2 two level system might be utilized as a qubit.

O 95.4 Thu 10:30 P

Electronic property of organic multilayers: Vanadyl phthalocyanine on Titanyl phthalocyanine monolayer/Ag(001) — Kyungju Noh[1,2], Luciano Colazzo[2], Andreas Heinrich[1,2], Fabio Donati[1,2], and •Yujeong Bae[1,2] — [1]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [2]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea

In this study, we identify orbital energy levels of Vanadyl phthalocyanine (VOPc) on Ag(001) with Titanyl phthalocyanine (TiOPc) interlayer by scanning tunneling microscopy (STM). Comparative research of single VOPc with and without molecular interlayer showed decoupling effect of the TiOPc monolayer. Using conductance measurement, we resolved HOMO and LUMO of individual VOPc molecules regularly spaced on one monolayer of TiOPc, whereas VOPc on bare metal substrate was strongly coupled with the metal substrate. Moreover, VOPc on TiOPc molecular layer has consistent adsorption direction. In this highly organized structure, the VOPc molecules presumably preserve the spin, hence representing a potential surface-absorbed molecular qubit.

O 95.5 Thu 10:30 P

Probing the anisotropy of g-factor of a single atom on a surface in vector magnetic fields — •Thi Hong Bui[1,2], Jinkyung Kim[1,2], Won-jun Jang[3], Denis Krylov[1], Soonhyeong Lee[1], Sangwon Yoon[1], Deung-jang Choi[4], Christoph Wolf[1], Fernando Delgado[5], Chris P. Lutz[6], Andreas J. Heinrich[1,2], and Yujeong Bae[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, South Korea — [2]Department of Physics, Ewha Womans University, Seoul, South Korea — [3]Nano Electronics Lab, Samsung Advanced Institute of Technology, Suwon 13595, South Korea — [4]Material Physics Center (UPV/EHU), 20018 Donostia-San Sebastian, Spain Donostia International Physics Center (DIPC), Spain — [5]Instituto de estudios avanzados IUDEA, Departamento de Fisica, Universidad de La Laguna, 38203, Tenerife, Spain — [6]IBM Almaden Research Center, San Jose, CA 95120, USA

Combining the electron spin resonance with the scanning tunneling microscope enables us to approach to the quantum states of single atoms on a surface with the energy resolution of sub-nano electron volts [1]. Here, we report the huge anisotropy of a hydrogenated titanium (Ti) atom at a lower symmetry binding site on MgO/Ag(100) studied using a mK ESR-STM in a vector magnetic field. We were able to determine the three components of g-factor. Interestingly, we observed the magnitude of the ESR signal significantly changes depending on the angle of the external magnetic vector, which can be attributed to the correlation between the relative orientation of the tip spin and the Ti spin. [1] S. Baumann et al., Science 350, 417 (2015)

O 95.6 Thu 10:30 P

Probing magnetic excitation of a spin spiral — •Hung-Hsiang Yang[1], Masayuki Hamada[2], Yasuo Yoshida[3], and Yukio Hasegawa[2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, Karlsruhe, 76131, Germany — [2]Institute for Solid State Physics, University of Tokyo, 5-1-5, Kashiwa-no-ha, Kashiwa, Chiba 277-8581, Japan — [3]Department of Physics, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Magnetic excitation due to inelastic electron scattering plays a crucial role in spintronics devices concerning the spin lifetime of polarized electrons and the amount of spin transfer torque for switching magnetic configurations in magnetic tunnel junctions. One of the fundamental processes is magnon creation, which occurs when injected hot electrons induce spin-flip scattering of the magnetic material. To image and address the magnetic origin of the excitations, we have performed low-temperature spin-polarized inelastic electron tunneling spectroscopy (IETS) on double layer Mn thin films formed on W(110) substrate.

The atomically-thin magnetic layer exhibits a homogeneous spin spiral with antiferromagnetic coupling, which provides a good reference for spin-polarized scanning tunneling microscopy (STM). Characteristic peak-dip features in IETS, as well as their correlation with the spin spiral, are acquired. Additionally, we have observed contrast reversal in the IETS intensity when the tip magnetization direction is flipped, indicating that the excitation is spin-dependent and thus presumably due to magnon creation.

O 96: Poster Session VII: Poster to Mini-Symposium: Frontiers of electronic-structure theory IV

Time: Thursday 10:30–12:30 Location: P

O 96.1 Thu 10:30 P

Electronic structure of β-SiAlON: effect of Al/O doping and of finite temperature — •Saleem Ayaz Khan[1], Ondrej Sipr[2], Jiri Vackar[2], Robin Niklaus[3], Peter J Schmidt[4], Wolfgang Schnick[3], and Jan Minar[1] — [1]University of West Bohemia, Czech Republic — [2]Institute of Physics of the Czech Academy of Sciences — [3]LMU Munich, Germany — [4]Lumileds Development Center, Aachen, Germany

Electronic structure of a series of ordered and disordered $\beta\text{-Si}_{6-z}\text{Al}_z\text{O}_z\text{N}_{8-z}$ systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the spr-kkr code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping $\beta\text{-Si}_3\text{N}_4$ with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in $\beta\text{-Si}_{6-z}\text{Al}_z\text{O}_z\text{N}_{8-z}$ is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.

O 96.2 Thu 10:30 P

A Bethe-Salpeter equation and a GW approach with electron-phonon coupling: from exciton binding energies to charge mobilities. — •Paolo Umari — University of Padova, Padova, Italy

e have introduced a simple scheme in order to account for the coupling with longitudinal phonons within the first-principles Bethe-Salpeter approach based on many-body perturbation theory. This allows to evaluate the reduction of exciton binding energies observed in polar semiconductors. The electron-phonon coupling is modelled from the macroscopic dielectric response in the infrared which, in turn, is calculated through density functional perturbation theory. In this way, the additional computational cost determined by our method is negligible. I will first illustrate our approach in the case of bulk ZnS and show how the excitonic series of bulk Cu2O is well reproduced[1]. The method could clarify the role of dielectric screening in hybrid perovskites yielding exciton binding energies in agreement with experiment[2]. Finally, I will discuss the extension of our method to GW calculations and I will show how the renormalisation of band-gaps and effective masses, and electron and hole mobilities can be easily calculated. Results for the hybrid perovskite MAPbI3 are in agreement with the most accurate calculations which include explicitly the coupling with phonons.

[1]L. Adamska and P. Umari, Phys. Rev B accepted (2021) [2]P. Umari, E. Mosconi, F. De Angelis, J. Phys. Chem. Lett. 9, 620 (2018).

O 96.3 Thu 10:30 P

Sticking coefficient for atoms scattering off metallic surfaces — •Celso Ricardo Caldeira Rego — Institute of Nanotechnology KIT

Achieving a complete understanding of the quantum dynamical processes arising when an atom approaches a metallic surface remains a challenge in surface physics. Conventional approaches based on the Born-Oppenheimer approximation become inapplicable when some charge is transferred between the surface and the adatom, and the resulting image-charge potential accelerates the particle towards the surface. Here, we solve the time-dependent Schrödinger equation to compute the electronic contribution to the sticking coefficient for a generalized version of the Anderson-Newns Hamiltonian and obtain adsorption probabilities as large as 15%. Numerical simulations demonstrate that the creation of low-energy electron-hole pairs is an efficient dissipation mechanism that may absorb kinetic energy from the incident particle to cause adsorption. The recently proposed exact-factorization formalism affords a physical interpretation of the results.

O 96.4 Thu 10:30 P

The electron-phonon scenario of superconductivity of LiBi — •Sylwia Gutowska[1], Bartłomiej Wiendlocha[1], Karolina Górnicka[2], Michał Winiarski[2], Weiwei Xie[3], Robert J. Cava[4], and Tomasz Klimczuk[2] — [1]AGH University of Science and Technology in Krakow, Poland — [2]Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ul. Narutowicza 11/12, 80-233 Gdańsk, Poland — [3]Department of Chemistry, Louisiana State University, Baton Rouge Louisiana 70803, United States — [4]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, United States

The electron-phonon interaction scenario of superconductivity is investigated in case of LiBi, which is a compound made of the lightest and the heaviest elemental metal and which hosts the tetragonal structure with squared sublattices of Bi, unusual for Bi-based compounds, that prefer the hexagonal type of sublattices due to the 3 valence electrons of 6p nature of bismuth. Such a simple structure is a perfect candidate for an investigation in details of the influence of the electronic as well as the phonon structure on the electron-phonon interaction and the superconductivity. After that, we compare the results in terms of electron-phonon coefficient and critical temperature to the experimental values. We also study the isotope effect and the influence of external pressure on the structure and superconductivity of this compound.

O 96.5 Thu 10:30 P

Energy gap closure of crystalline molecular hydrogen with pressure — •Vitaly Gorelov[1], Markus Holzmann[2,3], David M. Ceperley[4], and Carlo Pierleoni[1,5] — [1]Université Paris-Saclay, UVSQ, CNRS, CEA, Maison de la Simulation, Gif-sur-Yvette, France — [2]Univ. Grenoble Alpes, CNRS, LPMMC, Grenoble, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Physics, University of Illinois Urbana-Champaign, USA — [5]Department of Physical and Chemical Sciences, University of L*Aquila, L*Aquila, Italy

We study the gap closure with pressure in Phases III and IV of molecular crystalline hydrogen. Nuclear quantum and thermal effects are considered from first principles with Coupled Electron Ion Monte Carlo. The fundamental electronic gaps are obtained from grand-canonical Quantum Monte Carlo methods properly extended to quantum crystals. Nuclear zero point effects cause a large reduction in the gap (~2eV). As a consequence the fundamental gap closes at 530GPa for ideal crystals while at 360GPa for quantum crystals. Since the direct gap remains open until * 450GPa, the emerging scenario is that upon increasing pressure in phase III (C2/c-24 crystal symmetry) the fundamental (indirect) gap closes and the system enters into a bad metal phase where the density of states at the Fermi level increases with pres- sure up to ~450GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen.

O 96.6 Thu 10:30 P

gauge-covariant derivatives of the Berry curvature and orbital moment by Wannier interpolation — •Xiaoxiong Liu[1], Miguel Ángel Herrera[2], Stepan Tsirkin[1], and Ivo Souza[2] — [1]Department of Physics, University of Zurich — [2]Centro de Física de Materiales, Universidad del País Vasco

The momentum-space derivatives of the Berry curvature Ω and intrinsic orbital magnetic moment m of the Bloch states arise in multiple problems, such as the nonlinear anomalous Hall effect [1] and magneto-transport within the Boltzmann-equation formalism [2]. To study them from first principles, we developed a Wannier interpolation scheme for evaluating "generalized derivatives" of the non-Abelian Ω and m matrices for a group of bands of interest.

The generalized derivative does not involve couplings within the group, and preserves the gauge covariance of the Ω and m matrices. This formulation leads to robust *Fermi-sea* formulas for the Berry curvature dipole [1] and kinetic magnetoelectric effect tensor [2], which converge much faster with the density of the integration k-grid than the *Fermi-surface* formulas implemented earlier [3] in the Wannier90 code. The implementation is done in our newly-developed code WannierBerri [4]. We demonstrate the method with ab initio calculations on real materials, as well as tight-binding toy models.

[1] Sodemann et al, PRL 115 (2015): 216806.
[2] Zhong et al, PRL 116 (2016): 077201.
[3] Tsirkin et al, PRB 97 (2018): 035158.
[4] wannier-berri.org

O 96.7 Thu 10:30 P

Soft-mode enhanced type-I superconductivity in LiPd_2Ge — •Gabriel Kuderowicz[1], Karolina Górnicka[2], Elizabeth M. Carnicom[3], Kamil Kutorasiński[1], Tomasz Klimczuk[2], Robert J. Cava[3], and Bartłomiej Wiendlocha[1] — [1]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Aleja Mickiewicza 30, 30-059 Kraków, Poland — [2]Faculty of Applied Physics and Mathematics and Advanced Materials Centre, Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

Recently synthesized intermetallic compound LiPd_2Ge exhibits superconductivity below T_c=1.96 K. It belongs to the Heusler family which consist of more than 1000 compounds with various kinds of physical properties. Following the discovery of LiPd_2Ge we synthesized isostructural and isoelectronic LiPd_2Si and LiPd_2Sn. In this work we present DFT calculations of electronic structure, phonons and electron-phonon coupling. All three compounds have strong softening of the first acoustic mode. LiPd_2Ge has mostly pronounced softening and the highest value of the electron-phonon coupling constant $\lambda = (0.53 - 0.56)$ and highest T_c. Therefore, we suggest the correlation between superconductivity and the soft mode. We were looking for sources of phonon instabilities and observed deviations from harmonic potential.

O 97: Poster Session VII: Poster to Mini-Symposium: Molecular scale investigations of liquid-vapor interfaces II

Time: Thursday 10:30–12:30 Location: P

O 97.1 Thu 10:30 P

Interfacial Water Ordering Is Insufficient to Explain Ice-Nucleating Protein Activity — •Max Lukas[1], Ralph Schwidetzky[1], Anna T. Kunert[2], Ellen H.G. Backus[1,3], Ulrich Pöschl[2], Janine Fröhlich-Nowoisky[2], Mischa Bonn[1], and Konrad Meister[1,4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Max Planck Institute for Chemistry, Mainz, Germany — [3]University of Vienna, Vienna, Austria — [4]University of Alaska Southeast, Juneau, United States

Bacterial ice nucleation proteins (INPs) are the known to be the most efficient ice nucleators known. Here we study the solution structure of INPs from Pseudomonas syringae and find that there is no significant conformational change upon cooling. In contrast, upon heating on temperature exceeding ~55 °C the structure changes irreversibly, accompanied by a complete loss of ice nucleation activity. Structural ordering of interfacial water as it is observed by nonlinear sum-frequency generation (SFG) spectroscopy upon cooling is similar for active and heat-inactivated protein solutions. Our results demonstrate that the INPs' outstanding ice nucleation efficiency can not sufficiently be explained with increased water ordering at low temperatures and that the intact 3D protein structure is crucial for the underlying mechanism - taken altogether pointing to the importance of supramolecular interactions.

O 97.2 Thu 10:30 P

Photon impact induced luminescence spectroscopy of a liquid microjet — •Dana Bloss[1], Andreas Hans[1], Christian Ozga[1], Philipp Schmidt[1], Xaver Holzapfel[1], Arno Ehresmann[1], Petr Slavícek[2], Bernd Winter[3], and André Knie[1] — [1]Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Department of Physical Chemistry, University of Chemistry and Technology Prague, Technicka 5, 16628 Prague, Czech Republic — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Methods for Material Development, Albert-Einstein- Straße 15, 12489 Berlin, Germany

Liquids and especially liquid water have been subject to intense research for a long time due to their role in many chemical and biological systems. However, the investigation of liquid targets with fundamental methods of atomic and molecular physics, such as soft X-ray induced fluorescence spectroscopy, were a big challenge due to the required vacuum conditions. With the development of the liquid microjet technique the investigation of pure liquids or solutions after irradiation with synchrotron radiation became possible, which allows the exploration of the electronic structure of such complex systems. Here we present our results of dispersed luminescence from liquid water and demonstrate the possibilities of this detection method using this prototype system. One of the observed emission could be assigned to gas phase excited by Auger electrons escaping the liquid-vapor interface.

O 97.3 Thu 10:30 P

Structure of Aqueous Solutions via X-ray spectroscopies based on non-local Auger processes — •Eva Muchova and Petr Slavíček — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

Novel Auger-type X-ray spectroscopies are bringing new insights in the structure and electronic properties of aqueous solutions. It allows studying the chemical environment in solutions, e.g. the mutual effects of ions and solvent on each other, as well as ultrafast processes following ionization. The spectroscopy is also depth-sensitive and can reveal structural changes in interfaces. Sensitivity to ion pairing is achieved mainly by analysis of secondary electron spectroscopies, especially when newly identified non-local electron decay processes. The experiments, however, require a complex theoretical interpretation. In the contribution, we can show for a series of Na+, Mg2+ and Al3+ ions how the non-local Auger spectroscopy (mainly intermolecular Coulomb decay process, ICD) can provide details of speciation, e.g. show different type of interaction between ions and between ions and solvent. We can further discuss recent development of theoretical toolkit for non-local processes which we combine with multiscale methods like QM/MM or QM:QM in order to realistically model the environment.

O 97.4 Thu 10:30 P

Kinetics of Nano-Droplet Halide Emission from Salty Interfaces — •Philip Loche[1], Douwe J. Bonthuis[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

Ozone is one of many atmospheric trace gases whose presence is crucial for sustaining life on earth. Most of the ozone is located in the stratosphere (12 km - 55 km) where it absorbs short-wave radiation from the Sun and thus protects living organisms from potentially fatal genetic damage. Ozone depletion especially in the arctic can lead to temperature changes and influence the Southern Hemisphere mid-latitude circulation. The ozone concentration in the lower atmos-phere is correlated with the halide concentration which is emitted from seawater.

