Surface Science Division
Fachverband Oberflächenphysik (O)

Wolf Widdra
Martin-Luther-Universität Halle-Wittenberg
von-Danckelmann-Platz 3
06120 Halle
wolf.widdra@physik.uni-halle.de

Overview of Invited Talks and Sessions

(Lecture halls HSZ/AUDI, HSZ/0201, HSZ/0204, HSZ/0401, HSZ/0403, TRE/PHYS, TRE/MATH, and WILL/A317; Poster P2)

Invited Talks

O 2.3	Mon	11:00–11:30	HSZ/0201	**Superconducting Fermi arcs.** — •Andrii Kuibarov, Susmita Changdar, Oleksandr Suvorov, Luminita Harnagea, Bernd Büchner, Sergey Borisenko
O 5.1	Mon	10:30–11:00	HSZ/0403	**Can the mineral-water interface save the world? Mineral carbonation, enhanced weathering and negative emissions** — •Philip Pogge von Strandmann
O 5.4	Mon	11:30–12:00	HSZ/0403	**Machine learning exploration of water binding and ice nucleation at silicate and carbon surfaces** — •Mie Andersen
O 7.1	Mon	10:30–11:00	TRE/MATH	**Magnetic Order in 2D Materials Beyond Bulk Constraints** — •Jeison Fischer
O 8.3	Mon	11:00–11:30	WILL/A317	**Controlling nanostructures on surfaces via intermolecular interactions** — •Yunjun Cao
O 14.1	Mon	15:00–15:30	TRE/MATH	**Spin and time-resolved ARPES and the orbital angular momentum of light** — Pierre Nonnon, Romain Géneaux, Karol Hricovini, Christine Richter, David Bresteau, •Mauro Fanciulli
O 15.1	Mon	15:00–15:30	WILL/A317	**Tuning Spin-1/2 Interactions in Graphene: From Long-Range Coupling to Altermagnetic Order** — •Beatriz Viña-Bausá, Manuel A. García-Blázquez, Antonio T. Costa, Joao C. G. Henriques, Roberto Carrasco, Eva Cortés-del Río, Diego Expósito, Pierre Mallet, Jean-Yves Veuillen, Joaquín Fernandez-Rossier, Juan J. Palacios, Iván Brihuega
O 33.1	Tue	10:30–11:00	HSZ/0201	**During-synthesis functionalization of graphene layers** — •Cristina Africh
O 36.1	Tue	10:30–11:00	HSZ/0403	**Acidity in nanoconfinement from ab initio and NNPs simulations** — Anthony Baldo, Muhammad Saleh, Kevin Leung, •Marialore Sulpizi
O 36.4	Tue	11:30–12:00	HSZ/0403	**Living Interfaces: Dissolution and Precipitation Processes at Mineral-Brine Interfaces Revealed by AFM** — •Igor Siretanu, Vincenzo Alagia, Saravana Kumar, Shilpa Mohanakumar, Max Nederstigt, Chinmay Shukla, Michel Duits, Frieder Mugele
O 37.1	Tue	10:30–11:00	TRE/PHYS	**Calculations of excited electronic states by converging on saddle points on the electronic energy surface** — •Hannes Jonsson
O 37.4	Tue	11:30–12:00	TRE/PHYS	**Many-Body Theory meets Electrochemistry: Electronic Structure of Cathode Materials** — •Silke Biermann
O 39.3	Tue	11:00–11:30	WILL/A317	**Electric double layer of platinum electrodes** — •Marc Koper
O 39.6	Tue	12:00–12:30	WILL/A317	**First-principles modelling of electrochemical interfaces** — •Axel Gross
O 51.1	Tue	14:30–15:00	TRE/MATH	**Ultrafast aqueous electric double-layer dynamics** — •Mischa Bonn
O 51.3	Tue	15:15–15:45	TRE/MATH	**Interface-specific nonlinear THz spectroscopy** — •Chuanshan Tian

O 52.1	Tue	14:30–15:00	WILL/A317	**Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope** — •Friedrich Esch
O 55.3	Wed	11:00–11:30	HSZ/0204	**Cationic Mixing in Ultrathin Oxide Films: How substrate and oxygen conditions control nanoalloying.** — •Jacek Goniakowski
O 57.1	Wed	10:30–11:00	HSZ/0403	**From Plasmonic Near-Fields to Electron Dynamics - A Photoemission Perspective** — •Pascal Dreher
O 60.1	Wed	10:30–11:00	WILL/A317	**Disentangling the origins of spin polarization in (inverse) photoemission from solid surfaces** — •Jürgen Henk
O 64.1	Wed	15:00–15:30	HSZ/0403	**Cantilever based Scanning Force Microscopy: Ultimate Sensitivity and Quantitative Imaging of Nanoscale Spin Textures** — •Hans J. Hug
O 64.6	Wed	16:30–17:00	HSZ/0403	**Single-spin sensing: A molecule-on-tip approach** — •Laurent Limot
O 66.1	Wed	15:00–15:30	TRE/MATH	**Ultrafast exciton dynamics in 2D semiconductors and electric field gated devices** — •Jan Philipp Bange
O 67.1	Wed	15:00–15:30	WILL/A317	**New frontiers of one step model of photoemission for quantum materials** — •Jan Minar
O 78.1	Thu	10:30–11:00	HSZ/0401	**The Wendelstein 7-X plasma vessel vacuum system from a scientific perspective** — •Georg Schlisio, Torsten Bräuer, Stylianos Varoutis, Paul McNeely, Dirk Hartmann, Chandra Prakash Dhard, Dirk Naujoks, Victoria Hak, the W7-X team
O 82.1	Thu	10:30–11:00	WILL/A317	**Low-energy inverse photoelectron spectroscopy (LEIPS): probing unoccupied states and conduction band structure in functional materials** — •Hiroyuki Yoshida
O 82.2	Thu	11:00–11:30	WILL/A317	**Enhanced Sensitivity in Low-Energy Inverse Photoemission Spectroscopy with an Off-Axis Parabolic Mirror for Efficient Light Collection** — •Yongsup Park, Jong-Am Hong, Kyu-Myung Lee, Min-Jae Maeng
O 85.1	Thu	15:00–15:30	HSZ/0401	**From light to pressure: Laser-based quantum technologies for the realization of high-precision pressure and vaccum standards** — •Tom Rubin
O 86.1	Thu	15:00–15:30	HSZ/0403	**Ultrafast Dynamics at Surfaces with Machine Learning Surrogates** — •Reinhard Maurer
O 94.1	Fri	9:30–10:00	HSZ/0204	**Surface Chemistry on Copper Oxides** — •Dario Stacchiola
O 97.1	Fri	9:30–10:00	TRE/PHYS	**Questions of Selectivity in Electrocatalysis** — •Vanessa J. Bukas
O 98.1	Fri	9:30–10:00	TRE/MATH	**Electron-phonon interactions in the time domain: from nonequilibrium phonon dynamics to theoretical spectroscopy** — •Fabio Caruso

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

See SYFC for the full program of the symposium.