Here, we use molecular simulations to study the kinetics of Cl- by the evaporation from the air-water interface. We show that the emission of ions is a 2-state process. First hydrated ions are emitted, forming water fingers with the surface up to a distance of ~2 nm from the Gibbs dividing surface. If ions overcome this distance, they lose their hydration shell after ~20 nanoseconds and distances of several μm. From the determined reaction rate coefficient of evaporation we obtain the total flux of chloride ions per year from the earth's ocean and estimate that it would take roughly 90 years until the current chloride concentration in the lower atmosphere is reached.

O 98: Annual Meeting of the Surface Science Division

Time: Thursday 13:00–13:30 Location: R1

Topics: Report of the Chairman; Elections; Miscellaneous

O 99: Gerhard Ertl Young Investigator Award: Finalists session

Time: Thursday 13:30–15:30 Location: R1

O 99.1 Thu 13:30 R1

Magnetic resonance imaging in a scanning tunneling microscope — •Philip Willke[1,2,3,4], Aparajita Singha[2,3], Xue Zhang[2,3], Kai Yang[4], Yujeong Bae[2,3,4], Taner Esat[2,3], Christopher Lutz[4], Andreas Heinrich[2,3], and Taeyoung Choi[2,3] — [1]Karlsruhe Institute of Technology, Physikalisches Institute, Karlsruhe, Germany — [2]IBS Center for Quantum Nanoscience, Seoul, Republic of Korea — [3]Ewha Womans University, Seoul, Republic of Korea — [4]IBM Almaden Research Center, San Jose, USA

Combining electron spin resonance (ESR) with scanning tunneling microscopy (STM) allowed for spin resonance experiments on individual atoms on surfaces[1], for remote sensing of atomic spins[2] and for accessing the nuclear spin of single atoms in an STM[3]. In this talk, we focus on the interaction of the atomic spin system on the surface with the magnetic STM tip. We show that the tip field allows to tune the system into resonance similar to the external magnetic field, and can even fully replace the latter[4]. By utilizing this tip magnetic field, we establish magnetic resonance imaging of single atoms[5], exceeding the spatial resolution of other scanning field-gradient techniques by one to two orders of magnitude. We find that MRI scans of different atomic species and with different probe tips lead to unique resonance images revealing the magnetic interaction between tip and atom. [1] Baumann et al., Science, 350, 417-420 (2015). [2] Choi et al., Nat. Nano 12, 420-424(2017). [3] Willke et al., Science 362, 336-339 (2018) [4] Willke, Singha, Zhang et al., Nano Lett. 19, 8201-8206 (2019) [5] Willke et al. Nat. Phys. 15, 1005-1010 (2019).

O 99.2 Thu 14:00 R1

Ab-initio studies of exciton g factors: Monolayer transition metal dichalcogenides in magnetic fields — •Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

The effect of a magnetic field on the optical absorption in semiconductors has been measured experimentally and modeled theoretically for various systems in previous decades. We present a new first-principles approach [1] to systemat-

ically determine the response of excitons to magnetic fields, i.e. exciton g factors. By utilizing the GW-Bethe-Salpeter equation methodology we show that g factors extracted from the Zeeman shift of electronic bands are strongly renormalized by many-body effects which we trace back to the extent of the excitons in reciprocal space. We apply our approach to monolayers of transition metal dichalcogenides (MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2) with strongly bound excitons for which g factors are weakened by about 30%.
[1] Phys. Rev. Lett. 124, 226402 (2020)

O 99.3 Thu 14:30 R1

Manipulating charge states of individual molecules on insulators — •Shadi Fatayer, Florian Albrecht, Nikolaj Moll, and Leo Gross — IBM Research - Zurich

The physicochemical properties of molecules adsorbed on surfaces are charge-state dependent. Insulating films serve as an ideal platform to study the physics and chemistry of charged molecules, because these films avoid charge leakage. However, investigating individual charged molecules on insulators is experimentally challenging. The atomic force microscope (AFM), operable on insulating substrates and capable of single-electron sensitivity and atomic resolution, is suitable to be used with insulators. Here, I will present how different aspects of charged molecules can be accessed with the AFM: (i) How using the AFM as a single-electron current meter allows for tunneling spectroscopy to be performed on insulators and electron-transfer properties probed, (ii) how molecules in excited states can be prepared, (iii) how reversible chemical reactions can be performed via charging molecules and (iv) the insights gained via resolving the atomic structure of individual molecules in different charge states.

O 99.4 Thu 15:00 R1

Probing surface electronic structure and reaction intermediates in situ — •Kelsey Stoerzinger — Oregon State University, Corvallis, Oregon USA — Pacific Northwest National Laboratory, Richland, Washington USA

Catalysts are important constituents in numerous energy conversion and storage processes. Rational design of catalysts with greater activity for higher efficiency devices requires an understanding of the material surface's electronic structure in situ, as well as the reaction intermediates involved.

Many surface science techniques, such as X-ray photoelectron spectroscopy (XPS), collect information from inherently surface-sensitive low-energy processes, requiring operation in ultrahigh vacuum. This constraint is lifted for ambient pressure XPS, which can probe the surface in equilibrium with the gas phase at pressures up to ~a few Torr, or with thin liquid layers using a higher incident photon energy. I will discuss the insights obtained with this technique regarding the electronic structure of well-defined epitaxial oxides in equilibrium with a gaseous atmosphere of small molecules (e.g. O2, H2O, CO2, CH3OH, NO), the adsorption of such species, and their subsequent transformation upon driving a desired reaction by heat, voltage, or additional reactant. Adsorption and reactivity can be manipulated by the oxide composition and electronic structure, crystallographic orientation, strain, and local environment in amorphous materials. This molecular-level understanding of interfacial interactions can guide the rational design of high-surface-area oxide catalysts for technical applications.

O 100: Mini-Symposium: Infrared nano-optics II

Time: Thursday 13:30–15:30 Location: R2

Paper discussion O 100.1 Thu 13:30 R2

Broad spectral tuning of ultra-low-loss polaritons in a van der Waals crystal by intercalation — •Pablo Alonso-González — University of Oviedo

Phonon polaritons (PhPs) -light coupled to lattice vibrations- hold great promises for an unprecedented control of the flow of energy at the nanoscale because of their strong field confinement and long propagation. Moreover, recent experiments in polar van der Waals (vdW) crystals such as h-BN and alfa-MoO3, have demonstrated PhPs with anisotropic propagation, and ultra-long lifetime in the picosecond range. However, a main drawback of these PhPs is the lack of tunability of the narrow and material-specific spectral range where they exist (the so-called Reststrahlen Band (RB)), which severely limits their implementation in nanophotonics technologies. Here, we demonstrate that intercalation allows for a broad spectral shift of RBs in a vdW crystal, and that the PhPs excited within them show ultralow losses (lifetime of 5 ps) similar to PhPs in the non-intercalated crystal (lifetime of 8 ps). As a difference to previous attempts, which fail in keeping the polaritonic activity of the intercalated compound, our results are possible by employing an intercalation method based on single crystal growth, that we carried out in the vdW semiconductor alfa-V2O5, thereby also adding a new member to the library of vdW materials supporting PhPs. We expect this intercalation method to be applied in other vdW materials, opening the door for the use of PhPs in broad spectral bands that eventually cover the whole mid-IR range, which seems to be elusive with currently known polaritonic materials.

Paper discussion with expert panel members

Prof. S. Law (U Delaware), Prof. M. Raschke (JILA, UC Boulder), Prof. Y. Abate (U Georgia) and Prof. L. Wehmeier (TU Dresden)

O 100.2 Thu 14:15 R2

Configure phonon polaritons in van der Waals materials — •Siyuan Dai — Auburn University, Auburn, United States

The manipulation of light at small scales is one of the ultimate goals for nanophotonics. For this purpose, polaritons * hybrid light-matter waves that propagate in a confined length scale * are typically involved. Recent results of polaritons in van der Waals materials reveal a series of advances, including atomic scale localization, dynamic tunability, relative low-loss and topologically protected states. These advances are attributed to the unique physical properties in reduced dimensions and the configurability through van der Waals structuring and stacking. In this talk, I will show new merits of phonon polaritons that can be obtained through van der Waals configuration. I will talk about the tunability implemented into phonon polaritons by van der Waals heterostructuring hexagonal boron nitride with graphene and vanadium dioxide, where the polaritons can be tuned dynamically and reversibly via electrostatic gating and temperature control. I will also talk about the geometry and topology configuration of phonon polariton wavefront by twisting stacked slabs of molybdenum trioxide.

O 100.3 Thu 14:30 R2

Charge-transfer plasmon polaritons at graphene/α-RuCl3 interfaces — •Daniel J. Rizzo[1], B.S. Jessen[1], Z. Sun[1], F.L. Ruta[1], J. Zhang[2], J.-Q. Yan[3,4], L. Xian[2], A.S. McLeod[1], M.E. Berkowitz[1], K. Watanabe[5], T. Tanaguchi[5], S.E. Nagler[4], D.G. Mandrus[3,4], A. Rubio[2], M.M. Fogler[6], A.J. Millis[1], J.C. Hone[1], C.R. Dean[1], and D.N. Basov[1] — [1]Columbia University, New York, NY — [2]Max Planck Institute, Hamburg, German — [3]Univ. of Tennessee, Knoxville, TN — [4]Oak Ridge National Laboratory, Oak Ridge, TN — [5]NIMS, Japan — [6]UCSD, San Diego, CA

Charge transfer at the interface of two atomically-thin layers with different work functions offers a means of tuning 2D charge densities without the inherent limitations of traditional electrostatic gates that possess thick gate insulators. Specifically, the large work function of the Mott insulator α-RuCl3 (6.1 eV) makes it an ideal 2D electron acceptor.

In our study, we exploit this behavior to generate charge-transfer plasmon polaritons (CPPs) in graphene/α-RuCl3 heterostructures. Using near-field optical microscopy we measure the CPP dispersion, yielding a quantitative measure of the graphene Fermi energy (~0.6 eV) and thus the charge exchanged between α-RuCl3 and graphene (~2.7x10^13 cm-2). Concurrently, we observe dispersive edge modes and internal circular CPPs which reveal abrupt (<50 nm) changes in the graphene optical conductivity and charge density. Analysis of the CPP losses implies the presence of emergent optical conductivity in the doped interfacial layer of α-RuCl3. These results have broad implications for the study of highly-doped 2D materials.

Paper discussion O 100.4 Thu 14:45 R2

Nanocavities and polaritons in twisted and indirectly nanostructured 2D materials — •Frank Koppens — ICFO - The Institute of Photonics Sciences

Two-dimensional (2D) materials offer extraordinary potential for control of light and light-matter interactions at the atomic scale. In particular, twisted 2D materials has recently attracted a lot of interest due to the capability to induce moiré superlattices and discovery of electronic correlated phases. In this talk, we present nanoscale optical techniques such as near-field optical microscopy and photocurrent nanoscopy, and reveal with nanometer spatial resolution unique observations of the optical properties of twisted 2D materials. We report on the topological domain wall boundaries [1] of small-angle twisted graphene and interband collective modes in charge neutral twisted-bilayer graphene near the magic angle [2]. The freedom to engineer these so-called optical and electronic quantum metamaterials is expected to expose a myriad of unexpected phenomena.

We will also show record-small nanoscale polaritonic cavities [3,4], where the resonances are not associated to the eigenmodes of the cavity. Rather, they are multi-modal excitations whose reflection is greatly enhanced due to the interference of constituent modes. We demonstrate mid-IR cavities with volumes more than a billion below the free-space mode volume, while maintaining quality factors above 100.

[1] Hesp et al., Arxiv 1910.07893;
[2] Hesp et al., Arxiv 2011.05060;
[3] Epstein et al., Science (2020);
[4] Herzig Sheinfux et al., in preparation

Paper discussion with expert panel members
Prof. J.D. Caldwell (Vanderbilt U), Prof. J. Khurgin (Johns Hopkins U), Prof. S. De Liberato (U South Hampton) and Prof. M. Liu (Stony Brook U)

O 101: Poster Session VIII: Oxides and insulators: Adsorption and reaction of small molecules II

Time: Thursday 13:30–15:30 Location: P

O 101.1 Thu 13:30 P

Probing structural changes upon carbon monoxide coordination to single metal adatoms — •Paul T. P. Ryan[1,2,3], Matthias Meier[3,4], Zedenek Jakub[3], Jan Balajka[4], Jan Hulva[3], David J. Payne[2], Tien-Lin Lee[1], Cesare Franchini[4], Francesco Allegretti[5], Gareth S. Parkinson[3], and David A. Duncan[1] — [1]Diamond Light Source, Didcot, OX11 0QX UK — [2]Department of Materials, Imperial College London, SW7 2AZ UK — [3]Institute of Applied Physics, TU Wien, Austria — [4]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Austria — [5]Physics Department E20, Technical University of Munich, 85748 Garching, Germany

The application of highly accurate, but yet computationally cheap, density functional theory (DFT) calculations allows for the fine tuning of catalyst development. However, it is necessary to have stringent benchmarks against which these calculations are tested. In this work, the adsorption height of Ag adatoms on the $Fe_3O_4(001)$ surface after exposure to CO was determined using normal incidence X-ray standing waves. CO coordinated Ag adatoms (Ag^{CO}) were found to be pulled out of the surface to an adsorption height of 1.15 ± 0.08 Å, compared to the previously measured height of 0.96 ± 0.03 Å for bare Ag adatoms[1]. Utilising DFT+vdW+U calculations with the substrate unit cell dimension fixed to the experimental value, the predicted adsorption height for Ag^{CO} was 1.16 Å, in remarkably good agreement with the experimental results. [1] M. Meier et. al., Nanoscale 10, 2226 (2018)

O 101.2 Thu 13:30 P

Polarons in single atom catalysts: case study of Me_1=[Au_1,Pt_1,Rh_1] on TiO_2(110) — •Panukorn Sombut[1], Lena Haager[1], Marlene Atzmueller[1], Zdenek Jakub[1], Michele Reticcioli[2], Matthias Meier[1,2], Gareth S. Parkinson[1], and Cesare Franchini[2,3] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]University of Vienna, Vienna, Austria — [3]Universitá di Bologna, Bologna, Italy

Identification of the exact local environment of a single-atom catalyst (SAC) on metal oxide surfaces is crucial for understanding the reactivity as well as the catalytic properties of such systems. On $TiO_2(110)$, the stability and reactivity of adsorbed adatoms is further complicated by the presence of Oxygen vacancies and associated polaron charge, as both can affect the energetic, electronic configuration and local geometry of adsorbed adatoms. In this work the adsorption of group 9 to 11 transition metal adatoms (Rh, Pt and Au) are computationally studied by means of density functional theory (DFT, plus on-site Hubbard U), and compared with results obtained by experimental surface techniques such as scanning tunneling microscopy (STM), for Rh_1, and with available literature (Au_1 and Pt_1). Despite the many works on this subject, it is still unclear why Au and Pt are experimentally observed to adsorb in the O vacancy, contrary to Rh. By investigating the most stable adsorption site, oxidation state and the intermingled interaction among adatoms, O vacancies and polarons our data attempt to decipher the physical and chemical origin of the observed trend and to provide a conclusive interpretation of the puzzling observation.

O 101.3 Thu 13:30 P

Direct assessment of the acidity of individual surface hydroxyls on In_2O_3(111) — •Margareta Wagner[1,2], Bernd Meyer[3], Martin Setvin[1,4], Michael Schmid[1], and Ulrike Diebold[1] — [1]TU Wien, Vienna, Austria — [2]CEITEC BUT, Brno, Czech Republic — [3]FAU Erlangen-Nürnberg, Erlangen, Germany — [4]Charles University, Prague, Czech Republic

Non-contact atomic force microscopy is a versatile tool to investigate properties of individual atoms or molecules. Here we report a novel approach to determine the acidity of individual surface hydroxyls, which is directly linked to the proton affinity (PA) of the involved O atoms. The PA – the tendency to gain or lose a proton – is crucial *e.g.* in acid-base catalysis and the electro- and photocatalytic splitting of water.

The testcase of this study is the stoichiometric $In_2O_3(111)$ surface, which has four inequivalent surface O atoms $O_s(\alpha\text{-}\delta)$. Water dissociation leads to a pair of OH groups: the surface $O_SH(\beta)$ and the water O_WH. The remaining surface O atoms $O(\alpha,\ \gamma,\ \delta)$ can be protonated via manipulation with the tip. We probe the strength of their H bond with a functionalized tip of a nc-AFM via $F(z)$-spectroscopy and find quantitative agreement with density-functional theory (DFT) calculations. By relating the results to known PAs of gas-phase molecules, we can calibrate our data and determine the PA of different surface sites of $In_2O_3(111)$ with atomic precision. Measurements on hydroxylated TiO_2 and zirconia extend our method to other oxides. The trends of the site-specific PA values agree well with the expectations based on area-averaging techniques.