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber, Manuel Meierhofer, Ulrich Höfer
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes
SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — Daniel Lesko, Tobias Weitz, Weizhe Li, Selina Nöcker, Celina Hüttner, Tamara Pröbster, Simon Wittigschlager, Christian Heide, Ofer Neufeld, •Peter Hommelhoff

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

O 1.1–1.1	Mon	9:30–10:15	TRE/PHYS	**Topical Talk Wulfhekel (joint session O/TT)**
O 2.1–2.7	Mon	10:30–12:30	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states I**
O 3.1–3.7	Mon	10:30–12:15	HSZ/0204	**Scanning probe techniques: Method development I**
O 4.1–4.7	Mon	10:30–12:15	HSZ/0401	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules I**
O 5.1–5.6	Mon	10:30–12:30	HSZ/0403	**Focus Session: Mineral-water interfaces I**
O 6.1–6.8	Mon	10:30–12:30	TRE/PHYS	**Organic molecules on inorganic substrates: Adsorption and growth I**
O 7.1–7.7	Mon	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)**
O 8.1–8.7	Mon	10:30–12:30	WILL/A317	**Nanostructures at surfaces:1D, 2D, networks I**
O 9.1–9.12	Mon	15:00–18:00	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties I**
O 10.1–10.11	Mon	15:00–17:45	HSZ/0204	**2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)**
O 11.1–11.8	Mon	15:00–17:00	HSZ/0401	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules II**
O 12.1–12.11	Mon	15:00–17:45	HSZ/0403	**Scanning probe microscopy: light matter interaction at atomic scales**
O 13.1–13.12	Mon	15:00–18:00	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry I**
O 14.1–14.11	Mon	15:00–18:00	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces I**
O 15.1–15.11	Mon	15:00–18:00	WILL/A317	**Spins on surfaces at the atomic scale I**
O 16.1–16.2	Mon	18:00–20:00	P2	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster**
O 17.1–17.12	Mon	18:00–20:00	P2	**Spins on surfaces at the atomic scale – Poster**

O 18.1–18.6	Mon	18:00–20:00	P2	**New methods: Theory – Poster**
O 19.1–19.10	Mon	18:00–20:00	P2	**Vacuum Science & Technology: Theory and Applications – Poster**
O 20.1–20.1	Mon	18:00–20:00	P2	**Electronic structure theory – Poster**
O 21.1–21.2	Mon	18:00–20:00	P2	**Surface magnetism – Poster**
O 22.1–22.6	Mon	18:00–20:00	P2	**Surface dynamics – Poster**
O 23.1–23.10	Mon	18:00–20:00	P2	**Catalysis and surface reactions – Poster**
O 24.1–24.7	Mon	18:00–20:00	P2	**Solid-liquid interfaces: Reactions and electrochemistry – Poster**
O 25.1–25.2	Mon	18:00–20:00	P2	**Solid-liquid interfaces: Structure, spectroscopy – Poster**
O 26.1–26.5	Mon	18:00–20:00	P2	**Plasmonics and nanooptics: Fabrication, characterization and applications – Poster**
O 27.1–27.7	Mon	18:00–20:00	P2	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy – Poster**
O 28.1–28.8	Mon	18:00–20:00	P2	**Oxide and insulator surfaces: Structure, epitaxy and growth – Poster**
O 29.1–29.3	Mon	18:00–20:00	P2	**Oxides and insulators: Adsorption and reaction of small molecules – Poster**
O 30.1–30.4	Mon	18:00–20:00	P2	**Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster**
O 31.1–31.6	Mon	18:00–20:00	P2	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster**
O 32.1–32.1	Tue	9:30–10:15	TRE/PHYS	**Topical Talk Witte**
O 33.1–33.7	Tue	10:30–12:30	HSZ/0201	**Graphene: Growth, structure and substrate interaction (joint session O/HL)**
O 34.1–34.8	Tue	10:30–12:30	HSZ/0204	**Catalysis and surface reactions I**
O 35.1–35.7	Tue	10:30–12:15	HSZ/0401	**Organic molecules on inorganic substrates: Adsorption and growth II**
O 36.1–36.6	Tue	10:30–12:30	HSZ/0403	**Focus Session: Mineral-water interfaces II**
O 37.1–37.6	Tue	10:30–12:30	TRE/PHYS	**Electronic structure theory I**
O 38.1–38.8	Tue	10:30–12:30	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces II**
O 39.1–39.6	Tue	10:30–12:30	WILL/A317	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces I**
O 40.1–40.21	Tue	14:00–16:00	P2	**Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)**
O 41.1–41.4	Tue	14:00–16:00	P2	**Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)**
O 42.1–42.9	Tue	14:00–16:00	P2	**Electronic structure of surfaces: Spectroscopy, surface states – Poster**
O 43.1–43.17	Tue	14:00–16:00	P2	**Scanning probe microscopy: light matter interaction at atomic scales – Poster**
O 44.1–44.17	Tue	14:00–16:00	P2	**Scanning probe techniques: Method development – Poster**
O 45.1–45.11	Tue	14:00–16:00	P2	**Organic molecules on inorganic substrates: Adsorption and growth – Poster**
O 46.1–46.11	Tue	14:00–16:00	P2	**Organic molecules on inorganic substrates: electronic, optical and other properties – Poster**
O 47.1–47.4	Tue	14:30–15:30	HSZ/0201	**New methods: Theory**
O 48.1–48.6	Tue	14:30–16:00	HSZ/0204	**Metal & Semiconductor substrates: Structure, epitaxy and growth**
O 49.1–49.5	Tue	14:30–15:45	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy I**
O 50.1–50.7	Tue	14:30–16:15	TRE/PHYS	**Electronic structure theory II**
O 51.1–51.3	Tue	14:30–15:45	TRE/MATH	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II**
O 52.1–52.5	Tue	14:30–16:00	WILL/A317	**Oxide and insulator surfaces: Structure, epitaxy and growth I**
O 53.1–53.1	Wed	9:30–10:15	TRE/PHYS	**Topical Talk Parkinson**
O 54.1–54.8	Wed	10:30–12:30	HSZ/0201	**Nanostructured surfaces and thin films**
O 55.1–55.7	Wed	10:30–12:30	HSZ/0204	**Oxide and insulator surfaces: Structure, epitaxy and growth II**
O 56.1–56.7	Wed	10:30–12:15	HSZ/0401	**Scanning probe techniques: Method development II**