O 101.4 Thu 13:30 P

Signatures of oxygen vacancies in O1s core level shifts — Alvaro Posada-Borbon, Noemi Bosio, and •Henrik Grönbeck — Chalmers University of Technology, Gothenburg, Sweden

Density functional theory calculations are used to investigate O1s surface core level shifts for MgO(100), ZnO(10-10), In2O3(111) and CeO2(111). Shifts are calculated for the pristine surfaces together with surfaces containing oxygen vacancies and dissociated H2 and H2O. Pristine surfaces show small negative shifts with respect to the bulk components and oxygen vacancies are found to have minor effects on the O1s binding energies of neighboring oxygen atoms. OH-groups formed by H2 or H2O dissociation yield binding energies shifted to higher energies as compared to the oxygen atoms in the bulk. The results exemplify the difficulties in assigning core-level shifts and suggest that assignments of shifts in O1s binding energies to neighboring oxygen vacancies for the explored oxides should be reconsidered.

O 101.5 Thu 13:30 P

Thermal stability and CO-induced mobility of single Pt adatoms supported on the $\alpha - Fe_2O_3(1\bar{1}02)$ surface — •Ali Rafsanjani-Abbasi[1], Florian Kraushofer[1], Moritz Eder[2], Jiri Pavelec[1], Lena Haager[1], Giada Franceschi[1], Michele Riva[1], Michael Schmid[1], Ulrike Diebold[1], and Gareth S. Parkinson[1] — [1]Institute of Applied Physics, TU Wien, Wiedner Hauptstraße 8-10/E134, 1040 Wien, Austria — [2]Chair of Physical Chemistry, TU München, Lichtenbergstraße 4, 85748 Garching, Germany

Pt-based catalysts are the most efficient catalysts for the hydrogen evolution reaction and are also widely used for photocatalytic and CO-oxidation reactions. However, the high cost of Pt and its susceptibility to carbon monoxide poisoning are two drawbacks on its role as a catalyst. Downsizing catalyst clusters to single atoms is an effective way to reach maximum efficiency, and so-called *"Single-Atom Catalysis"* is now an important field of research [1]. Nevertheless, stabilization of single Pt atoms on a support without compromising catalytic activity is still a key challenge.

Here, we present a study of the thermal stability and CO-induced mobility of single Pt atoms on the $\alpha - Fe_2O_3(1\bar{1}02)$ surface, at elevated temperatures and in a CO-containing environment. Thermally-induced and CO-induced sintering of the Pt single atoms are traced by means of STM and XPS. In addition, in time-lapse series the mobility and rearrangement of single Pt adatoms have been determined with varying carbon monoxide pressure in the background.

1. G. S. Parkinson, Catal. Lett. 149, 1137 (2019).

O 101.6 Thu 13:30 P

Momentum for Catalysis: How Surface Reactions Shape the RuO_2 Flat Surface State — Vedran Jovic[1,2], Armando Consiglio[3], Kevin E. Smith[4], Chris Jozwiak[1], Aaron Bostwick[1], Eli Rotenberg[1], Domenico Di Sante[3], and •Simon Moser[1,3] — [1]Advanced Light Source, USA — [2]GNS Science, New Zealand — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [4]Boston University, USA

The active (110) surface of the benchmark oxygen evolution catalyst RuO_2 spans a flat-band surface state (FBSS) between the surface projections of its Dirac nodal lines (DNL) that define the electronic properties of this functional semimetal. Monitoring well known surface adsorption processes of H_2, O_2, NO and CO by in-operando angle resolved photoemission spectroscopy, we selectively modify the oxidation state of individual Ru surface sites and identify the electronic nature of the FBSS: Stabilized by bridging oxygen O_{br} p_z, the FBSS disperses along <001> oriented chains of bridging Rubr $4d_{z2}$ orbitals, collapses upon O_{br} removal, yet, remains surprisingly unaffected by the oxidation state of the undercoordinated 1f-cus-Ru species. This directly reflects in the ability of RuO_2 (110) to oxidize CO and H_2 along with its inability to oxidize NO, demonstrating the FBSS's active role in catalytic charge transfer processes at the oxygen bridge sites. Our synergetic approach provides momentum resolved insights to the interplay of a catalyst's delocalized electronic band structure and the localized orbitals of its surface reactants - a route towards a microscopic understanding of heterogeneous catalysis.

O 101.7 Thu 13:30 P

Selective electrochemical reduction oxalic acid on anatase surfaces — •Gergely Juhasz — Tokyo Institute of Technology, Tokyo, Japan

Direct electrochemical reduction of carboxylic acids to alcohols is rare and has several potential applications such as raw material synthesis or energy storage. We studied the mechanism of the recently reported electrochemical reduction of oxalic acid on anatase nanoparticle surfaces. The questions we focused on were why the reduction occurs only on one of the carboxylic groups, what would be the necessary conditions to perform full 8 electron reduction, and why the reaction occurs only on anatase surfaces.

Calculations with DFTB methods revealed that the molecules can be reduced only on a carboxylic group that is not attached to the surface, and the other group works as an anchor and stays electrochemically inactive. This explains the preference for 4 electron reduction and the selectivity of the process. Further calculations showed that the majority of titanium-oxide surfaces prefer to bind both carboxylic groups of the oxalic acid, therefore they remain electrochemically inactive.

O 101.8 Thu 13:30 P

Surface reactivity to hydrogen of Ag- and Cu- modified CeO2 — •Stefania Benedetti[1], Avinash Vikatakavi[1,2], Giulia Righi[1,2], Paola Luches[1], Sergio D'Addato[1,2], Rita Magri[1,2], and Annabella Selloni[3] — [1]CNR, Istituto Nanoscienze, 41125 Modena, Italy — [2]Dipartimento di Fisica, Informatica e Matematica, Universita' di Modena e Reggio-Emilia, 41125 Modena, Italy — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08540, United States

In this work we investigate the H2 dissociation on Ag- and Cu- modified CeO2 surfaces to increase oxide activity for application in catalytic reactions in electrochemical devices to replace Pt. We have followed by XPS the Ag oxidation state, the concentration of Ce3+ ions, O vacancies, and OH- groups during thermal reduction cycles in H2 and in UHV of thin CeO2 films. As expected, the reactivity of ceria toward H2 dissociation improves when Ag is included. However, thermal treatment under H exposure decreases the concentration of Ce3+ ions in Ag-modified ceria with respect to pure oxide in the same conditions, while the number of surface O vacancies is larger for the Ag-modified surface [1]. Thanks to DFT calculations, we explain this behavior in terms of a reduction of the surface Ag, which acquires some of the extra electrons created by the O vacancies and the adsorbed H atoms. Results are compared to films with substitutional Cu atoms. In this case Ce3+ concentration increases by a factor of 2 compared to pure oxide and activation temperature decreases to 570 K. [1] S. Benedetti et al., ACS Applied Materials & Interfaces, 2020, 12, 24, 27682-27690

O 102: Poster Session VIII: Organic molecules on inorganic substrates: electronic, optical and other properties IV

Time: Thursday 13:30–15:30 Location: P

O 102.1 Thu 13:30 P

Measuring the Change in Reactivity of a Single Molecule — •Jack Henry, Phil Blowey, and Adam Sweetman — University Of Leeds, Leeds, United Kingdom

Decades of surface science studies on adsorbed molecules have shown the surface a molecule is adsorbed on can effect the molecules electronic and geometric structure [1-3]. In this work, the influence of molecule-substrate bonding on the interactions experienced by a scanning probe microscope (SPM) tip were investigated.

A system comprised of C_{60} molecules adsorbed on the Cu(111) surface was studied using simultaneous non-contact atomic force microscopy (NC-AFM) and scanning tunnelling microscopy (STM). This system is ideal for invesitgating the effect molecule-substrate bonding has on the physico-chemical properties of a molecule as the C_{60}- Cu(111) interface can be controlled to form two distinct structures [4-6]. The physico-chemical properties of the C_{60} molecules were investigated using NC-AFM spectroscopy. A comparison was made by looking at the force minima in collected spectra, along with the corresponding junction conductance. Complementary ab initio simulations of the spectra were performed in density functional theory (DFT) to gain a deeper understanding of the experimental results.

[1] L. Gross et al. Science 325, 110 (2009); [2] J. Repp et al. PRL 94, 026803 (2005); [3] F Mohn et al. University Of Regensburg (2012); [4] W. Wu Pa et al. PRL 104, 036103 (2010); [5] J. A. Larsson et al. PRB 77, 115434 (2008); [6] J. Brand et al. Nano.Lett. 19, 7845-7851 (2019);

O 102.2 Thu 13:30 P

Identifying the Origin of Local Flexibility in a Carbohydrate Polymer — •Kelvin Anggara[1], Yuntao Zhu[2], Giulio Fittolani[2,4], Yang Yu[2], Theodore Tyrikos-Ergas[2,4], Martina Delbianco[2], Stephan Rauschenbach[1,3], Sabine Abb[1], Peter Seeberger[2,4], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research — [2]Max Planck Institute for Colloids and Interfaces — [3]University of Oxford — [4]Freie Universität Berlin — [5]École Polytechnique Fédérale de Lausanne

Correlating structures and properties of a polymer to its monomer sequence is key to understand how its higher hierarchy structures are formed and how its macroscopic material properties emerge. Carbohydrate polymers, such as cellulose and chitin, are the most abundant materials found in nature whose structures and properties have only been characterized at sub-micrometer level. Here, by imaging single cellulose chains at nanoscale, we determine the structure and local flexibility of cellulose as a function of its sequence (primary structure) and conformation (secondary structure). Changing the primary structure by chemical substitutions and geometrical variations in the secondary structure allow the chain flexibility to be engineered at the single linkage level. Tuning local flexibility opens opportunities for the bottom-up design of carbohydrate materials.

O 102.3 Thu 13:30 P

CoTPP molecules deposited on passivated Fe-(100)-p(1x1)O: a photoemission tomography study — •David Janas[1], Henning Sturmeit[1], Iulia Cojocariu[2], Vitaliy Feyer[2], Stefano Ponzoni[1], Giovanni Zamborlini[1], and Mirko Cinchetti[1] — [1]Experimentelle Physik VI, TU Dortmund, Otto-Hahn-Straße 2, 44227 Dortmund, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Leo-Brandt-Straße, 52425 Jülich, Germany

In order to enhance the performances of organic spintronic devices, a detailed knowledge of the physical properties at the interface is crucial [1]. In this context, photoemission tomography (PT), which combines ab-initio calculations and angle-resolved photoelectron spectroscopy (ARPES), stands out as a powerful tool to unravel the orbital structure of molecular thin films at metal/organic interfaces [2].

In our work we apply PT to investigate the interaction of paramagnetic molecules, namely CoTPP, on the passivated Fe-(100)-p(1x1)O surface. Recently, it was shown that the interactions at this interface lead to an emergent magnetic ordering of the molecular layer. Here, we use PT to further characterize this intriguing system. In particular, we precisely determine the energy level alignment at the interface, the nature of the frontier orbitals, and the azimuthal orientation of the CoTPP with respect to the substrate.

[1] Cinchetti, M., Dediu, V. & Hueso, L. Activating the molecular spinterface. Nature Mater 16, 507-515 (2017)

[2] Puschnig, P. et al. Reconstruction of molecular orbital densities from photoemission data. Science 326, 702-706 (2009)

O 102.4 Thu 13:30 P

Orientation Dependent Charge Transfer: Heptacene on Coinage Metals — •Andreas Windischbacher[1], Thomas Georg Boné[1], Marie Sophie Sättele[2], Holger F. Bettinger[2], Heiko Peisert[2], Thomas Chassé[2], Georg Koller[1], and Peter Puschnig[1] — [1]University of Graz, Graz, Austria — [2]University of Tübingen, Tübingen, Germany

Over the past decade, pi-conjugated, aromatic molecules have gained increased attention in material science as their electron donating or accepting nature can be exploited to tune the charge rearrangement in hybrid organic-inorganic systems. Major research efforts have been directed towards the description of effects related to this electron transfer between a surface and its adlayer, often focusing on the metal's workfunction and the adsorbate's electron affinity.

In our contribution, we want to demonstrate the decisive impact of the adsorbate orientation on the charge transfer properties of a molecule-metal interface. We utilize density functional calculations to simulate the adsorption of heptacene, seven linearly fused benzene rings, on coinage metal surfaces M(110), M=Ag, Cu. Considering various adsorption configurations and unit cells, we elucidate the electronic structures of our systems, observing an unusually strong dependence on the orientation of the molecule. Complementary photoemission experiment data confirm the theoretical predictions.

O 102.5 Thu 13:30 P

SF-IETS studies on CuCu4(shi)4 metallacrown complex — •Robert Ranecki[1], Stefan Lach[1], Angeliki Athanasopoulou[2], Eva Rentschler[2], and Christiane Ziegler[1] — [1]Dept. of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Inst. of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, Germany

Exchange coupled magnetic centers on surfaces are expected to provide an excellent platform for the development of spintronic technologies. For such structures, the detection of spin excitations by low-temperature scanning tunnelling spectroscopy has enabled investigations on coupling individual spins [2]. Up to now, however, only a few Spin-Flip Inelastic Tunneling Spectroscopy (SF-IETS) measurements have been performed on single molecules encapsulating several spin centers [1]. Here, we present Scanning Tunneling Spectroscopy (STS) studies on an electrospray deposited 12-MC-4 metallacrown pentacopper(II) nanomagnet. We observe symmetric around zero-bias features on differential conductance spectra, an evident hallmark of inelastic tunneling. We use third-order electron transport model [2], assuming exchange coupling constants determined by the broken symmetry approach [3], to describe the experimental spectra. The obtained results provide access to intramolecular coupling of spins in a single molecular system with competing superexchange interactions.

[1] S.Kahle, et al. Nano letters 12, 518-521 (2012).
[2] M.Ternes, et al. J. Phys. Condens. Matter 21 053001 (2009).
[3] Y.Pavlyukh et al. Phys. Rev. B 99 144418 (2019).

O 102.6 Thu 13:30 P

Time-resolved orbital imaging of the CuPc/TiSe$_2$ interface — •Kiana Baumgärtner[1], Markus Scholz[2], Christian Metzger[1], Dmytro Kutnyakhov[3], Nils Wind[4], Michael Heber[3], Lukas Wenthaus[3], Kai Rossnagel[3,5], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg, Germany — [2]European XFEL, Germany — [3]DESY, Hamburg, Germany — [4]Universität Hamburg, Germany — [5]Universität Kiel, Germany

In the last decade [1], the interpretation of the momentum distribution from static angle-resolved photoemission experiments has improved our understanding of charge transfer processes at the molecule-substrate interface [2] as well as the geometric alignment in these systems [3]. In this contribution I will present our experimental findings on time-resolved orbital imaging of the excited CuPc/TiSe$_2$ interface which were conducted at a HHG-laser facility with a momentum microscope. Previous studies on the transition-metal dichalcogenide TiSe$_2$ have shown exciting electronic behavior on the fs to ps time scale upon optical excitation [4]. With the introduction of CuPc as a charge donor new interaction channels arise at the interface and showcase the electronic as well as structural interplay at the interface. [1] P. Puschnig et al., Science 326, 702 (2009). [2] G. Zamborlini et al., Nat. Comm. 8, 335 (2017). [3] M. Grimm et al., Phys. Rev. B 98, 195412 (2018). [4] T. Rohwer et al., Nature 471, 490 (2011).

O 102.7 Thu 13:30 P

A multifunctional organic interface: decoupling the spin tuning from molecule-metal hybridization — •H. Sturmeit[1], I. Cojocariu[2], M. Jugovac[2], A. Windischbacher[3], P. Puschnig[3], C. Piamonteze[4], A. Sala[5,6], G. Comelli[5,6], A. Cossaro[5], A. Verdini[5], L. Floreano[5], M. Stredansky[5,6], E. Vesselli[5,6], C. Hohner[8], M. Kettner[8], J. Libuda[8], C. M. Schneider[2,7], G. Zamborlini[1], M. Cinchetti[1], and V. Feyer[2,7] — [1]TU Dortmund, Dortmund, Germany — [2]Forschungszentrum Jülich, Jülich, Germany — [3]Karl-Franzens-Universität, Graz, Austria — [4]Paul-Scherrer-Institute, Villigen, Switzerland — [5]Lab. TASC IOM-CNR, Trieste, Italy — [6]University of Trieste, Trieste, Italy — [7]Universität Duisburg-Essen, Duisburg, Germany — [8]Friedrich-Alexander-Universität, Erlangen, Germany

The possibility to separately address and control the spin and charge properties at a metal/organic interface could pave the way to a new generation of multifunctional devices. Here, by using a theoretical and experimental spectro-microscopy approach, we introduce a system with decoupled, and therefore independently tunable, spin and electronic properties. A single layer of nickel tetraphenyl porphyrin molecules strongly interacts with the copper (100) surface, causing a massive charge transfer and the uncommon Ni(I) oxidation state. We find that by dosing nitrogen dioxide (NO$_2$) the Ni(II) oxidation state of the gas phase molecule can be restored while the substrate-induced high-spin configuration is preserved.