O 57.1–57.7	Wed	10:30–12:30	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy II**
O 58.1–58.8	Wed	10:30–12:30	TRE/PHYS	**Organic molecules on inorganic substrates: Adsorption and growth III**
O 59.1–59.8	Wed	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)**
O 60.1–60.7	Wed	10:30–12:30	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission I**
O 61.1–61.11	Wed	15:00–17:45	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties II**
O 62.1–62.11	Wed	15:00–17:45	HSZ/0204	**Graphene: Electronic structure, excitations, etc. (joint session O/TT)**
O 63.1–63.11	Wed	15:00–17:45	HSZ/0401	**Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)**
O 64.1–64.9	Wed	15:00–17:45	HSZ/0403	**Surface Magnetism**
O 65.1–65.12	Wed	15:00–18:00	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry II**
O 66.1–66.10	Wed	15:00–17:45	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces III**
O 67.1–67.11	Wed	15:00–18:00	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission II**
O 68.1–68.6	Wed	18:00–20:00	P2	**Nanostructured surfaces and thin films – Poster**
O 69.1–69.13	Wed	18:00–20:00	P2	**Nanostructures at surfaces:1D, 2D, networks – Poster**
O 70.1–70.7	Wed	18:00–20:00	P2	**2D materials: Stacking and heterostructures – Poster (joint session O/TT)**
O 71.1–71.23	Wed	18:00–20:00	P2	**2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
O 72.1–72.6	Wed	18:00–20:00	P2	**2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)**
O 73.1–73.6	Wed	18:00–20:00	P2	**Graphene: Growth, structure and substrate interaction – Poster**
O 74.1–74.9	Wed	18:00–20:00	P2	**Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
O 75.1–75.1	Thu	9:30–10:15	TRE/PHYS	**Topical Talk Bibes (joint session O/TT)**
O 76.1–76.7	Thu	10:30–12:15	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states II**
O 77.1–77.7	Thu	10:30–12:15	HSZ/0204	**Nanostructures at surfaces:1D, 2D, networks II**
O 78.1–78.6	Thu	10:30–12:15	HSZ/0401	**Vacuum Science & Technology: Theory and Applications I**
O 79.1–79.7	Thu	10:30–12:15	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy III**
O 80.1–80.5	Thu	10:30–13:00	TRE/PHYS	**Gerhard Ertl Young Investigator Award Competition**
O 81.1–81.7	Thu	10:30–12:15	TRE/MATH	**Catalysis and surface reactions II**
O 82.1–82.6	Thu	10:30–12:30	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission III**
O 83.1–83.10	Thu	15:00–17:30	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties III**
O 84.1–84.11	Thu	15:00–17:45	HSZ/0204	**2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**
O 85.1–85.7	Thu	15:00–17:00	HSZ/0401	**Vacuum Science & Technology: Theory and Applications II**
O 86.1–86.10	Thu	15:00–17:45	HSZ/0403	**Surface dynamics**
O 87.1–87.9	Thu	15:00–17:15	TRE/PHYS	**Solid-liquid interfaces: Structure, spectroscopy**
O 88.1–88.11	Thu	15:00–17:45	TRE/MATH	**Catalysis and surface reactions III**
O 89.1–89.12	Thu	15:00–18:00	WILL/A317	**Spins on surfaces at the atomic scale II**
O 90	Thu	17:15–18:15	HSZ/0401	**Members' Assembly of the Vacuum Science and Technology Divison (VA)**
O 91	Thu	19:00–19:30	HSZ/AUDI	**Members' Assembly**
O 92	Thu	19:30–20:30	HSZ/AUDI	**Post-Deadline Session**
O 93.1–93.10	Fri	9:30–12:00	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states III**
O 94.1–94.11	Fri	9:30–12:30	HSZ/0204	**Oxides and insulators: Adsorption and reaction of small molecules**

O 95.1–95.12	Fri	9:30–12:30	HSZ/0401	**2D Materials: Stacking and heterostructures (joint session O/HL/TT)**
O 96.1–96.12	Fri	9:30–12:30	HSZ/0403	**Plasmonics and nanooptics: Fabrication, characterization and applications**
O 97.1–97.11	Fri	9:30–12:30	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry III**
O 98.1–98.10	Fri	9:30–12:15	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces IV**
O 99.1–99.12	Fri	9:30–12:30	WILL/A317	**Spins on surfaces at the atomic scale III**
O 100.1–100.1	Fri	13:15–14:00	TRE/PHYS	**Closing Talk Steinrück**

Members' Assembly of the Vacuum Science and Technology Divison (VA)

Thursday 17:15–18:15 HSZ/0401

Members' Assembly of the Surface Science Division

Thursday 18:00–19:00 HSZ/AUDI

O 1: Topical Talk Wulfhekel (joint session O/TT)

Time: Monday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 1.1 Mon 9:30 TRE/PHYS

Vortices, inter-band coupling and inelastic QPI in two band superconductors — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology

The majority of superconductors have more than one Fermi surface, on which the electrons pair below the critical temperature, yet their behavior can be well described by a single-band Bardeen-Cooper-Schrieffer theory. This is mostly due to interband scattering, especially in superconductors in the dirty limit, rigidly linking the pairing amplitude of the bands. We here lift this constrain and study the behavior of the ultra-pure two-band superconductor Pb. We show that at low temperatures, it is neither of type I nor type II and superconducting vortices of arbitrary flux quanta can be formed. We show that on the non-spherical Fermi surfaces, a modified index theory is needed for the description of in gap states in vortices. Further, the two condensates are only weakly coupled and can be individually manipulated. By studying stacking fault tetrahedra, we demonstrate local tuning of interband coupling ranging from weak to strong and the modification of the superconducting order parameters from two well separated gaps to one merged gap around defects. The experiments critically test the theory of multiband superconductors and give a route to access a wide range of predicted quantum effects in these systems. Finally, we demonstrate that quasi particle interference is also possible in the inelastic tunneling channel enabling the imaging of standing phonons with STM.

O 2: Electronic structure of surfaces: Spectroscopy, surface states I

Time: Monday 10:30–12:30 Location: HSZ/0201

O 2.1 Mon 10:30 HSZ/0201

Unveiling the spin texture of the topological surface state in Sb(111) — •Xin Liang Tan[1], Arthur Ernst[2], Anders Christian Mathisen[1], Stefanie Suzanne Brinkman[1], Fabian Göhler[1], Chul Hee Min[1], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway — [2]Institut für Theoretische Physik, Johannes Kepler Universität, A 4040 Linz, Austria

Spin-resolved momentum microscopy is a powerful tool for mapping the complete Fermi surface and spin texture of two-dimensional electronic states. Here, we present spin- and momentum-resolved Sb(111) surface state, a benchmark system exhibiting strong spin-orbit coupling and a non-trivial topology. Using a continuous-wave vacuum-ultraviolet laser (h$\nu = 6eV$) for photoexcitation, we achieve efficient k-space mapping of the in-plane spin-polarization components over the full surface Brillouin zone. We will present experimental data obtained for different light polarizations. Our results are compared to first-principles calculations.

[1] X.L. Tan et al., Ultramicroscopy 253, 113820 (2023).
[2] C. Tusche et al., Ultramicroscopy 159, 520 (2015).
[3] D. Hsieh et al., Science 323, 919-922(2009).
[4] H. Ishida. Phys., Rev. B 90, 235422 (2014).

O 2.2 Mon 10:45 HSZ/0201

Surface Electronic Structure of Magnetic Kagome Metal GdV$_6$Sn$_6$ — •Robin P. Forster[1], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Gustav Bihlmayer[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]JCNS Forschungszentrum-Jülich — [3]PGI-1 Forschungszentrum-Jülich

The magnetic Kagome metal GdV$_6$Sn$_6$ combines in a single material phenomena such as van Hove Singularities [1,2,3], local moments of the 4f electrons of Gd, and itinerant V 3d electrons [4], providing a platform to study their complex magentic and electronic interactions. We have performed termination-dependent micro-ARPES measurements of paramagnetic GdV$_6$Sn$_6$ with 20 μm real-space resolution at 20 K [5]. A series of scans over a photon energy range between 75 eV and 200 eV enabled the distinction between surface and bulk states. We have chosen $h\nu$ of 80 and 130 eV for detailed ARPES scans. In addition, XPS measurements and DFT-GGA slab calculations were performed, which can be used to investigate surface terminations. Preliminary circular-dirchroic ARPES maps exhibit multiple sign inversions that stem from a combination of initial state orbital angular momenta and photoemission final state scattering [6]. [1] PRL 127, 266401 (2021) [2] RRL 17, 2300083 (2023) [3] Sci. Adv. 8, 38 (2022) [4] JPSJ 90, 124704 (2021) [5] PRB 104, 235139 (2021) [6] arXiv:2410.19652 (2024).

Invited Talk O 2.3 Mon 11:00 HSZ/0201

Superconducting Fermi arcs. — •Andrii Kuibarov, Susmita Changdar, Oleksandr Suvorov, Luminita Harnagea, Bernd Büchner, and Sergey Borisenko — Leibnitz Institute for Solid State and Materials Research, Dresden, Germany

PtBi$_2$ is a trigonal non-centrosymmetric material that has recently drawn attention as a natural platform for topological superconductivity, without the need for engineered heterostructures. Recent STM studies have strengthened this claim by showing a superconducting gap with size up to 20 meV and critical temperature around 45 K.

Using angle-resolved photoemission spectroscopy, we demonstrate that both terminations of PtBi$_2$ expose Fermi arc surface states, which become superconducting at approximately 15 K with a gap size up to 3 meV, while the bulk of the material remains metallic, making PtBi$_2$ a surface-only superconductor. Further momentum-resolved gap measurements have shown that the superconducting gap on the Fermi arcs is anisotropic, with the superconducting node located in the center of six Fermi arcs, making it the first *i-wave ($l = 6$)* superconductor. This anisotropy implies the formation of Majorana surface cones and predicts robust zero-energy flat-band Majorana states at the hinges of the crystal.

O 2.4 Mon 11:30 HSZ/0201

From low- to high-energy photoelectron diffraction: Novel theoretical approaches and Kikuchi diffraction analysis — •Trung-Phuc Vo[1], Olena Tkach[2], Didier Sébilleau[3], Olena Fedchenko[2], Hans-Joachim Elmers[2], Gerd Schönhense[2], and Ján Minár[1] — [1]Univ. of West Bohemia in Pilsen, Czech Republic — [2]Univ. of Mainz, Germany — [3]Univ. of Rennes, France

Time-of-flight momentum microscopy (ToF-MM) enables simultaneous energy- and momentum-resolved mapping of the full photoelectron distribution. Its sensitivity to the strong energy dependence of Kikuchi patterns [1,2] requires advanced theoretical modeling, especially across the broad energy range accessible with modern large-k-field setups [3]. We present a fully relativistic multiple-scattering study of fine diffraction features in core-level photoemission from Ge(100) and Si(100) over kinetic energies from 106 to 4174 eV [4]. Our one-step calculations avoid cluster-size convergence issues and include inelastic scattering to describe pattern broadening. For the first time, we reproduce circular dichroism in the angular distribution of Si(100) 1s with asymmetries up to 31%, and capture both bulk- and surface-sensitive diffraction features. The simulations show good agreement with experimental data obtained using circularly polarized light, demonstrating the robustness of our approach for high-energy photoemission and PED analysis.

[1] O. Tkach et al., Ultramicroscopy 250, 113750 (2023); [2] T.-P. Vo et al., AIP Conf. Proc. 3251, 020005 (2024); [3] T.-P. Vo et al., arXiv:2504.14758 (2025); [4] T.-P. Vo et al., npj Comput. Mater. 11, 159 (2025).