O 102.8 Thu 13:30 P

SF-IETS studies on CuCu4(shi)4 metallacrown complex — •Robert Ranecki[1], Stefan Lach[1], Angeliki Athanasopoulou[2], Eva Rentschler[2], and Christiane Ziegler[1] — [1]Dept. of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Inst. of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, Germany

Exchange coupled magnetic centers on surfaces are expected to provide an excellent platform for the development of spintronic technologies. For such structures, the detection of spin excitations by Low-Temperature Scanning Tunnelling Spectroscopy (LT-STS) has enabled investigations on coupling individual spins [1]. Up to now, however, only a few Spin-Flip Inelastic Tunneling Spectroscopy (SF-IETS) measurements have been performed on single molecules encapsulating several spin centers [2]. Here, we present LT-STS studies on an electrospray deposited 12-MC-4 pentacopper(II) metallacrown system. We observe symmetric around zero-bias features on differential conductance spectra, an evident hallmark of inelastic tunneling. We use third-order electron transport model [1], assuming exchange coupling constants determined by the broken symmetry approach [3], to analyze our experimental data. The obtained results provide access to intramolecular coupling of spins in a single molecular system with competing superexchange interactions.

[1] M.Ternes, et al. J. Phys. Condens. Matter 21 053001 (2009).
[2] S.Kahle, et al. Nano letters 12, 518-521 (2012).
[3] Y.Pavlyukh et al. Phys. Rev. B 99 144418 (2019).

O 103: Poster Session VIII: Surface reactions II

Time: Thursday 13:30–15:30 Location: P

O 103.1 Thu 13:30 P

Enhancement of homochirality in on-surface designed indenofluorene polymers — •Cristina Martín Fuentes, Jose Ignacio Urgel, Jose Maria Gallego, Jose Santos, Rodolfo Miranda, Nazario Martín, and David Écija — IMDEA nanociencia, Cantoblanco 28049, Madrid, Spain

A crucial aspect in polymer science is to find out route to enhance homochirality when the monomer precursor is chiral or prochiral.

Inspired by our recent results regarding the homocoupling of acene species exploiting the =CBr^2 functional group and its reactivity on surfaces, we synthesized a prochiral precursor molecule presenting an indenofluorene backbone with two CBr$_2$ groups. Upon sublimation on surfaces the homocoupling reaction took place at room temperature. Three different substrates were employed: Au(111), Ag(111) and Ag(100), to elucidate the chemical role of the metal and of the substrate termination.

On all the surfaces, long polymers were found based on cumulene bridges. On Au(111) the polymers display racemic segments, a result of the random mixture the two molecular enantiomers. However, on Ag(100) and Ag(111), the polymers display more homochiral segments than the ones formed on Au(111) by a factor of 2. We can conclude that, depending on the substrate, it is possible to steer the homochirality of the designed molecular wires. Our results represent a step further towards a better control of the on-surface synthesis of homochiral polymers.

O 103.2 Thu 13:30 P

On-surface synthesis of doubly-linked one-dimensional pentacene ladder polymer — •Kalyan Biswas[1], José I. Urgel[1], Ana Sánchez-Grande[1], Shayan Edalatmanesh[2], José Santos[1], Borja Cirera[1], Pingo Mutombo[2], Koen Lauwaet[1], Rodolfo Miranda[1], Pavel Jelínek[2], Nazario Martín[1], and David Écija[1] — [1]IMDEA Nanoscience, 28049 Madrid, Spain — [2]Institute of Physics of the Czech Academy of Science, CZ-16253 Prague, Czech Republic

π-conjugated polymers have received great attention in basic and applied research fields as promising new materials for the fabrication of semiconducting devices due to their unique electronic properties. The traditional solution synthesis of such material has been extended to the new synthetic discipline of on-surface synthesis, being based on the reaction of molecular precursors on surfaces in ultra-high vacuum conditions. Here, we provide a synthetic protocol toward the on-surface synthesis of ethynylene-like doubly-connected pentacene polymers by sublimation of pentacene derivatives with =CBr$_2$ moieties and subsequent annealing on Au(111). The characterization of the polymers was performed by low-temperature scanning tunneling microscopy and non-contact atomic force microscopy, complemented with density functional theory calculations, revealing the formation of an unprecedented ethylene-like bridged pentacene ladder polymer. We envision that our study will be of general relevance for the synthesis and characterization of π-conjugated polymers opening new avenues with prospects for applications in molecular optoelectronics.

O 103.3 Thu 13:30 P

Formation of Polymeric Chains via On-Surface Coupling of Aldehydes — •Nan Cao[1], Maryam Ebrahimi[1,2], Alexander Riss[1], Eduardo Corral-Rascon[1], Aleksandr Baklanov[1], Willi Auwärter[1], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, D-85748 Garching, Germany — [2]Department of Chemistry, Lakehead University, P7B 5E1 Thunder Bay, Ontario, Canada

On-surface reactions provide new prospects for the formation of well-defined nanostructures stabilized by covalent bonds. Within the last decade, inspired by classic organic reactions, many pathways were demonstrated on single crystal surfaces under ultrahigh vacuum conditions. Precursors and products can be directly characterized by scanning probe techniques with atomic resolution in real space. Here, we report on a new coupling reaction using aromatic aldehyde species. The deposition of aldehyde precursors on Ag(111), followed by a post-annealing treatment, resulted in the formation of ordered polymeric chains. Scanning tunneling microscopy (STM) provides insights into the structural evolution before and after the coupling reaction. Our non-contact atomic force microscopy and high-resolution STM data illustrate the linkage of carbonyl groups in the periphery of the reactants. Based on these insights, and taking into account complementary X-ray photoelectron spectroscopy measurements and density functional theory calculations, we develop a coherent picture of the reaction pathway. Our findings introduce a new avenue for the on-surface synthesis of ordered covalent nanostructures.

O 103.4 Thu 13:30 P

Investigating the mechanism underlying an order-disorder transition for molecular assemblies of tetraphenylporphyrin (TPP) on Au(111) — •Matthew Edmondson[1], Eleanor Frampton[1,2], Chris J. Judd[1], Neil R. Champness[2], David A. Duncan[3], Robert Jones[2], and Alex Saywell[1] — [1]School of Physics & Astronomy, University of Nottingham — [2]School of Chemistry, University of Nottingham, Nottingham, UK — [3]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK

Porphyrins display a rich array of chemical and physical properties which can be tuned by incorporating a metal atom via solution-phase synthesis or on-surface protocols.[1] Self-metalation (uptake of metal atoms from a supporting substrate) has been observed for surface confined porphyrin species, such as for 2H-tetraphenylporphyrin (2H-TPP) on Cu(111),[2] and offers an alternate synthetic pathway for the formation of metalated TPP (M-TPP) which is driven by interaction with the substrate.

Here we report on the interaction between 2H-TPP and Au(111) and present details of an order-disorder transition of 2H-TPP assemblies. Chemical analysis via X-ray photoelectron spectroscopy (XPS) suggests the formation of an Au-TPP species as part of this process. Characterisation using a combination of scanning probe microscopy, XPS, and X-ray standing wave techniques provide both chemical and structural information on the evolution of this on-surface reaction.

[1] J. M. Gottfried, Surface Science Reports, 2015, 70, 259-379.
[2] K. Diller et al., Journal of Chemical Physics, 2012, 136, 14705.

O 103.5 Thu 13:30 P

Interfacial chemical bonding of protective (Ti,Al)N coatings grown on polycarbonate — •Lena Patterer, Soheil Karimi Aghda, Damian Mauritius Holzapfel, and Jochen Michael Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

Due to its superior mechanical properties as well as oxidation resistance, (Ti,Al)N coatings are commonly used as protective coatings for cutting and forming tools. However, less attention has been drawn so far to its application as protective coatings onto polymer components. To identify the chemical reactions and the corresponding bond formation at the (Ti,Al)N | polycarbonate interface, a detailed X-ray photoelectron spectroscopy analysis is performed on pulsed direct current magnetron sputtered (DCMS) (Ti,Al)N coatings deposited onto polycarbonate. To this end, the coating thickness was less than 2 nm to ensure that the chemical state information including the interfacial region is probed. By comparing to the chemical state information of the uncoated polycarbonate, the formation of CNx as well as of C-O-(Ti,Al) bonds is identified. Hence, it is reasonable to assume that these bonds serve as chemical link across the interface and firmly anchor the (Ti,Al)N coating on the polycarbonate substrate.

O 103.6 Thu 13:30 P

Production of oxidized C_{60} on carbonaceous substrates — •Georgios Pantazidis[1], Andrew Cassidy[1], John David Thrower[1], and Liv Hornekaer[1,2] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

In this poster, data characterising the production of C_{60} oxides on a graphitic surface, in conditions that mimic interstellar environments, are presented. Experiments were performed in an ultra-high vacuum chamber with a base pressure of 5×10^{-10} mbar. Thin films of C_{60} were prepared by *in situ* dosing on a highly oriented pyrolytic graphite (HOPG) substrate. Oxygen atoms were produced *via* thermal cracking through a hot capillary which is heated to *ca.* 1850 K. Surface science techniques like temperature programmed desorption (TPD), scanning tunnelling microscopy (STM) and X-ray photoelectron spectroscopy (XPS), were used for the experimental investigation. Findings suggest that $C_{60}O_x$ are formed, with oxygen atoms chemisorbing on the C_{60} molecule, forming ether and epoxide functional groups. Upon thermal annealing, the $C_{60}O_x$ fragment into C_yO_z and species like CO and CO_2, which lead to the formation of thermally stable remnants on top of the HOPG, creating a porous carbonaceous substrate (m-HOPG). When the $C_{60}O_x$ were produced on the m-HOPG substrate, the reactivity towards oxygen atoms was higher and, apart from ether and epoxide groups, carbonyl groups were also present, suggesting a more complex chemistry, aided by the porous substrate.

O 103.7 Thu 13:30 P

Highly selective synthesis of enetriyne via tetramerization of terminal alkynes on Ag(100) — Nan Cao[1], •Biao Yang[1], Jonas Björk[2], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, D-85748 Garching, Germany — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, 58183 Linköping (Sweden)

Enetriyne, a conjugated species of eneyne family, is a prominent constituent in the antibiotic and antitumor sector. On-surface synthesis under ultrahigh vacuum, which can be monitored by real space scanning probe microscopy and other techniques, has been widely used as a powerful tool to disentangle and control reaction pathways on well-defined interfaces. We herein report a novel approach of enetriyne formation with high selectivity via tetramerization of terminal alkynes on Ag(100). Taking advantage of a hydroxyl directing group, we managed to steer the reaction process and obtain a uniform product. Firstly, upon O2 exposure the adsorbed precursor's terminal alkyne moieties deprotonate, which entails the formation of organometallic dimer. Secondly, controlled annealing of the pretreated sample induces the formation of the tetrameric species, which self-assembles in regular islands stabilized by lateral weak interactions. We combine STM, XPS studies and DFT calculations to examine the newly formed covalent compounds and suggest a reaction mechanism. Our study provides a protocol, involving a directing group, gas-mediated pretreatment, and an excitation reaction to precisely fabricate a functional enetriyne species.

O 104: Poster Session VIII: Scanning probe techniques: Method development III

Time: Thursday 13:30–15:30 Location: P

O 104.1 Thu 13:30 P

Ultra-high vacuum millikelvin scanning tunnelling microscope with adiabatic demagnetisation refrigeration — •Taner Esat[1,2], Peter Coenen[1,2], Andrea Raccanelli[3,2], Vasily Cherepanov[1,2], Xiaosheng Yang[1,2], Peter Borgens[1,2], Stefan Tautz[1,2], and Ruslan Temirov[1,2,4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]Cryo-Lab, Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [4]II. Physikalisches Institut, Universität zu Köln, Germany

We describe the design of an ultra-high vacuum scanning tunnelling microscope that operates at millikelvin temperatures and high magnetic fields of up to 8 Tesla. Employing adiabatic demagnetisation refrigeration technique instead of the traditionally used 3He dilution refrigeration, we have built a very modular setup with outstandingly high stability, allowing STM experiments in very well controlled variable temperature conditions down to 26 millikelvin. To demonstrate the microscope's performance, we show the temperature-dependent scanning tunnelling spectroscopy data acquired on a superconducting Al(100) surface and discuss the factors determining the effective electronic temperature of the STM junction.

O 104.2 Thu 13:30 P

The Quantum Corral - Bond to an artificial atom — •Fabian Stilp[1], Andreas Bereczuk[2], Julian Berwanger[1], Nadine Mundigl[1], Klaus Richter[2], and Franz J. Giessibl[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

In 1993 Crommie, Lutz and Eigler first created a quantum corral, an adatom structure that confines surface state electrons on metal surfaces, and investigated discrete energy states inside the corral using scanning tunneling microscopy (STM) [1]. We revisit the same corral, a ring of 48 iron atoms on a Cu(111) surface with a diameter of 14.26 nm, with atomic force microscopy (AFM) to investigate the bonding of this artificial atom to the front atom of the AFM-tip. The measured forces on the order of 100 femtonewtons reveal a covalent attraction to metal tips and Pauli repulsion to CO terminated tips. This is familiar to the interactions of these tips with natural atoms, so one would also expect repulsive interaction for closer distances between the front atom of the metal tip and the quantum corral. It is not possible to measure this repulsive force, because the tip is not stable for closer tip-sample distances, but one can place the front atom of the metal tip inside the corral and investigate the change of the corral states with STM. The response of the states to this additional adatom indicates the expected repulsive force.

[1] Crommie et al. Science 262, 218 (1993)

O 104.3 Thu 13:30 P

Optimising conditions for high resolution SPM at room temperature — •Timothy Brown, Phil Blowey, and Adam Sweetman — University of Leeds, Leeds, UK

Non-contact atomic force microscopy has yielded enormous progress in the established field of scanning probe microscopy (SPM), with its ability to characterise materials at the atomic scale, and study chemical structures of individual molecules. Long acquisition times are typically required for system stability, which is often accomplished by operating at cryogenic temperatures. However if high resolution characterisation of species at room temperature is required, thermal non-equilibrium between the tip and sample poses a limit on acquisition time. Atom tracking can counteract the effects of thermal drift between the tip and sample. Measuring the displacement, and subsequent compensation thereof, using a feedforward correction, can be used as a means to correct the drift, a technique pioneered by Abe. et. al (2007). The net drift is liable to change continuously due to the surroundings, thus diminishing the accuracy of the applied correction. We describe a protocol, similar to that of Rahe. et. al (2011), by which the temperature in a ultra-high vacuum scanning tunnelling / atomic force microscope is stabilised at room level using a tuned feedback circuit, such that atom tracking, can be continuously used in order to take scripted, dense 3D data sets, even at room temperature.

References:

1. Abe, M. et al. Applied Physics Letters. 90, 203103 (2007).
2. Rahe, P. et al. Review of Scientific Instruments 82, 063704 (2011).

O 104.4 Thu 13:30 P

Single Atom Electron Spin Resonance Spectroscopy at High Magnetic Fields — •Piotr Kot, Robert Drost, Maximilian Uhl, and Christian Ast — Max Planck Institute for Solid State Research, Stuttgart, DE

In the last several years electron spin resonance spectroscopy (ESR) and scanning tunneling microscopy (STM) have been combined, introducing a new technique for studying spin dynamics on the atomic scale. Here, we present a next-generation ESR-STM with operating frequencies between 60GHz and 90GHz, which allows us to probe larger Zeeman energies than what has been previously reported. The instrument operates at a base temperature of 300mK, much lower than typical Zeeman energies in the operational frequency range. Spin systems are therefore thermally initialised to their ground state. We envision to take advantage of this to maximise the ESR-STM signal and ultimately implement coherent control at the nanoscale.

O 104.5 Thu 13:30 P

Statistical analysis of AFM images of nanofiber mats by grey-scale resolved Hurst exponent distributions — •Tomasz Blachowicz[1], Krzysztof Domino[2], Michal Koruszowic[1], Jacek Grzybowski[3], and Andrea Ehrmann[4] — [1]Silesian University of Technology, Institute of Physics - Centre for Science and Education, Gliwice, Poland — [2]Polish Academy of Sciences, Institute of Theoretical and Applied Informatics, Gliwice, Poland — [3]Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice, Poland — [4]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, Bielefeld, Germany

Two-dimensional periodic or random structures can be classified by diverse methods. Nevertheless, quantitative descriptions of such surfaces are still problematic. While the statistical analysis of periodic fibrous structures by Hurst exponent distributions was suggested some years ago [1], the quantitative analysis of atomic force microscopy (AFM) images of nanofiber mats was only recently described [2]. Here we present the influence of typical AFM image post-processing steps, such as polynomial background subtraction, aligning rows, deleting horizontal errors or sharpening, on the grey-scale-resolved Hurst exponent distribution. Our results show that while characteristic features of these false-color images may be shifted by grey-channel and Hurst exponent, they can still be used to identify AFM images and, in the next step, to quantitatively describe AFM image of nanofibrous surfaces.

[1] T. Blachowicz et al., Physica A 452, 167-177 (2016)

[2] T. Blachowicz et al., Tekstilec 63, 104-112 (2020)

O 104.6 Thu 13:30 P

Nonlinearities in force microscopy cantilever oscillations — •Lukas Böttcher[1], Dominique Schneider[1], Jens Starke[2], Ingo Barke[1], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock, 18059 Rostock — [2]Institute of Mathematics, University of Rostock, 18051 Rostock

In dynamic force microscopy nonlinearities of the nanoprobe-surface interaction at small separations lead to deformed and bistable resonance curves of the cantilever oscillation [1-4]. To understand and control instable imaging conditions we acquire distance dependent frequency sweeps of the amplitude in dynamic atomic force-microscopy and determine frequencies of instability. We address the behavior on hard versus soft surfaces.

[1] Gleyzes et al. (1991), Appl. Phys. Lett. 58 (25), S. 2989*2991

[2] Hölscher, Schwarz (2007), International Journal of Non-Linear Mechanics 42 (4), S. 608*625

[3] Raman, et al. (2009), In: Morita, Giessibl und Wiesendanger (Hg.): Noncontact Atomic Force Microscopy: Volume 2. Berlin, Heidelberg: Springer Berlin Heidelberg, S. 361*395

[4] Stark (2010), Materials Today 13 (9), S. 24*32

O 105: Poster Session VIII: Graphene and beyond II

Time: Thursday 13:30–15:30 Location: P

O 105.1 Thu 13:30 P

Low-energy ion implantation of Cobalt in graphene investigated by scanning tunneling microscopy — •Anna Sinterhauf[1], Benno Harling[1], Manuel Auge[2], Felix Junge[2], Philip Willke[3], Hans Hofsäss[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Universität Göttingen — [2]II. Physikalisches Institut, Universität Göttingen — [3]Physikalisches Institut, Karlsruher Institut für Technologie (KIT)

To tailor the properties of a graphene sheet by band structure engineering, the issue of doping is decisive to turn graphene into a true device material. For this purpose, a direct incorporation of foreign atoms into the graphene layer by low-energy ion beam implantation has shown to be a versatile method [1] as demonstrated for B and N. Here, we report on the successful implantation of Cobalt atoms into the graphene lattice achieved by low-energy Cobalt implantation at an ion energy of 20eV. After transfer through air, reinsertion into UHV and annealing at 400°C for 30 minutes, the structural and electronic properties of the ion implanted epitaxial graphene are investigated by scanning tunneling microscopy and spectroscopy (STS). Contrary to B and N [2], we find a negligible charge transfer from Co to graphene in agreement with theoretical considerations [2]. In addition, at the topographic position of the defects, STS reveals a pronounced peak in dI/dV-spectra at zero bias voltage. Financial support by the DFG through project We 1889/13-1 is gratefully acknowledged.

[1] P. Willke et al., Nano Lett. 15(8), 5110-5115, 2015

[2] E. J. G. Santos et al., Phys. Rev. B 81, 125433, 2010

O 105.2 Thu 13:30 P

LEEM/PEEM investigation of ambient oxidized g/ge(110) — •Ka Man Yu[1,2], Chanan Euaruksakul[3], Thipusa Wongpinij[3], Robert M. Jacobberger[4], Michael S. Arnold[4], Max G. Lagally[4], and Michael S. Altman[1] — [1]Hong Kong University of Science and Technology, Hong Kong SAR — [2]University of Kaiserslautern, 67663 Kaiserslautern, Germany — [3]Synchrotron Light Research Institute, Nakhon Ratchasima 30000, Thailand — [4]University of Wisconsin-Madison, Wisconsin 53706, United States

Germanium (Ge) is an excellent candidate for MISFET devices due to its high intrinsic charge carrier mobility. However, in contrast to the native oxide on Si, the native oxide on Ge hinders practical applications. The recent finding that a graphene monolayer can diminish the oxidation rates of Ge under ambient conditions identifies a possible scheme for overcoming a key challenge to the development of Ge-based electronic devices. Further knowledge of how oxygen permeates graphene to react with Ge is crucial to achieving this goal. In this work, the oxidation of Ge(110) under a graphene monolayer that is caused by ambient exposure was investigated using LEEM and PEEM. Three oxide domains are identified: a mixed monolayer or dispersed submonolayer comprised of GeO_x/GeO_{1+y}, thin and thicker GeO_{1+y} over a buried GeO_x interfacial layer in contact with the Ge bulk. The permeability of graphene to oxygen is attributed to defects at boundaries between the prevalent $R0$ and $R30$ graphene grains, within grains and at wrinkles. A statistical treatment for isochromatic correction of energy-resolved PEEM images will also be presented.

O 105.3 Thu 13:30 P

The role of two-dimensional pressure in sulfur intercalation underneath graphene on ruthenium — •Lars Buss[1,2], Jens Falta[2], Moritz Ewert[1], Bin Shao[3], Tim Wehling[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [3]Beijing Computational Science Research Center (CSRC), Beijing, China — [4]Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Micrometer-sized single-layer graphene can epitaxially be grown on transition-metal substrates with excellent crystalline quality. However, due to strong binding these substrates have a detrimental influence on the intrinsic properties of the graphene. By lifting the interlayer coupling, e. g., via intercalating foreign atoms, its unique electronic properties can be restored. We have investigated the intercalation of sulfur underneath graphene on Ru(0001) with low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). We find that sulfur deposited at elevated temperatures enters through the edge of the island, leading to wrinkle formation in the decoupled graphene. Interestingly, the presence of the graphene limits the possible S/Ru(0001) reconstructions that may form underneath, preventing less dense reconstructions like the $p(2 \times 2)$ and $(\sqrt{3} \times \sqrt{3})$ reconstructions. Based on density functional theory calculations, these findings are explained by a 2D pressure exerted by the overlying graphene, which results from the strong graphene-substrate interaction, only rendering the denser reconstructions of the S/Ru phase diagram energetically favorable.

O 105.4 Thu 13:30 P

Probing Quantum Hall edge channels by scanning tunneling spectroscopy — •Tjorven Johnsen[1], Sayanti Samaddar[1], Astrid Weston[2,3], Matthew J. Hamer[2,3], Kenji Watanabe[4], Takashi Taniguchi[4], Roman Gorbachev[2,3,5], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University, Germany. — [2]Department of Physics and Astronomy, University of Manchester, UK. — [3]National Graphene Institute, University of Manchester, UK. — [4]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan. — [5]Henry Royce Institute for Advanced Materials, University of Manchester, UK.

The topology of the quantum Hall effect is imprinted in the edge channel (EC) transport, but microscopic details of the EC topography at the scale of the magnetic length are largely unknown. Here we use scanning tunneling spectroscopy to probe the quantum Hall ECs at integer fillings along a gate-tunable graphene pn interface. ECs with finite width at the Fermi level become apparent along the continuous potential gradient across the interface. They meander along the interface in width and lateral position due to the inhomogeneous local electrostatic environment. However, the appearance of charging lines testifies the simultaneous presence of a tip-induced quantum dot that is influencing the electrostatics at the interface similarly as in scanning gate experiments and, hence, modifies the measurement results in detail. To disentangle the contributions from ECs and quantum dot, we employed electrostatic model simulations that explain multiple details of the observed charging lines and the local density of states features.

O 105.5 Thu 13:30 P

Local spots of viscous electron flow in graphene at room temperature and moderate mobility — •Sayanti Samaddar[1], Jeff Strassdas[1], Kevin Janssen[2], Tjorven Johnsen[1], Zhenxing Wang[3], Daniel Nuemaier[3,4], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]Research Centre Jülich, Peter Grünberg Institute, 52425 Jülich, Germany, — [3]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen — [4]University of Wuppertal, 42285 Wuppertal, Germany,

Dominating electron-electron scattering enables viscous electron flow exhibiting hydrodynamic current density patterns such as Poiseuille profiles or vortices. The viscous regime has recently been observed in graphene by non-local transport experiments and mapping of Poiseuille profiles up to room temperature. Here, we probe the current-induced surface potential maps of graphene field effect transistors using scanning probe microscopy at room temperature. We discover the appearance of μm large areas close to charge neutrality, where the current induced electric field opposes the externally applied field. By estimating the scattering lengths from the gate dependence of local electric fields, we find that these areas exhibit a dominating electron-electron scattering as expected for viscous flow. We map the respective meandering electric fields and carefully rule out artifacts such as by source-drain voltage induced local doping. Our results imply that viscous electron flow is omnipresent in graphene devices, even at moderate mobility.

O 105.6 Thu 13:30 P

Control of interface alloying between silicene and a silver substrate — •Johannes Küchle[1], Aleksandr Baklanov[1], Felix Haag[1], David Duncan[2], Paul Ryan[2,3], Ari Seitsonen[4], Willi Auwärter[1], and Francesco Allegretti[1] — [1]Physics Department E20, Technical University of Munich, 85748 Garching, Germany — [2]Diamond Light Source, OX11 0DE Didcot, UK — [3]Imperial College London, SW7 2AZ London, UK — [4]Département de Chimie, École Normale Supérieure, 75005 Paris, France

Silicene, the silicon analogue of graphene, is a promising material with unique structural and electronic properties, which has been in the focus of intense research during the past decade. With the epitaxial fabrication via deposition of silicon on solid substrates being the best-established growth method, silicene is susceptible to strong interfacial interactions that may drastically alter its functional properties. However, these interactions are still largely unexplored. Here, we present our recent experiments with soft X-ray photoelectron spectroscopy (SXPS) at various Si coverages in combination with X-ray standing waves, indicating that during the growth of the most commonly studied (4 x 4) superstructure of silicene on Ag(111) Si-Ag surface alloying occurs. Accordingly, our scanning tunneling microscopy (STM) studies resolve a yet unreported phase, which we interpret as a Si-Ag alloy structure, extending underneath the silicene layer. Moreover, we show that growing silicene on a sacrificial Ag_2Ge surface alloy strongly suppresses the Si-Ag alloy component in SXPS, resulting in new, distinct phases, as detected by low energy electron diffraction and STM.

O 105.7 Thu 13:30 P

Two phases of monolayer tantalum sulfide on Au(111) — Daniela Dombrowski[1,2], Abdus Samad[3], Clifford Murray[4], Marin Petrović[5], Pascal Ewen[1], Thomas Michely[4], Marko Kralj[5], Udo Schwingenschlögl[3], and •Carsten Busse[1,2] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [2]Department Physik, Universität Siegen, Germany — [3]KAUST, Physical Science and Engineering Division, Thuwal, Saudi Arabia — [4]II. Physikalisches Institut, Universität zu Köln, Germany — [5]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Zagreb, Croatia

Transition metal chalcogenides (TMCs) are 2d materials with a broad variety of electrical properties and phenomena like charge density waves, superconductivity and Mott transitions. Like their bulk parent materials, 2d-TMCs exhibit polymorphism. This includes the well-known 2H- and $1T\text{-}MX_2$ phases but also more complex structures such as self-intercalated bilayers or chalcogene-poor compounds with sulfur vacancies. The structure has a strong influence on the properties. For example, group 6 TMCs in the 2H-phase are semiconducting, while they are metallic in the 1T-phase.

We use a combination of physical and chemical vapor deposition to grow two different phases of tantalum sulfide on Au(111). STM, STS and ARPES results corroborated by DFT allow us to identify the phases as $2H\text{-}TaS_2$ and a novel phase found for sulfur-poor conditions where the bottom sulfur layer is missing.

O 105.8 Thu 13:30 P

Single-domain h-BN monolayer growth on an incommensurable surface: Pt(110) — •Dominik Steiner[1], Marco Thaler[1], Florian Mittendorfer[2], and Erminald Bertel[1] — [1]Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Institute of Applied Physics and Center of Computational Material Science, University of Technology, Vienna, Austria

Lattice matching has been widely considered to be a prerequisite for perfect epitaxial growth. In contrast, we demonstrate by LEED, STM and DFT calculations large-scale, single-domain hexagonal Boron Nitride (h-BN) growth on the incommensurable Pt(110) surface [1]. In a competition between the h-BN and the Pt bulk geometry the former dominates the arrangement of the Pt(110) surface atoms. This adaptivity of the Pt(110) surface is key to the perfect film growth.

STM and LEED studies show that single-domain growth occurs only above a threshold temperature of ~1120 K. At T<1120 K, a defective multi-domain film on a rough Pt-surface is obtained. Referring to the results of Lee et al. for h-BN growth on liquid Au [2] we proposed that the Pt surface atoms form a quasi-liquid layer above the threshold temperature, thus enabling the alignment of h-BN nuclei. Our recent studies of the growth mechanism, however, indicate a more complex mechanism leading to single-domain growth.

[1] Steiner et al., ACS Nano 2019, 13 (6), 7083-7090.

[2] Lee at al., Science 2018, 362 (6416), 817.

O 105.9 Thu 13:30 P

Moiré-driven charge accumulation in few-layer antimony films on InSb(111)A — Bing Liu[1,3], •Tim Wagner[1,3], Martin Kamp[1,3], Stefan Enzner[2,3], Philipp Eck[2,3], Giorgio Sangiovanni[2,3], and Ralph Claessen[1,3] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany

Few-layer antimony films are a promising topological material which has been widely investigated on various substrates. Here we show few-layer films which have been successfully synthesized on a InSb(111)A substrate. The epitaxially grown antimony layers keep the bulk Sb lattice constant, i.e., do not adapt to that of the substrate. According to density functional theory calculations considering this Moiré situation in a simplified unit cell, the lattice mismatch at the interface gives rise to charge accumulations at positions where the atoms of film and substrate are in phase. Although situated at the interface, these charge localizations are predicted to extend perpendicular to the interface over several antimony layers. Experimentally, this can be confirmed in scanning tunneling microscopy with a Moiré pattern visible up to the seventh layer. Spectroscopy measurements of antimony films with various thicknesses show Sb bulk behavior, i.e., the scattering of the topological surface state, down to five film layers. At lower thicknesses, this scattering is suppressed, which may be attributed to the increased influence of the Moiré-driven charge accumulations at the interface.

O 105.10 Thu 13:30 P

Proximity effects in the charge density wave order and superconductivity in single-layer NbSe2 — •Wen Wan[1], Paul Dreher[1], Alla Chikina[2], Haojie Guo[3], Rishav Harsh[1], Marco Bianchi[2], Marco Gobbi[4], Jose-Maria Gomez-Rodriguez[3], Antonio Javier Martinez-Galera[3], Philip Hofmann[2], Jill A. Miwa[2], and Miguel Ugeda[1] — [1]Donostia International Physics Center, San Sebastián-Donostia, Spain — [2]Department of Physics and Astronomy, Aarhus University — [3]Dpto. Física de la Materia Condensada, Universidad Autónoma de Madrid — [4]CIC Nanogune

Collective electronic states such as the charge density wave (CDW) order and superconductivity respond dramatically to external perturbations. In two-dimensional materials hosting such states, the closeness to unavoidable supporting substrates may lead to significant changes in their properties. Here we explore the impact of proximity effects on the CDW and superconducting states in single-layer NbSe2. We performed the electronic characterization of single-layer NbSe2 on several substrates of opposite metallicity by means of STM/STS at 350 mK, ARPES and 4-point probe transport measurements. In particular, we have epitaxially grown single-layer NbSe2 by MBE on two different metals, Au(111) and BLG/SiC(0001), and two insulators, bulk WSe2 and monolayer h-BN/Ir(111). While both phases disappear on Au(111), they persist on BLG/SiC. The fate of the CDW and superconducting phases is more intricate on insulating substrates, which are largely affected, however, despite of the electronic decoupling of the 2D superconductor with the substrate states.

O 105.11 Thu 13:30 P

The true corrugation of monolayer h-BN on Rh(111) — Luis Henrique de Lima[1,2], Thomas Greber[3], and •Matthias Muntwiler[2] — [1]Universidade Federal do ABC, Santo Andre, Brazil — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]Universität Zürich, Zürich, Switzerland

Monolayer hexagonal boron nitride (h-BN) grown on the (111) surface of rhodium exhibits an intriguing corrugation pattern called "nanomesh" with a lattice constant of 3.2 nm. Despite numerous experimental and theoretical studies, structural details such as the corrugation amplitude have been difficult to determine quantitatively due to the differences in chemical and electronic environments in the strongly bound pore regions and the weakly bound wire regions of the corrugated structure. For reliable results it is important to probe the structure with a method that is inherently sensitive to the positions of the atomic cores rather than electron density.