O 2.5 Mon 11:45 HSZ/0201

Fermiology and spin polarization of the topological surface states in PtBi$_2$ — •Stefanie Suzanne Brinkman[1], Anders Christian Mathisen[1], Xin Liang Tan[1], Kristian Maeland[2], Øyvind Finnseth[1], Fabian Göhler[1], Chul Hee Min[1], Grisha Shipunov[3], Anna Isaeva[2], Jorge Ismael Facio[4], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, NTNU, Norway — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands — [4]Instituto Balseiro, National University of Cuyo, Argentina

Weyl semimetals host topologically protected Weyl nodes in the bulk, that are connected by Fermi arcs on the surface. In PtBi$_2$, recent reports indicate superconductivity in the surface Fermi arcs at elevated temperatures [1]. In this talk, we will present results from spin- and angle-resolved VUV photoemission experiments for both inequivalent surface terminations of PtBi$_2$. Our measurements, combined with first-principles calculations, establish vastly different low-energy dispersion relations of the Fermi arcs depending on surface termination. Furthermore, we provide evidence for spin polarization of the Fermi arcs. We will discuss the implications of our results for the emergence of unconventional superconductivity on the surface of PtBi$_2$.

[1] Andrii Kuibarov et al., Evidence of superconducting Fermi arcs. Nature **626**, 294-299 (2024)

O 2.6 Mon 12:00 HSZ/0201

Multi-technique research ecosystem structured around electronic band structure analysis — Takahiro Hashimoto[1], Andreas Janzen[2], •Hrag Karakachian[2], Eleni Anargirou[2], Timo Wätjen[1], and Martin Schmid[1] — [1]Scienta Omicron AB, Danmarksgatan 22, 75323 Uppsala, Sweden — [2]Scienta Omicron GmbH, Limburger Strasse 75, 65232 Taunusstein, Germany

The discovery and control of novel quantum materials are essential to the progress of modern technology. These materials frequently show complex behaviours that demand multiple, complementary techniques to fully understand their properties. For example, the electronic band structure, which is central to understanding emerging quantum materials, is typically investigated using angle-resolved photoemission spectroscopy (ARPES) or momentum microscopy.

Here, we describe how a surface-science research ecosystem centred on ARPES can be established by integrating state-of-the-art capabilities such as molecular beam epitaxy (MBE) for thin-film growth, X-ray photoemission spectroscopy (XPS) for chemical-state analysis, and scanning probe microscopy (SPM) for real-space imaging. Materials innovation is accelerated by combining these complementary techniques, leveraging both laboratory-based and user-facility instrumentation, and developing new tools to extend commercial systems.

We will present several research scenarios focused on electronic band-structure analysis and highlight application examples involving 2D materials and topological materials.

O 2.7 Mon 12:15 HSZ/0201

The TXPES Beamline at SESAME * A New Facility for Advanced Soft X-ray Photoelectron Spectroscopy — •ZEYNEP REYHAN OZTURK — SESAME

The Turkish X-ray Photoelectron Spectroscopy (TXPES) beamline, newly installed at the SESAME synchrotron, is dedicated to advanced soft X-ray photoelectron spectroscopy (XPS/UPS) for surface and interface analysis. Designed for high-resolution measurements across a broad photon energy range, TXPES enables detailed investigation of electronic structure, chemical composition, and oxidation states in complex materials.

The end station features interconnected UHV chambers for sample preparation, analysis, and in situ or near-ambient pressure experiments. Equipped with a hemispherical analyzer, ion gun, LEED, and LEIS, it allows comprehensive surface characterization with variable depth sensitivity.

TXPES provides a powerful platform for studying surface oxidation, adsorption, catalysis, and band alignment under controlled environments, including realistic gas conditions via its high-pressure cell. Currently in commissioning, the beamline will support diverse research on functional oxides, thin films, catalysts, and magnetic materials, highlighting the collaborative effort between Turkish institutions and SESAME toward full user operation.

O 3: Scanning probe techniques: Method development I

Time: Monday 10:30–12:15 Location: HSZ/0204

O 3.1 Mon 10:30 HSZ/0204

Single-Molecule Insights into On-Surface C-C Bond Formation: Radical Control via Sequential Dehalogenation — Qigang Zhong[1], Daniel Kohrs[2], Jannis Jung[3], Daniel Ebeling[1], Doreen Mollenhauer[3], Hermann Wegner[2], and •Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Giessen, Germany

On-surface synthesis through dehalogenative coupling provides a powerful route to construct carbon-carbon bonds with atomic precision. Using a combination of scanning tunneling microscopy (STM), atomic force microscopy (AFM), and density functional theory (DFT), we investigated the radical intermediates and coupling pathways of brominated polyaromatic precursors, specifically BBPN and BPIN, on Ag(111). Controlled thermal and tip-induced dehalogenation enabled the selective generation of phenyl and naphthyl radicals, which were subsequently characterized at the single-molecule level. Statistical analysis of tip-induced reactions reveals that cyclization leading to C-C bond formation occurs preferentially when the first dehalogenation takes place at the naphthyl group. Computational modeling demonstrates that radical alignment and flexibility govern the feasibility of C-C coupling. These findings highlight the interplay between precursor structure, radical generation sequence, and surface interactions in steering on-surface coupling chemistry.

O 3.2 Mon 10:45 HSZ/0204

Scanning probe microscopy investigation on cyclocarbons — •Jakob Eckrich[1], Lisanne Sellies[1], Marco Vitek[3], Yueze Gao[2], Fabian Paschke[1], Florian Albrecht[1], Leonard-Alexander Lieske[1], Harry L. Anderson[2], Igor Rončević[3], and Leo Gross[1] — [1]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [2]Oxford University, Oxford, UK — [3]University of Manchester, Manchester, UK

I will discuss our recent investigations of cyclocarbons by means of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Cyclocarbons, molecular carbon allotropes consisting of a ring of two-fold coordinated carbon atoms, have been synthesized on surface using tip-induced chemistry [1-3], and the formation of larger cyclocarbons by dimerization of precursors was shown [3]. This talk will focus on the generation and investigation of large cyclocarbons.

[1] K. Kaiser et al., Science, 365, 1299-1301 (2019) [2] L. Sun et al., Nature, 623, 972-976 (2023) [3] F. Albrecht et al., Science, 384, 677-682 (2024)

O 3.3 Mon 11:00 HSZ/0204

Machine Learning Models Tailored for Scanning Probe Microscopy Topographic Data — •Lovis Hardeweg, Johanna Matusche, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Modern machine learning methods have great potential to automate processes in scanning probe microscopy (SPM). An important step for any automated operation of SPM is the accurate extraction of meaningful information, such as the position and type of adsorbates, from topographic data. Existing frameworks, that localize and identify adsorbates on the surface [1], often rely on large models developed by the traditional computer vision community. Therefore, their application to SPM topographies has certain drawbacks.