In this contribution, we determine the corrugation of h-BN nanomesh from synchrotron based angle- and energy-resolved photoelectron diffraction measurements with chemical state resolution. By comparing measured data to multiple-scattering simulations true adsorbate-substrate distance can be measured with high precision, avoiding pitfalls of apparent topography observed in scanning probe techniques.

L. H. de Lima et al., 2D Mater. 7, 035006 (2020)

O 105.12 Thu 13:30 P

Transitions from single-layer MoS_2 to bilayer growth: A LEEM study — •Moritz Ewert[1,2,3], Lars Buss[1,2], Francesca Genuzio[4], Tevfik Onur Menteş[4], Andrea Locatelli[4], Jens Falta[2,3], and Jan Ingo Flege[1,2,3] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Institute of Solid State Physics, University of Bremen, Germany — [3]MAPEX Center for Materials and Processes, University of Bremen, Germany — [4]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Molybdenum disulfide (MoS_2) is well-known to change from an indirect to a direct semiconductor as a single layer.

We present insights from in-situ low-energy electron microscopy (LEEM) on the extended growth of MoS_2 on the Au(111) surface at elevated temperatures of 720°C. Our continuous growth method leads to the formation of micron-sized single-layer MoS_2 islands. The single-domain character of these islands is confirmed by employing dark-field imaging and micro-diffraction (LEED). This also reveals the distribution of 90:10 of the two expected MoS_2 mirror domains on Au(111). Selected-area angle-resolved photoelectron spectroscopy (ARPES) measurements of these mirror domains underline the threefold symmetry of the two mirror domains and indicate the presence of MoS_2 bilayer. Using X-ray photoemission electron microscopy (XPEEM) and intensity-voltage LEEM (I(V))-LEEM we identify the bilayer nucleation areas at nearly full surface coverage and propose a model pathway for their formation.

O 105.13 Thu 13:30 P

1H-MoS_2 edge reconstructions and functionalization — •Yuman Sayed-Ahmad-Baraza[1], Ruben Canton-Vitoria[2], Mario Pelaez-Fernandez[3], Carla Bittencourt[4], Raul Arenal[3], Nikos Tagmatarchis[2], and Chris Ewels[1] — [1]Institut des Matériaux Jean Rouxel (IMN), Université de Nantes, CNRS, 2 rue de la Houssinière, BP 32229, 44322 Nantes, cedex 3, France — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 3 Athens, Greece — [3]Laboratorio de Microscopias Avanzadas, Instituto de Nanociencia de Aragon, Universidad de Zaragoza, 50018 Zaragoza, Spain — [4]Chimie des Interactions Plasma-Surface, University of Mons, 20 Place du Parc, 7000 Mons, Belgium

Single-layer 1H-MoS_2 presents a rich variability of edges. We present DFT studies of the structure and stability of reconstructed Mo-100%S and Mo-50%S zigzag edges [1]. For Mo-100%S we identify a family of metastable edges consisting in Mo atoms linked by disulfide ligands. For Mo-50%S, we find a lattice distortion with 3x periodicity, compatible with a Peierls' distortion and the formation of 3-centre local bonds. Additionally, we present DFT studies of the covalent functionalization of MoS_2 with 1,2-dithiolanes. We find preferential functionalisation at the edges, stable against a vacancy healing reaction; consistent with our experimental results [2]. 1. Y. Sayed-Ahmad-Baraza and C. P. Ewels, Chem. - Eur. J. 26, 6686 (2020). 2. Y. Sayed-Ahmad-Baraza, R. Canton-Vitoria, M. Pelaez-Fernandez, R. Arenal, C. Bittencourt, C. P. Ewels, and N. Tagmatarchis, Npj 2D Mater. Appl. 1, (2017).

O 106: Poster Session VIII: Poster to Mini-Symposium: Electrified solid-liquid interfaces III

Time: Thursday 13:30–15:30 Location: P

O 106.1 Thu 13:30 P

Gouy-Chapman and beyond: A new double layer model for Pt — •Katharina Doblhoff-Dier — Leiden University, Leiden, The Netherlands

The Gouy-Chapman-Stern model and its various extensions (e.g., modified to include finite-size effects) are expected to represent the electric double layer structure in dilute electrolytes rather well. Consequently, these models form the basis of many constant-potential methods available in the various electronic structure codes. However, recent experimental results [1,2] show that the double layer capacitance of Pt(111) surfaces, and (to a lesser extent) of Au(111), does not follow the predictions made by these simplistic models. Consequently, we need to rethink the structure of the electric double layer. A reasonable match between theory and experiment can be attained when extending the standard Gouy-Chapman-Stern-like capacitance models by i) the hyperpolarizability caused by water adsorbing at the interface and ii) a weak attractive ion-surface interaction. These little effects strongly alter the potential vs. electric relation of the interface as well as the z-dependence of the near-surface electric field. Inclusion of these effects therefore does not only suggest a renewed picture of the double layer structure, the correct description of these properties is also relevant in order to obtain accurate adsorption energies of polar molecules and reaction barriers from first principle calculations.

[1] K. Ojha, N. Arulmozhi, D. Aranzales, and M.T. M. Koper; Angew. Chem. Int. Ed. 59, 711 (2020)

[2] K. Ojha, K. Doblhoff-Dier, M.T.M. Koper (unpublished)

O 106.2 Thu 13:30 P

Entropy changes during adsorption of pyridine on Au(111) in aqueous solutions — •Katarina Josifovska, Marco Schönig, and Rolf Schuster — Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe

The adsorption of pyridine on gold surfaces has been often studied by applying various electrochemical, microscopic and spectroscopic techniques. Corresponding to reported data, pyridine adsorption occurs in anodic direction in two different structural orientations [1,2,3].

In attempt to describe the adsorption, we used different concentrations of pyridine in aqueous solutions over Au(111), on which we conducted electrochemical microcalorimetric measurements in our home-build calorimeter [4]. We measured the Peltier heat which provides direct information on the reaction entropy of the electrochemical processes, scanning the whole adsorption region.

Negative entropy was found for the anodic processes, with a strong minimum of ca. -170 J/mol*K that was observed at about the same potential at which the reorientation occurs. This entropy reduction is in line with adsorption of weakly solvated neutral molecules from the solution, but also other processes, such as ion transport, entropy from double layer polarization, and/or accompanying solvent reorientation might contribute.

[1] L. Stolberg et al., J. Electroanalytical Chem. 1991, 241, 307. [2] J. Li et al., J. Am. Chem. Soc. 2015, 137, 2400. [3] S. Iqbal et al., Electrochimica Acta 2015, 186, 427. [4] R. Schuster, Curr. Opin. Electrochem. 2017, 1, 88.

O 106.3 Thu 13:30 P

Thermodynamic and kinetic data of the hydrogen evolution reaction (HER) from electrochemical microcalorimetry. — •Marco Schönig and Rolf Schuster — Karlsruher Institut für Technologie, Deutschland

The hydrogen evolution reaction (HER) is an often investigated model electrocatalytic reaction. However, there are still open questions, like the influence of the alkaline metal cations in alkaline solution[1].

We measured the exchanged heat during the HER on Pt upon short potential or current pulses. The evolved heat is made up of reversible and irreversible contributions, which can be disentangled by measuring with different pulse polarities[2]. From the reversibly exchanged heat we derived the reaction entropy. The irreversible contribution to the exchanged heat corresponds to the overpotential. Thus, from the calorimetric data we can derive the overpotential as a function of current density, which allows for the determination of the exchange current density of the reaction and provides an alternative to the determination of kinetic parameters from Tafel plots.

The determined reaction entropies agree well with the standard reaction entropy of the HER in the respective solutions [3]. For the exchange current density, we found 1.3 mA/cm2 for 0.1 M LiOH. For 0.1 M KOH and 0.1 M CsOH lower values were found, which is in accordance with trends observed in the literature[1].

[1] A.S. Bandarenka et al., ChemElectroChem 2018, 5, 2326.[2] R. Schuster, Curr. Opin. Electrochem. 2017, 1, 88.[3] B.E. Conway et al., J.Chem. Soc, Faraday Trans. 1 1978, 74,1373.

O 106.4 Thu 13:30 P

$Ni(OH)_2$ modified Cu(111): interfacial water structure and electrocatalysis — •Andrea Auer[1], Francisco J. Sarabia[2], Daniel Winkler[1], Victor Climent[2], Juan Feliu[2], and Julia Kunze-Liebhäuser[1] — [1]Institute of Physical Chemistry, University Innsbruck, Austria — [2]Instituto Universitario de Electroquímica, Universidad de Alicante, Spain

The design of bimetallic electrodes is one key tactic to tune their activity and selectivity for electrocatalysis. Here, irreversible adsorption of Ni ions[1] was used to prepare $Ni(OH)_2$ modified Cu(111) electrodes with different coverages and to study their effect on the hydrogen evolution reaction (HER) and CO reduction in alkaline media. To investigate the structure-activity relation, electrochemical scanning tunneling microscopy was performed and shows morphological changes upon modification consistent with adsorption of $Ni(OH)_2$ on the step edges. The presence of $Ni(OH)_2$ on Cu(111) leads to an enhancement in the rate of the HER, similar to $Ni(OH)_2$/Pt(111) electrodes[1], but also changes the selectivity of the CO reduction. Intriguingly, laser induced temperature jump experiments reveal that the $Ni(OH)_2$ modification influences the charge distribution at the interface by a decrease of the electric field strength. This implies an easier reorganization of the interfacial water molecules facilitating charge transfer through the double layer, and thus enhancing the electrocatalytic reaction.

[1] F. J. Sarabia, P. Sebastián-Pascual, M. T. M. Koper, V. Climent, J. M. Feliu, *ACS Appl. Mater. Interfaces* **2019**, 11, 1, 613-623.

O 106.5 Thu 13:30 P

Amino acids adsorption at electrified gold/aqueous interface — •Denys Biriukov[1,2] and Zdenek Futera[2] — [1]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo nám. 2, 16610 Prague 6, Czech Republic — [2]Institute of Physics, Faculty of Science, University of South Bohemia, Branišovská 1760, 370 05 České Budějovice 2, Czech Republic

Molecular detailization of gold/aqueous interfaces in an external electric field stimulates various applications in electrochemistry. In this contribution, we investigate the adsorption of several, particularly charged amino acids, since they represent principal components of proteins and other molecular junctions. Using all-atom molecular dynamics simulations and free energy calculations, we show that positively charged amino acids exhibit larger interfacial changes than negatively charged when an external electric field is applied. The reason is the ability of the side-chain of positively charged amines to replace water molecules in the first adsorption layer at Au (111) surface. Charge-neutral amino acids are also capable to penetrate into the interfacial water structure, so their response to an applied electric field reflects that of positively charged amino acids. However, it is overall less significant due to charge-neutrality of the molecule. Contrary, negatively charged carboxylates adsorb with their carboxyl group further from the surface, i.e., an applied electric field acting on the side-chain is screened by the solvent. This leads to reduced electric field effects and weaker adsorption in general. Current results provide a useful information, which may help to interpret complex electrokinetic phenomena.

O 106.6 Thu 13:30 P

In-situ optical detection of charge distributions at electrified solid-liquid interfaces — •Christoph Cobet, Saul Vazquez-Miranda, Luis Rosillo-Orozco, and Kurt Hingerl — Johannes Kepler University, Altenbergerstr 69, 4040, Linz, Austria

Polarization optical methods like Spectroscopic Ellipsometry are used by us to determine the distribution of charges, i.e. electrons and ions, and their potential dependent variation in the uppermost atomic layers of a working electrode as well as in the inner Helmholtz plane above. Our focus lad initially on planar surfaces with regular atomic structure to discriminate the different contributions to the optical response. On the one hand, the aforementioned optical probes are extremely sensitive to electronic surface/interface changes even in the presence of sub-monolayer changes. On the other hand, exactly this advantage often makes it problematic to extract quantitative information. But we will show that valuable additional information is accessible which is in parts complimentary to results of conventional methods such as impedance spectroscopy, EC-STM or novel XPS approaches. This will be demonstrated for single crystalline metal (Cu) as well as metal-oxide (ZnO) surfaces; both drosophila-like examples of catalytic surfaces where the optical resonances of Drude electrons, of electrons in surface states and of electronic states in the electrostatic as well as strain field at electrified solid-liquid interfaces contribute to the measured signal. [1] S. Vazquez-Miranda, et.al.: J. Phys. Chem. C 124, 5204 and 25403 (2020); [2] M.-H. Chien, et.al.: J. Phys. Chem. C 122, 8984 (2018), [3] G. Barati, et.al.: Langmuir 30, 14486 (2014)

O 106.7 Thu 13:30 P

Electrochemical properties of Ru(0001) - pH effects, anions effects and anodic H_2 formation — •Albert K. Engstfeld[1], Simon Weizenegger[2], Zenonas Jusys[2], Joachim Bansmann[2], Jakub Drnec[3], and R.Jürgen Behm[2] — [1]Institute of Electrochemistry, Ulm University, Ulm — [2]Institute of Surface Chemistry and Catalysis, Ulm University, Ulm — [3]ESRF, Grenoble, France

The electrochemical properties of Ru electrodes in aqueous electrolyte are very complex since it interacts strongly with anion species and shows overlapping surface redox processes. Furthermore, it has recently been shown in $HClO_4$ electrolyte that hydrogen adsorbed in the hydrogen evolution region, is desorbed in the positive-going scan by hydroxyl displacement from the surface, to form H_2 at potentials more positive than the equilibrium potential of $E(\frac{1}{2}H_2/H^+) = 0$ V, instead of forming H^+.[1] Here we present the electrochemical properties of Ru(0001) in acid and alkaline electrolytes. The electrodes were prepared under UHV conditions and investigated in an electrochemical flow cell combined with differential electrochemical mass spectrometry (DEMS). With the DEMS data, we provide direct evidence for hydrogen adsorption in H_2SO_4 electrolyte, which was so far not considered. Additional surface X-Ray diffraction (SXRD) measurements in H_2SO_4 reveal a strong hysteresis in the potential dependent structural properties and adlayer composition. The herein reported processes are suggested to be characteristic for other strongly interacting metals in general. [1] Scott & Engstfeld, et al, CatSciTechnol, 10 (2020) 6870

O 107: Poster Session VIII: Poster to Mini-Symposium: Manipulation and control of spins on functional surfaces IV

Time: Thursday 13:30–15:30 Location: P

O 107.1 Thu 13:30 P

First Principles modelling of Supramolecular Spin-valves — •Jorge Olivares, Artem Fediai, and Wolfgang Wenzel — Karlsruhe Institute of technology, Institute of Nanotechnology, Karlsruhe, Germany

Molecular spintronics uses the spin degree of freedom to develop technology that can control electrical currents in nanodevices. A good understanding of the underlying physics in nanoscale systems and reliable technical tools for simulating them are required to exploit the full capacity of the spin degree of freedom in molecules. Experimental setups have shown a remarkable spin-dependent behaviour of the current (Magnetoresistance) through a carbon nanotube decorated with single molecular magnets (SMMs). We present results of ab-initio simulations on Carbon nanotubes (CNT) decorated by two terbium phthalocyanine (SMMs). The transmission coefficient and density of states were calculated using the Non-Equilibrium Green's function (NEGF) formalism. We show the dependence of the transmission coefficient with respect to the relative spin orientation of the SMMs. Our results show how the different spin states of the system CNT+SMMs affects the transmission through a CNT as well as the advantages and limitations of an non-interactive approach. The system under study, allows us to extend our approach to any periodic sytem and different types of SMMs, opening a field of ab-initio studies of nano-electronic spintronic devices in the non-interacting and possibly to the interacting regimes.

O 107.2 Thu 13:30 P

Inducing carbon magnetism in nanographenes — •Elia Turco[1], Shantanu Mishra[1], Pascal Ruffieux[1], and Roman Fasel[1,2] — [1]Empa-Swiss Federal Laboratories for Materials Science and Technology, Dubendorf, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland.

Magnetism is historically associated to d- and f-block elements of the periodic table, which form the basis for modern information storage technologies. However, recent advances on the bottom-up synthesis of low-dimensional materials revealed the emergence of non-trivial magnetic states in all-carbon compounds. The low spin-orbit and hyperfine couplings in carbon, along with the possibility of electric-field control of magnetism, provides unique opportunities in emerging technologies such as quantum computation. The electronic structure of nanographenes can be selectively controlled through variation in size, shape and edge structure, allowing to experimentally realize new quantum properties, including magnetism. In this contribution, we investigate the on-surface synthesis of z-shaped nanographenes belonging to the zethrene family. Single molecule scanning probe measurements reveal the transition from a closed-shell to an open-shell singlet ground state with increasing zethrene length. In the longest analogue, singlet to triplet spin excitation are detected via inelastic electron tunneling spectroscopy, unveiling a magnetic exchange coupling of 50 meV. These results open new perspectives for the realization of organic magnetic devices operating at practical temperatures.