Here, we present two machine learning architectures that are adapted specifically for their application to high-resolution low-temperature SPM data. The first model predicts a semantic segmentation on samples with heterogeneous surface material, Ag(001) and MgO/Ag(001) in particular. The second model is trained to identify adatoms, molecules and possible clusters adsorbed on the surface. Both models achieve high accuracy. Additionally, due to their reduced size, they require fewer resources during training and application than models, that have not been purpose-built for their respective tasks.

[1] J. Am. Chem. Soc, 147, 39, 35232-35243 (2025)

O 3.4 Mon 11:15 HSZ/0204

Exploring Dissipation in Single-Molecule Manipulation —

•Norio Okabayashi[1], Alfred J. Weymouth[2], Sophia Schweiss[2], Thomas Frederiksen[3,4], and Franz J. Giessibl[2] — [1]Kanazawa University, Ishikawa 920-1192, Japan — [2]University of Regensburg, Regensburg D-93053, Germany — [3]Donostia International Physics Center, San Sebastián 20018, Spain — [4]Basque Foundation for Science, Bilbao 48013, Spain

Single-molecule manipulation with scanning probe microscopy (SPM) offers a well-defined platform for studying nanoscale friction. While previous work has focused mainly on the forces driving molecular motion [1], the corresponding dissipation processes remain less explored. Here, we investigate a single CO molecule on Cu(110) using STM, AFM, LFM, and DFT at low temperatures. DFT identifies the preferred adsorption sites and the switching pathway (top-bridge-top), which are confirmed experimentally by IETS and by dissipation signals during AFM and LFM oscillations. In AFM [2], dissipation appears only along specific manipulation paths, whereas in LFM it also arises along trajectories associated with molecular switching. The switching rate is evaluated from STM as a function of lateral tip position, giving the manipulation probability per LFM oscillation cycle. Combining this cycle-resolved rate with the measured dissipation per cycle allows us to quantify the energy dissipated per manipulation event. [1] M. Ternes et al., Science 319, 1066 (2008); [2] N. Okabayashi et al., PRL 131, 148001 (2023).

O 3.5 Mon 11:30 HSZ/0204

A direct measurement of weak lateral trapping over a C$_6$ ring — •Alfred John Weymouth[1], Maximilian Titl[1], Shinjae Nam[1], Lukas Hörmann[2], Oliver Hofmann[3], and Franz J. Giessibl[1] — [1]University of Regensburg, Germany — [2]University of Warwick, U.K. — [3]TU Graz, Austria

Six-membered carbon rings (C$_6$ rings) can be found in a multitude of systems from graphite to organic molecules. Graphitic surfaces are so flat that they have been used to explore superlubricity, where one important aspect of their frictional response is the trapping of a single atom in an individual C$_6$ ring. This trapping also plays a role in the lateral movement of adsorbates on these surfaces. However, studies investigating trapping on these surfaces often focus only on strongly-bound adsorbates. We experimentally measure the trapping of a weakly-bound single atom asperity using lateral force microscopy with a CO-tip and simulate this system with DFT-based methods. Surprisingly, we observe a uniform lateral spring constant within individual C$_6$ rings over heights of tens of picometers for a range of systems. To precisely determine the surface trapping, we re-evaluate the lateral spring constant of the CO at the tip apex. With this value, we determined a very weak lateral spring constant of a particle within a C$_6$ ring.

O 3.6 Mon 11:45 HSZ/0204

Atomic scale energy dissipation as a function of temperature measured with LFM — •Sophia Schweiss[1], Lukas Hörmann[2], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Vienna, Vienna, Austria

One method of studying atomically resolved surfaces and adsorbates is small amplitude FM-AFM. With this technique, the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction are measured. Lateral force microscopy (LFM) is a related technique in which the tip oscillates laterally. Tip preparation for standard FM-AFM experiments at low temperature often includes the pickup of a CO molecule at the tip apex, which results in an inert tip with enhanced imaging properties. [1] These tip preparation techniques are also available for LFM. Over individual chemical bonds, LFM yields a measurable E_{diss} signal which we interpret as the CO snapping over the bond. [2]

Here, a CO-terminated tip is used to investigate the bonds of PTCDA molecules deposited on a Cu(111) surface with LFM. E_{diss} is measured for different temperatures in the range of 5.3 K to 6.5 K. Certain bonds exhibit a distinct T-dependence, whereas others do not.

[1] Gross et al., Science, 325, 1110 (2009)

[2] Weymouth et al., Phys. Rev. Lett., 124, 196101 (2020)

O 3.7 Mon 12:00 HSZ/0204

Bond-resolved STM with density-based methods — Emiliano Ventura-Macias[1], Jose Martinez-Castro[2], Guillermo Haas[1,3], •Jara Trujillo-Mulero[1], Pablo Pou[1], Markus Ternes[2], Ruslan Temirov[2], Frank Stefan Tautz[2], and Rubén Pérez[1] — [1]Departamento de Física Teórica de la Materia Condensada and Instituto de Física de la Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425, Jülich, Germany — [3]Grenoble INP-Phelma, 3 Parv. Louis Néel, 38000 Grenoble, France

Bond-resolved STM (BRSTM) combines scanning tunneling microscopy with the intramolecular resolution of CO-functionalized ncAFM. We introduce a simple, broadly applicable method for simulating BRSTM images and apply it to new measurements of PTCDA on Ag(111) acquired with unprecedented tip-sample control (~10 pm). Our approach integrates the Full-Density-Based Model (FDBM) for high-resolution AFM with Chen's derivative approximation, capturing both σ and π tunneling channels while accounting for CO-tip deflection. It accurately reproduces experimental images of PTCDA/Ag(111) and TOAT/Cu(111), including subtle distance-dependent features. We also show that substrate-induced changes in orbital occupation and CO relaxation significantly influence BRSTM contrast.

O 4: Metal & Semiconductor substrates: Adsorption and reaction of small molecules I

Time: Monday 10:30–12:15 Location: HSZ/0401

O 4.1 Mon 10:30 HSZ/0401

Increasingly incoherent: Effects of adatoms on the structure and characterisation of physisorbed aromatic molecules on Cu(111) — •Henry Thake[1], Matthew Stoodley[1,2], Mariia Radova[1], David A. Duncan[2,3], Lukas Hörmann[4], and Reinhard J. Maurer[1,4] — [1]University of Warwick, UK — [2]Diamond Light Source, UK — [3]University of Nottingham, UK — [4]University of Vienna, AT

X-ray standing wave (XSW) is a quantitative structural characterisation technique for hybrid metal-organic interfaces, providing species-dependent adsorption heights at picometer accuracy. Alongside adsorption heights, XSW measurements provide information on the coherence of the signal, directly related to the structural disorder of the overlayer. A series of recent XSW experiments on physisorbed poly-aromatic hydrocarbons (PAHs) revealed surprisingly low coherent fractions that are inconsistent with structural models produced by Density Functional Theory (DFT) calculations. In this talk, we investigate a hypothesis that this apparent increase in disorder may be related to molecular interactions with surface adatoms that are omnipresent at ambient conditions. Using a frozen transfer learned interatomic potential trained on DFT data of PAHs on Cu(111), we probe the influence of adatoms on dynamic adsorption at the interface. Spectroscopic measurements of these systems reveal perturbations in the electronic structure that are consistent with the co-adsorption of PAHs with adatoms. The inclusion of Cu adatoms to Cu(111) consistently increases the disorder for the PAHs, in line with XSW measurements.

O 4.2 Mon 10:45 HSZ/0401

Interfacial Processes in Ionic Liquid-Modified Catalysts — •Laura Ulm, Cynthia C. Fernández, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Solid catalysts with ionic liquid layers (SCILL) provide a powerful route to tailor the selectivity of catalytic reactions. In this context, we study the elementary reaction steps involved in the hydrogenation of 1,3-butadiene to 1-butene, a reaction in which high selectivity is crucial for hydrocarbon processing. We recently demonstrated that ionic liquids (ILs) selectively modify the adsorption of 1,3-butadiene over 1-butene, that is, the initial step of the hydrogenation of 1,3-butadiene on Pt(111). Herein, we now address the next reaction step, namely, how ultrathin layers of the IL [C$_8$C$_1$Im][PF$_6$] influence olefin displacement from Pt(111). Ultrathin films of IL with thicknesses < 1 nm are prepared in situ by physical vapor deposition. Using temperature-programmed X-ray photoelectron spectroscopy (TPXPS), we track structural and compositional film changes and olefin desorption with increasing temperature. We find that i) IL deposition onto a saturated 1-butene layer enhances the displacement and desorption of 1-butene by a factor of 2.8; ii) 1,3-butadiene remains unaffected by the IL; and iii) IL decomposition on Pt(111) is shifted to higher temperatures by 80 ± 10 K.

O 4.3 Mon 11:00 HSZ/0401

Investigating CO Oxidation on Rh(111)/(332) with High-Repetition-Rate Velocity Resolved Kinetics

— •Johannes Diedrich, Arved Dorst, and Tim Schäfer — Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Tammannstr. 6, 37077 Göttingen

Velocity resolved kinetics (VRK) allows measuring the temporal evolution of reaction products from surfaces. A recent development is high repetition rate (HRR)-VRK [1]. By using more ionization pulses per molecular beam pulse, the signal-to-noise ratio is significantly improved and data acquisition accelerated.

An ultra-high-vacuum apparatus used for conventional VRK was modified to HRR-VRK by using a 100 kHz femtosecond laser for multiphoton nonresonant ionization and a TimePix3 event camera. This setup enables measururement of the full time of flight spectrum for every laser pulse.

Preliminary results are presented for the oxidation of CO on Rh(111) and (332) facets. This system allows comparison of conventional and HRR-VRK for a previously investigated reaction [2]. Thermal and hyperthermal CO2 channels are distinguished and deviations from the single-exponential decay are discussed. In future work, the decomposition of hydrazine on Ir will be investigated to gain a deeper understanding of Ir-based monopropellant thruster catalysts.

[1] F. Nitz et al., Rev. Sci. Instrum. 96, 055106 (2025).

[2] A. C. Dorst, PhD diss. (Georg-August-University Goettingen 2025).

O 4.4 Mon 11:15 HSZ/0401

First-principles structure search study of multi-component alloys for electrocatalysis

— Lei Jia, •Guo-Xu Zhang, and Zhenbo Wang — MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin, P. R. China

Multi-component alloys (MCA) have gained increasing attention as electrocatalysts due to their tunability of catalytic properties, while vast composites and diverse active sites make them highly challenging to identify configurations of molecules on surfaces. Here, we combined first-principles calculations with an active machine learning approach, Bayesian Optimization Structure Searching (BOSS), which enables efficient and accurate identification of molecular adsorbate structures on the MCA surfaces. This strategy utilizes smart sampling of adsorption energy surface (AES), constructs a surrogate model to predict the AES landscapes, and continuously refines the models to search global and local minima of adsorption configurations. The performance of first-principles calculations with BOSS was illustrated by benchmark data against single-atom, binary and ternary alloy catalysts. The good predictive power of our method suggests an effective way towards large-scale molecular adsorption for MCA electrocatalysts.

O 4.5 Mon 11:30 HSZ/0401

Surface effects during plasma-activated nitrogen splitting for catalytic ammonia formation

— •Sabine Auras and Roland Bliem — ARCNL, Amsterdam, The Netherlands

Plasma-assisted catalysis (PAC) enables the activation of stable molecules, e.g. N_2 or CO_2, by generating reactive species that interact with a catalyst, thereby lowering dissociation barriers and creating new reaction pathways. For ammonia synthesis, PAC is particularly attractive as it can operate under milder conditions than the conventional Haber-Bosch process, potentially improving efficiency while reducing energy input. However, plasma fundamentally alters the reaction environment, which limits the applicability of concepts from thermal catalysis. Therefore, in-situ studies of surface properties and adsorbate evolution are needed to understand the surface chemistry under plasma conditions. Here, we present the first in situ XPS data of Ru and Rh surfaces during N_2 plasma exposure, as well as mixed N_2/H_2 plasmas. To correlate surface processes and plasma properties, we further characterize the plasma composition by optical emission spectroscopy and monitor gas-phase products using mass spectrometry. The results reveal distinct differences in how activated N_2 species interact with the catalytic surface. This allows us to identify surface intermediates, assess reaction kinetics, and propose a mechanism for NH_3 formation, taking into account the role of different plasma species. Our findings highlight the need for a combined approach to identify the role that plasma and catalytic surfaces play - and thus to understand the interactions driving plasma-assisted catalysis.