O 107.3 Thu 13:30 P

Supercurrent Reversal through Atomic Scale Yu-Shiba-Rusinov States — •Christian R. Ast[1], Sujoy Karan[1], Haonan Huang[1], Ciprian Padurariu[3], Björn Kubala[3], Gonzalo Morrás[2], Alfredo Levy Yeyati[2], Juan Carlos Cuevas[2], Joachim Ankerhold[3], and Klaus Kern[1,4] — [1]MPI für Festkörperforschung, Stuttgart — [2]Universidad Autónoma de Madrid, Spain — [3]Universität Ulm — [4]EPFL, Lausanne, Switzerland

Magnetic impurities on superconductors give rise to discrete bound states inside the superconducting gap known as Yu-Shiba-Rusinov (YSR) states. Varying the impurity-superconductor coupling induces a quantum phase transition (QPT) as the YSR state energy passes through zero. The concomitant sign change in the Josephson current – a long sought for hallmark of this QPT – has remained elusive so far. Using scanning tunneling microscopy (STM), we demonstrate such a 0 to π transition of a Josephson junction through a YSR state as we continuously change the impurity-superconductor coupling. We detect the sign change in the Josephson current by exploiting a second transport channel as a reference in analogy to a superconducting quantum interference device (SQUID), which provides a rudimentary phase sensitivity for the STM. The change in the Josephson current through the QPT is significant and demonstrates the role of the impurity spin as well as the parity change across the QPT.

O 107.4 Thu 13:30 P

Spin dependent transmission of nickelocene-Cu contacts probed with shot noise — Michael Mohr[1], Ricarda Reuter[1], Manuel Gruber[1], David Jacob[2], Paula Abufager[3], Nicolás Lorente[4], •Alexander Weismann[1], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastián, Spain — [3]Instituto de Física de Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Universidad Nacional de Rosario, 2000 Rosario, Argentina — [4]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), E-20018 Donostia-Sebastián, Spain

The current I through nickelocene molecules and its noise are measured with a low-temperature scanning tunneling microscope on Cu(100). DFT and many-body calculations are used to analyze the data. During contact formation, two types of current evolution are observed, namely an abrupt jump to contact and a smooth transition. These data along with dI/dV spectra are interpreted in terms of a transition from a spin-1 to a spin-$\frac{1}{2}$ state that is Kondo-screened. Many-body calculations show that the smooth transition is also consistent with a renormalization of spin excitations of a spin-1 molecule by Kondo exchange coupling. The shot noise is significantly reduced compared to the Schottky value of $2eI$. The noise can be described in the Landauer picture in terms of the spin polarization of the transmission of ≈ 35 % through two degenerate d_π-orbitals of the nickelocene molecule.

O 107.5 Thu 13:30 P

Power optimization for spin-orbit torque induced magnetization switching in a monodomain magnetic particle — •Sergei Vlasov[1], Igor Lobanov[1], Grzegorz Kwiatkowski[2], Valery Uzdin[1], and Pavel F. Bessarab[1,2] — [1]ITMO University, St. Petersburg, Russia — [2]University of Iceland, Reykjavik, Iceland

The discovery of the spin-orbit torque (SOT) has opened a wide range of opportunities for the efficient manipulation of the magnetization, which is advantageous for spintronics applications. In particular, SOT produced by an in-plane current in a heavy-metal layer can be used to induce magnetization switching in a supported ferromagnetic element, thus providing means for bit operations in nonvolatile magnetic memories.

In this study, we demonstrate employing the optimal control theory that the energy cost of the SOT-induced magnetization switching can be reduced by properly tuning the current pulse. We present a complete analytical solution to the energy-efficient reversal of a macrospin under SOT. We calculate optimal control paths (OCPs) of the magnetization reversal and reconstruct the time-dependent amplitude and frequency of both components of the in-plane current. We also demonstrate the stability of calculated optimal switching protocols with respect to perturbations in materials properties and temperature.

This work was funded by the Russian Science Foundation (Grant No.19-72-10138) and the Icelandic Research Fund (Grant No. 184949-052).

O 107.6 Thu 13:30 P

Spin-polarized photoelectron emission from chiral cobalt oxide layers — •Onur Gül[1], Paul Möllers[1], Daniel Nürenberg[1], Koyel Banerjee Ghosh[2], Wenyan Zhang[2], Francesco Tassinari[2], Yitzhak Mastei[2], Ortal Lidor-Shalev[2], Simon Wei[3], Emil Wierzbinski[3], David Waldeck[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Westfälische Wilhems-Universität, 48149 Münster, Germany — [2]Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Revohoz, Israel — [3]Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

Chiral catalyst surfaces were recently shown to enhance the chemical selectivity of an electrocatalytic water splitting reaction by aligning the electron spins in the laboratory frame. [1] [2]

In this contribution we present results of spin-resolved photoemission experiments conducted with chiral cobalt oxide thin films. The photoelectrons were excited with laser pulses at $\lambda = 213$ nm, generated as the fifth harmonic of a Nd:YVO$_4$ laser, and the average spin polarization was determined in a Mott scattering apparatus. While only unpolarised electrons were emitted from the achiral layers, the electrons emitted from chiral layers exibit up to 30 percent spin polarization, suggesting that the spin polarization is indeed a consequence of the chirality of the layers.

[1] S. Ghosh et al,, J. Phys. Chem. C, 123 (2019) [2] K. B. Ghosh et al., J. Phys. Chem. C, 124 (2020)

O 107.7 Thu 13:30 P

Chiral cupric oxide layers as spin-polarizing water splitting catalysts — •Paul Möllers[1], Daniel Nürenberg[1], Koyel Banerjee Ghosh[2], Wenyan Zhang[2], Francesco Tassinari[2], Yitzhak Mastai[2], Ortal Lidor-Shalev[2], Simon Wei[3], Emil Wierzbinski[3], David Waldeck[3], Ron Naaman[2], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, Westfälische Wilhelms- Universität, 48149 Münster, Germany — [2]Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100 Rehovot, Israel — [3]Chemistry Department, University of Pittsburgh, Pittsburgh, PA 15260, United States

Spin-polarized catalytic surfaces can greatly enhance the selectivity of chemical reactions, e.g., in an electrocatalytic water splitting process. The spin polarization can be can be generated by the introduction of a chiral catalyst surface. [1,2] Here, we confirm that spin-polarized photocurrents can be obtained from chiral cupric oxide (CuO) films, and explore the underlying mechanism. Chiral CuO films were electrochemically deposited on polycrystalline gold substrates using a method pioneered by Switzer et al [3]. Photoelectrons were excited with laser pulses at 213 nm, and their average spin polarization was measured in a Mott scattering apparatus. The polarization exceeds $P = +10\,\%$ for 20 nm thin CuO films with 'L' chirality and, notably, is reversed for oxide films of opposite 'D' chirality.

[1] S. Ghosh et al., J. Phys. Chem. C, 123, 3024-3031 (2019)

[2] K. B. Ghosh et al., J. Phys. Chem. C, 124, 22610-22618 (2020)

[3] Kothari et al., Chem. Mater. 16, 4232-4244 (2004)

O 108: Poster Session VIII: Poster to Mini-Symposium: Frontiers of electronic-structure theory V

Time: Thursday 13:30–15:30 Location: P

O 108.1 Thu 13:30 P

Electron-phonon band gap renormalization in graphene nanoribbons — •Rodrigo Menchón[1] and Aran Garcia-Lekue[1,2] — [1]Donostia International Physics Center (DIPC), San Sebastian, Spain — [2]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

During the last decade, on-surface synthesis techniques have paved the way to the creation of atomically precise carbon-based nanostructures, e.g. 1D stripes referred to as graphene nanoribbons (GNRs).[1] Alongside these experimental advancements, first-principle simulations have been pivotal for understanding and predicting the electronic properties of GNRs. In particular, GNRs with so-called armchair edges are specially well-studied due to their semiconductor character.[2,3] This makes them very promising for electronic applications, and, at the same time, demands a high quality description of their semiconducting gap. Within this scenario, it would be interesting to address electron-phonon induced energy renormalization effects and their dependance upon temperature.[4] In this work, starting from Density Functional Theory simulations the electron self-energies and the band gap renormalization of armchair GNRs resulting from the electron-phonon interactions are determined. Our method might be extended to other semiconducting families of GNRs, 0D systems (e.g. carbon macromolecules) or 2D materials (e.g. nanoporous graphene).

References: [1] S. Clair et al., Chem. Rev. 2019, 119, 7, 4717 (2019). [2] L. Talirz et al., Adv. Mater. 2016, 28, 6222 (2016). [3] J. Lawrence et al., ACS Nano 2020, 14, 4, 4499 (2020). [4] F. Brown-Altvater et al., Phys. Rev. B 101, 165102 (2020).

O 108.2 Thu 13:30 P

Anomalous low-velocity electronic stopping in proton-irradiated graphene — •Alina Kononov[1] and Andre Schleife[2] — [1]Department of Physics, University of Illinois at Urbana-Champaign — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign

Ion beams in high-resolution imaging and patterning techniques can be used efficiently to manipulate and characterize 2D materials. Low particle velocities are particularly interesting, since in this regime the drag force induced on an incident ion by electrons is rife with material-specific effects. Examples include the threshold velocity for semiconductors and insulators below which an ion cannot excite electrons across the band gap and electronic stopping vanishes. In addition, directional bonding in these materials makes electronic stopping sensitive to the ion's trajectory even for slow ions, when core electrons are negligible. Graphene, thus, presents a highly interesting case with directional bonding but no band gap. Our real-time time-dependent density functional theory simulations of proton-irradiated graphene reveal a shoulder in the low-velocity stopping of channeling protons which does not occur for protons traversing a centroid path. From analyzing the post-impact band occupations and projectile charge state, we infer that resonant charge capture from certain valence bands by channeling protons is responsible for this feature. Our prediction of a new form of anomalous low-velocity stopping has implications for ion beam imaging, where such trajectory-dependent behavior could be exploited to achieve high resolution. (Supported by NSF OAC 17-40219)

O 108.3 Thu 13:30 P

Ultrafast dynamics of hot carriers in bulk semiconductors and in accumulation layer: energy relaxation and screening effects. — •Jelena Sjakste — LSI, CEA/DRF/IRAMIS, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Electron-phonon coupling determines the charge transport properties in pure materials as well as the relaxation dynamics of photoexcited carriers. The rapid development of the computational methods based on density functional theory, on the one hand, and of the time- energy- and momentum- resolved spectroscopy, on the other hand, allows today an unprecedently detailed insight into the role of the electron-phonon coupling [1,2].

In this work, we will present our recent results, both experimental and theoretical, on hot electron relaxation in silicon [3]. Moreover, we will present our recent results, both experimental and theoretical, on the hot electron relaxation in InSe. InSe is a quasi-2D material which was shown recently to have potential interest for optoelectronics. In this work, we will discuss our new results on the relaxation dynamics and screening of the electron-phonon interaction in doped InSe [4].

References:

[1] J. Sjakste et al, J. Phys: Cond. Mat. 30, 353001 (2018).

[2] Tanimura et al, Phys. Rev. B 93, 161203 (R) (2016).

[3] Tanimura, Kanasaki, Tanimura, Sjakste, Vast, Phys. Rev. B 100, 035201 (2019).

[4] Chen, Sjakste et al, PNAS 117, 21962-21967 (2020).

O 108.4 Thu 13:30 P

Impact of the structural dynamics on the electronic properties of the metal organic frameworks — •Mariana Kozlowska[1], Ritesh Haldar[2], Shahriar Heidrich[1], Marcus Elstner[3], Christof Wöll[2], and Wolfgang Wenzel[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Functional Interfaces (IFG), KIT — [3]Institute of Physical Chemistry (IPC), KIT

Electronic properties of organic semiconductors (OSC) depend on the assembly of molecules and their vibrational flexibility in a material. These determine the microscopic intercommunication, resulting in a materials conduction. Here, we have employed a metal-organic framework (MOF) type of assembly strategy to engineer the arrangement of the (i) OSC pentacene and (ii) the DPA-TPE (diphenylamine-tetraphenylethylene) chromophore, and demonstrated the change of the electronic and spectroscopic properties of molecules and films towards assembly in the spatially ordered MOF structure.

Using the combination of DFT, DFT-B, QM/MM methods, the charge carrier mobility, starting from the band structure and the Marcus charge hopping, to the direct propagation of charge carriers using the time dependent Schrödinger equation, coupled to the classical motion of nuclei, were performed. This allowed to identify localized frustrated rotations of the pentacene, as the reason for the breakdown of band transport, and constraining of rotations in DPA-TPE, leading to the TADF emission upon crystallization in MOF.

O 108.5 Thu 13:30 P

Tailoring the electronic anisotropy of nanoporous graphene — •Xabier D. de Cerio[1] and Aran Garcia-Lekue[1,2] — [1]Donostia International Physics Center (DIPC), San Sebastian, Spain — [2]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Recent experimental advances have allowed the synthesis of atomically precise nanoporous graphene (NPG) through the lateral fusion of graphene nanoribbons (GNRs). Besides being a semiconductor, this novel 2D material exhibits a highly anisotropic electronic structure, which makes it appealing for electronic, optical, and sensing applications, and has thus generated great interest [Science 360, 199 (2018); Nano Lett. 19, 576 (2019); J. Am. Chem. Soc. 141, 13081 (2019)]. In this work, by means of Density Functional Theory (DFT) calculations, we determine the electronic anisotropy of a new family of NPG, in which atomic scale modification of lateral linkers leads to three different inter-ribbon coupling configurations. Our calculations predict different anisotropic behaviour for each coupling configuration. Additionally, we find that the rotation angle of phenyl rings in the linkers works as a continuos knob to manipulate the electronic crosstalk between adjacent GNRs. Supported by on-surface synthesis of this new nanostructure, we present a proof-of-concept study showing that engineering the linkers is an efficient way to tune the electronic anisotropy of NPG.

O 108.6 Thu 13:30 P

Topological semimetallic phase in PbO_2 promoted by temperature — •Bo Peng[1], Ivona Bravic[1], Judith MacManus-Driscoll[2], and Bartomeu Monserrat[1,2] — [1]Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

The past decade has witnessed multiple experimental realization and thousands of predictions of topological materials. However, it has been determined that increasing temperature destroys topological order, restricting many topological materials to very low temperatures and thus hampering practical applications. Here, we propose the first material realization of temperature promoted topological order. We show that a semiconducting oxide that has been widely used in lead-acid batteries, β-PbO_2, hosts a topological semimetallic phase driven by both thermal expansion and electron-phonon coupling upon increasing temperature. We identify the interplay between the quasi-two-dimensional nature of the charge distribution of the valence band with the three-dimensional nature of the charge distribution of the conduction band as the microscopic mechanism driving this unconventional temperature dependence. Thus, we propose a general principle to search for and design novel topological materials whose topological order is stabilized by increasing temperature. This provides a clear roadmap for taking topological materials from the laboratory to technological devices.

O 109: Poster Session VIII: Poster to Mini-Symposium: Machine learning applications in surface science III

Time: Thursday 13:30–15:30 Location: P

O 109.1 Thu 13:30 P

Development of a Neural Network Potential for Metal-Organic Frameworks — •Marius Herbold and Jörg Behler — Georg-August Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

Metal-organic frameworks (MOFs) are crystalline porous materials with many applications in chemistry and materials science, from gas separation to heterogeneous catalysis. Computer simulations of chemical processes in MOFs are severely limited by the use of classical force fields (FFs), because most FFs are unable to describe bond formation and breaking. In principle, electronic structure methods, like density-functional theory (DFT), can overcome this problem, but often the required systems are too large for routine applications of DFT. A high-dimensional neural network potential (NNP) combines the advantages of both worlds - the accuracy of first principle methods with the efficiency of simple empirical potentials. Here we present a method to construct a NNP for MOFs using size-converged fragments only.

O 109.2 Thu 13:30 P

Predicting hydration layers on surfaces using deep learning — •Yashasvi S Ranawat[1], Ygor M Jaques[1], and Adam S Foster[1,2] — [1]Department of Applied Physics, Aalto Uiversity, Finland — [2]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Surface characterisation at the nano-scale of a mineral-water interface has applications in understanding many technological and natural processes dominated by the mineral-water interactions, for example biominerelisation, corrosion etc. Atomic Force Microscopy (AFM) has the potential to characterise such surfaces. The image mechanism is governed by the complex interplay of the tip with the hydration layers over the surface and hence high resolution requirements pose a challenge. A direct link between the AFM images and water density over a surface has paved the way for theoretical molecular dynamics methods to simulate the density over a given surface, and therefore the AFM image. The computationally intense theoretical approaches have helped with the surface characterisation. However the search space, given a hydration layer image, is wide and the approach is prohibitively expensive. Here we introduce deep learning methods to swiftly and reliably predict the hydration layer over a given surface. These methods are tested on the polymorphs of calcium carbonate.

O 109.3 Thu 13:30 P

In Silico prediction of antibacterial activity of sesquiterpene lactones using density-functional theory and quantitative structure-activity relationship methods — •Fabian Puga[1], Alicja Mikolajczyk[2], Paola Ordoñez[1], and Henry Pinto[1] — [1]Yachay Tech University, Ecuador — [2]University of Gdansk, Poland

Antibiotic resistance is a problem that involves every humanity. Therefore, the development of new and effective anti-bacterial components is of vital importance. Organic molecules called Sesquiterpene Lactones (STL) have shown a wide spectrum of biological activities especially antibacterial activity against methicillin-resistant staphylococcus aureus (MRSA). Unfortunately, the experimental methods to study the effectiveness of plant-based antibiotics are expensive and time-consuming. In order to tackle these limitations in silico studies can be applied to accelerate the development of more efficient antibiotics. In this study, electronic structure calculations on 21 STL were performed to develop a model capable to predicting the antibacterial activity of new STL molecules. By using an optimal combination of density-functional tight-binding method and ab initio density-functional theory calculations, we were able to calculate the most energetically favorable conformers, their atomic structure and physical-chemical properties. Then using these values QSAR models considering experimental antibacterial activity were developed. Preliminary results suggest that models that includes the HOMO and electronic energy correlates better the antibacterial activity. These results could allow reliable prediction of antibacterial activity for new STL.

O 109.4 Thu 13:30 P

Excitonic Wave Function Reconstruction from Near-Field Spectra Using Machine Learning Techniques — •Fulu Zheng[1], Sidhartha Nayak[2], and Alexander Eisfeld[2] — [1]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A general problem in quantum mechanics is the reconstruction of eigenstate wave functions from measured data. In the case of molecular aggregates, information about excitonic eigenstates is vitally important to understand their optical and transport properties. Strong interactions between the transition dipoles of the molecules lead to delocalized excitonic eigenstates where an electronic excitation is coherently shared by many molecules [1]. Here we show that from spatially resolved near field spectra it is possible to reconstruct the underlying delocalized aggregate eigenfunctions [2, 3]. Although this high-dimensional nonlinear problem defies standard numerical or analytical approaches, we have found that it can be solved using a convolutional neural network. For both one-dimensional and two-dimensional aggregates the reconstruction is robust to various types of disorder and noise. The methodology can be easily applied to more complicated cases, promoting information extraction from experimental data in a wide variaty of applications.

[1] A. Eisfeld, C. Marquardt, A. Paulheim, and M. Sokolowski, Phys. Rev. Lett. 119, 097402 (2017).
[2] X. Gao and A. Eisfeld, J. Phys. Chem. Lett. 9, 6003 (2018).
[3] F. Zheng, X. Gao and A. Eisfeld, Phys. Rev. Lett. 123, 163202 (2019).

O 109.5 Thu 13:30 P

Prediction of energetics in nucleation and non-equilibrium growth using machine learning — •Thomas Martynec[1], Sabine H. L. Klapp[1], and Stefan Kowarik[2] — [1]Technische Universität Berlin — [2]Karl-Franzens-Universität Graz

Machine learning is playing an increasing role in the discovery of novel materials and may also facilitate the search for optimum growth conditions of crystals and thin films of these materials. We demonstrate that a convolutional neural network that is trained on snapshots of surface configurations can predict the underlying lateral binding energy and diffusion barrier. Specifically, a single KMC image of the morphology is sufficient to determine the energy barriers with high accuracy for energies in the range of 100 - 550 meV. The CNN can also make correct predictions for images with noise and lower than atomic-scale resolution. We expect our machine learning method to be of use for both, fundamental studies of growth kinetics and for faster optimization of low defect materials growth.

O 109.6 Thu 13:30 P

Predicting the activity and selectivity of bimetallic metal catalysts for ethanol reforming using machine learning — •Nongnuch Artrith — Columbia Center for Computational Electrochemistry, Columbia University, New York, NY, 10027 USA

Machine learning (ML) has proven a powerful tool for accelerating the computational characterization of energy materials. There is a growing number of case studies identifying descriptors of catalytic performance using ML instead of physical intuition. ML is ideally suited for the pattern detection in large uniform data sets, but consistent experimental data sets on catalyst studies are often small. Here we demonstrate how a combination of machine learning and first-principles calculations can be used to extract knowledge from a small set of experimental data.[1] The approach is based on combining a complex ML model trained on a computational library of transition-state energies with simple linear regression models of experimental catalytic activities and selectivities. Using the combined model, we identify the key C-C bond-scission reactions involved in ethanol reforming and perform a computational screening for ethanol reforming on monolayer bimetallic catalysts with architectures TM-Pt-Pt(111) and Pt-TM-Pt(111) (TM = 3d transition metals). The model also predicts four promising catalyst compositions for future experimental studies. The approach is not limited to ethanol reforming but is of general use for the interpretation of experimental observations as well as for the computational discovery of catalytic materials.[2] [1] N. Artrith, Z. Lin, J.G. Chen, *ACS Catal.* **10** (2020) 9438–9444. [2] N. Artrith, *Matter* **3** (2020) 985–986.

O 109.7 Thu 13:30 P

Using Neural Evolution algorithm to generate disordered High Entropy Alloys structures — •Conrard Giresse TETSASSI FEUGMO[1], Kevin Ryczko[2,3], Abu Anand[4], Chandra Singh[4], and Isaac Tamblyn[1,2,3] — [1]National Research Council Canada — [2]Department of Physics , University of Ottawa — [3]Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada — [4]Department of Materials Science and Engineering , University of Toronto

A new inverse design approach using pair distribution functions and atomic properties have been implemented. The generative model combines artificial neural networks (ANNs) and genetic algorithms (GAs) to build high disordered crystal structures. The method was introduced by Ryczko et. al. [J. Phys. Chem. C 124, 26117 (2020).] to optimize the doping of graphene-based three-terminal devices for valleytronic applications. Models have been optimized for multicomponent alloy systems such as High Entropy Alloys (HEAs) and structures have been compared to the Special quasi-random (SQSs). Unlike the SQSs, the average optimization time increase slow with the size of the system (ration 1.4). Moreover, the model is able to generate structures with more than 8000 atoms in a few hundred seconds. Finally selected generated structures have been using to compute properties such as the elastic constants, the bulk modulus, and the Poisson ratio, and the results are similar to the SQSs.

O 109.8 Thu 13:30 P

Automatic image evaluation of aberration-corrected HRTEM images of 2D materials. — •Christopher Leist, Haoyuan Qi, and Ute Kaiser — Central Facility for Electron Microscopy,of Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm, Germany

Aberration-corrected high-resolution transmission electron microscopy (HRTEM) allows for unambiguous elucidation of atomic structures down to sub-Angstrom scale. By determining the positions of each single atom, the distribution and local variation of bond lengths and angles can be evaluated statistically. However, conventional image analysis methods, e.g., handcrafted filter kernels, often requires heavy user supervision and tremendous time cost, posing strong limitations on the data volume for statistical analysis. The incompetence in handling big data volume also incurs the risk of user-induced selection bias, leading to overestimation of low-probability phenomena. Here, we developed a neural network of U-net architecture for automatic analysis of atomic positions in HRTEM images. A combination of networks can be applied to automatically evaluate image series, including automatic exclusion of image regions unusable for evaluation. This method results in large statistics thus reducing the impact of individual errors. The networks are trained with simulated data which reduces user bias and gives a time inexpensive way of generating the required training data. Its implementation on various 2D carbon materials is compared to one another. The distribution of bond angles in CVD graphene, determined by this method, shows excellent agreement with literature.

O 110: Poster Session VIII: Poster to Mini-Symposium: Dzyaloshinskii-Moriya Interaction (DMI) in magnetic layered systems

Time: Thursday 13:30–15:30 Location: P

O 110.1 Thu 13:30 P

Magnetic exchange interactions at proximity of a superconductor — •Uriel Allan Aceves Rodriguez[1], Sascha Brinker[1], Filipe Souza Mendes Guimaraes[2], and Samir Lounis[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [3]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Magnetic impurities coupled to superconductors give rise to a plethora of rich physics such as sub-gap states like Yu-Shiba-Rusinov states and Majorana zero modes, which constitute key mechanisms on the road towards a topological quantum computer. The interplay of spin-orbit coupling and (non-collinear) magnetism enrich the complexity and topological nature of the in-gap states hosted in proximity-induced superconductors. However, little is known about the impact of superconductivity on the different contributions to the magnetic exchange interactions, like the bilinear isotropic exchange and the Dzyaloshinskii-Moriya interaction — and in turn the impact on the magnetic textures. In this work, we propose a method for the extraction of the tensor of exchange interactions in the superconducting regime as described in the framework of the Bogoliubov-de Gennes method. We investigate various 3*d* monolayers deposited on the Nb(110) surface based on our multi-orbital tight-binding code TITAN.

–Work funded by Horizon 2020–ERC (CoG 681405–DYNASORE).

O 110.2 Thu 13:30 P

Stabilizing Zero-Field Skyrmions with Cobalt-decorated Edges in Ultrathin Films — •Jonas Spethmann, Elena Vedmedenko, Roland Wiesendanger, André Kubetzka, and Kirsten von Bergmann — Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Magnetic skyrmions are promising candidates to serve as information carriers in the emerging field of spintronic memory and logic devices. In such devices it is quintessential to prevent the loss of information. One common pathway towards skyrmion destruction is via the edge of the skyrmion material. This could prove detrimental in any potential skyrmion racetrack device, due to the magnus force driving the skyrmions towards the racetrack edge [1]. In our model system, a bilayer of Pd/Fe on the Ir(111) surface [2], skyrmion collapse at the edge becomes the prevalent skyrmion destruction pathway for small external magnetic fields [3]. We modify the Pd/Fe island edge by adding Co to the system and investigate it using spin-polarized STM. The Co-decorated edges strongly affect the magnetic ground state of Pd/Fe, by changing the spin spiral propagation direction. Surprisingly, we also observe single skyrmions and occasionally 2π skyrmions in the magnetic virgin state. Additionally, we find that at fields above 1 T skyrmions can pin to the Co edge without collapsing and utilize spin dynamics simulations to investigate this phenomenon.

[1] W. Jiang *et al.*, Nature Physics **13**, 162-169 (2018).
[2] N. Romming *et al.*, Science **341**, 636-639 (2013).
[3] P. F. Bessarab *et al.*, Sci. Rep. **8**, 3433 (2018).

O 110.3 Thu 13:30 P

First-principles study of exchange frustration and DMI in Rh/Co/Fe/Ir multilayers — •Felix Nickel, Sebastian Meyer, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel

Magnetic skyrmions are promising for data storage, logic devices, and neuromorphic computing. Materials, which can host nanoscale skyrmions in zero magnetic field at room temperature, are desirable for such applications. Recently, it has been shown that ultrathin Rh/Co films on Ir(111) exhibit skyrmions with diameters below 10 nm at zero magnetic field [1]. In magnetic multilayers, room temperature skyrmion with diameters of 30 nm - 90 nm have been reported [2]. The Dzyaloshinskii-Moriya interaction (DMI), the exchange interaction, and the magnetocrystalline anisotropy are the main characteristics that make materials capable of hosting such complex spin structures. Here, we present density functional theory calculations for transition-metal multilayers consisting of Co, Fe, Ir, and Rh layers. We varied the thickness and material for the magnetic layer (Co and Fe) and the spacer layer (Ir and Rh), as well as the stacking of the individual layers. We present how the magnetic interactions depend on those structural conditions. We demonstrate that it is possible to transfer the properties of the ultrathin film system Rh/Co/Ir(111) [1] to a multilayer system.

[1] Meyer *et al.*, Nat. Commun. **10**, 3823 (2019)
[2] Moreau-Luchaire *et al.*, Nat. Nanotechnol. **11**, 444 (2016)

O 110.4 Thu 13:30 P

Emergence of Magnetic Skyrmions in Ultrathin Films of Manganese on W(001) at High Magnetic Fields — •Reiner Brüning, Kirsten von Bergmann, André Kubetzka, and Roland Wiesendanger — Festkörper- und Nanostrukturphysik, Hamburg, Deutschland

Topological spin textures like skyrmions with diameters on the order of a few nanometers are promising objects for the application in the field of spintronics. Whereas typical skyrmion systems like Pd/Fe bilayers on Ir(111) [1] have hexagonal symmetry, here, we investigate a monolayer of Mn on the square lattice of W(001) using spin-polarized scanning tunneling microscopy at 4.2 K. At $B = 0$ T, the known magnetic ground state of a spin spiral with two rotational domains [2] is observed. The measurements at 9 T show that the external magnetic field initializes the transition from the spin spiral to small skyrmion areas and leads to a coexisting state of the spin spiral phase and the skyrmion phase. Thereby, the skyrmions arrange themselves in small areas in a hexagonal like order, according to the recent simulations of the sample system [3]. At high bias voltages of 1-2 V we observe square magnetic patterns, even in zero magnetic fields. We interpret these square patterns as time-averaged superpositions of rotational spiral domains, driven by excitations by the tunneling electrons.

[1] N. Romming *et al.*, Science, **341**, (2013)
[2] P. Ferriani *et al.*, Phys. Rev. Lett. **101**, 027201 (2008)
[3] A. K. Nandy *et al.*, Phys. Rev. Lett. **116**, 177202 (2016)

O 110.5 Thu 13:30 P

Dzyaloshinskii-Moriya interaction induced by an ultrashort electromagnetic pulse: Application to coherent (anti)ferromagnetic skyrmion nucleation — •Louise Desplat[1], Sebastian Meyer[2], Juba Bouaziz[3], Patrick M. Buhl[4], Samir Lounis[3], Bertrand Dupé[5,2,1], and Paul-Antoine Hervieux[1] — [1]Université de Strasbourg, CNRS, IPCMS, Strasbourg, France — [2]Nanomat/Q-mat/CESAM, Université de Liège, Belgium — [3]Peter Grünberg Institut and Institute for Advanced Simulation, FZ Jülich and JARA, Jülich, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [5]FNRS, Brussels, Belgium

We show how, at ultrashort timescales, a Dzyaloshinskii-Moriya interaction can be generated in metallic thin films by an electromagnetic pulse. This interaction originates from the spin-orbit coupling between the pulse-induced electric field and the spins of the delocalized electrons of the material[1]. We perform density functional theory calculations to estimate the strength of this field-induced interaction in Fe, Co, Ni, and Mn monolayers, as well as FePt and MnPt alloys. Last, using atomistic simulations, we demonstrate how an isolated (anti)ferromagnetic skyrmion can be coherently nucleated from the collinear background by an electric field pulse at the 100-fs timescale[2]. These results provide a new handle for an ultrafast, coherent control of noncollinear magnetic states.

[1] Imamura et al. PRB 69, 121303(R) (2014) ; Hinschberger et al., PRA 93, 042117 (2016) ; Bouaziz et al. New J. Phys. 19, 023010 (2017) [2] Desplat et al. ArXiv:2011.12055 (2020)

O 111: Key Note VIII

Time: Thursday 15:30–16:00 Location: R1

Plenary Talk O 111.1 Thu 15:30 R1

Light-matter interaction at the atomic scale — •Klaus Kern — MPI for Solid State Research, Stuttgart, Germany — Institute of Physics, EPFL, Lausanne, Switzerland

Light-matter interaction drives many different systems such as optoelectronic devices like light-emitting diodes and solar cells, biological structures like photosystem II, and potential future quantum devices. The absorption or emission of light is typically a local process occurring on the sub-nanometer scale. Concomitantly, the involved processes are fast and take place on attosecond to picosecond time scales. The interaction of electromagnetic radiation with matter at atomic scales can be studied by using a scanning tunneling microscope, whereby the two separate domains of spatial and temporal resolution at its atomic limits are accessed by coupling light into or extracting light from the tunnel junction. Electromagnetic radiation couples with matter through the interaction with charge carriers (electrons and holes), leading to excitations such as electronic transitions, collective oscillations, excitons, and spin flips. New approaches in which light interacts with the tunnel junction itself or with a quantum system in the junction now allow studying these excitations with highest spatial and temporal resolution. In this talk, I discuss the powerful union of photonics and scanning probe techniques and highlight the frontiers of current research.

O 112: Announcement of Gerhard Ertl Young Investigator Award and Concluding Remarks

Time: Thursday 16:00–16:15 Location: R1

Ulrike Diebold, TU Vienna, Vice-Chair Surface Science Division

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