O 4.6 Mon 11:45 HSZ/0401

Bonding properties of a CO molecule with metallic adatoms

— •Fabian Stilp, Marco Weiss, Mia Fuerst, Maximilian Krueger, Luis Vendolsky, Nicolas Wirth, Hendrik Weinert, and Franz J. Giessibl — Department of Physics, University of Regensburg, Germany

CO terminated AFM tips are often used to investigate molecules on surfaces as they are a powerful tool to make the internal structure of such molecules visible. Their chemical inertness results in high resolution of the single atoms and bonds in such molecule via Pauli repulsion. However, it was shown by Huber et al. [1] that CO terminated tips can form weak bonds to some species of adatoms on a Cu (111) sample such as Fe and Cu. In contrast, Si adatoms only interact via van der Waals attraction and Pauli repulsion.

Can one predict the strength of the bond between the CO molecule and an arbitrary atom just from its electron configuration? To set the rules for this prediction we expand our collection of AFM measurements with various atomic species.

In total the interaction between the CO molecule and the adatom shows up to five different regimes, two attractive and three repulsive. The forces are distinctly pronounced, which allows to group the atoms in four different types.

We analyze the different atomic species for their different barrier before forming the bond, directionality of the bond and electrostatic interactions.

[1] Huber et al., Science 366, 235-238 (2019).

O 4.7 Mon 12:00 HSZ/0401

Online monitoring of the oxygen adsorption on Cu(110) with PEEM and DRS

— •Robert Heller, Thorsten Wagner, and Peter Zeppenfeld — Johannes Kepler University, Institute of Experimental Physics, Surface Science Division, 4040 Linz, Austria

We studied the dissociative adsorption of oxygen on the Cu(110) surface using Photoelectron Emission Microscopy (PEEM) and Differential Reflection Spectroscopy (DRS) simultaneously. Unlike many experiments carried out already in the 1970s and 1980s, our approach focusses on real-time monitoring. For oxygen exposures up to ∼100L, at temperatures between 350K and 420K, the process saturates at an oxygen coverage of 0.5 with a well-ordered (2×1)O superstructure. At intermediate coverages, a regular pattern of alternating Cu and CuO stripes is formed [1].

We used a PEEM with a xenon lamp (Xe) to study changes in the electron yield (EY) during the exposure. Oxygen adsorption causes a decrease in EY and, hence, an increase in the work function. Since our DRS setup uses the same light source as the PEEM, we can synchronously record the change of the reflectance and reliably compare the two signals. Interestingly, the normalised adsorption curves are not identical, indicating that the PEEM and/or the DRS signals are not directly proportional to the oxygen coverage. This could be related to the effect of the formation of the nanostructured Cu-CuO stripe pattern upon oxygen adsorption [1].

[1] K. Kern et al., Phys. Rev. Lett. 67, 855 (1991).

O 5: Focus Session: Mineral-water interfaces I

The Focus Session discusses recent advances in the understanding of mineral-water interfaces. These interfaces are ubiquitous in nature, host of many geological and biological processes, intimately linked to the global carbon cycle, and therefore highly relevant for Earth*s climate. For example, silicate weathering removes carbon dioxide from the atmosphere on geological timescales, acting as a stabilizing feedback mechanism since weathering rates increase with temperature. In the oceans, carbonates dissolve and precipitate in response to changing atmospheric carbon dioxide concentrations, thus far mitigating part of the anthropogenic impact of CO_2 emissions. In addition, numerous industrial and technological processes involve mineral-water interfaces, including seawater desalination, scaling and incrustation prevention, as well as various biochemical applications. However, and despite their importance, many fundamental aspects of mineral-water interfaces remain poorly understood, including water binding and diffusion, structure formation, ice nucleation, growth, or desorption.

This DPG Focus Session will address these aspects at the molecular level, elucidating fundamental processes involving both single water molecules and bulk water in contact with mineral surfaces. The session brings together scientists investigating mineral-water systems under ultrahigh vacuum conditions as well as at mineral-water interfaces in bulk aqueous environments. We aim for a balanced Session with contribution from both renowned experts and young investigators active in the field.

Organized by Philipp Rahe (U Osnabrück), Angelika Kühnle (U Bielefeld), Jan Balajka (TU Vienna), Wolf Gero Schmidt (U Paderborn).

Time: Monday 10:30–12:30 Location: HSZ/0403

Invited Talk O 5.1 Mon 10:30 HSZ/0403

Can the mineral-water interface save the world? Mineral carbonation, enhanced weathering and negative emissions — •Philip Pogge von Strandmann — Johannes Gutenberg University, Mainz

The rising atmospheric CO2 concentrations are clearly having a significant impact on the climate, and will continue to do so. The currently only foreseeable method by which anthropogenic climate change will not be completely catastrophic (i.e. limited to 1.5-2°C warming), is if we implement global "negative emissions" technologies, that is the artificial removal of CO2. Two such technologies directly rely on the mineral-water interface: mineral carbonation and enhanced weathering. Both require the dissolution of silicate minerals in mildly acidic water, and the subsequent precipitation of carbonate secondary minerals, but without too much precipitation of silicate secondary minerals, which hinder the reaction. In fact, the reaction is more complex than that, because numerous reactions occur at the mineral-water interface: dissolution, sorption, exchange, co-precipitation and incorporation into interstitial sites in mineral lattices. Each of these reactions has significant consequences for the efficiency of the reaction and the CO2 drawdown. This presentation will examine these reactions, including the aspects we currently understand and can measure, and those where our knowledge and analytical abilities are still lacking.

O 5.2 Mon 11:00 HSZ/0403

Reconstruction of calcite (10.4) manifests itself in the tip-assisted diffusion of water — •Klausfering Lea, Schneider Florian, Bechstein Ralf, and Kühnle Angelika — Bielefeld University, 33615 Bielefeld, Germany

Calcite is the most common carbonate in the Earth*s crust and plays a fundamental role in environmental and industrial processes. The most stable cleavage plane of calcite is the (10.4) plane. This surface has already been extensively studied in liquid environments as well as under ultra-high vacuum (UHV) conditions. Under UHV conditions, the surface exhibits a (2 x 1) reconstruction. Due to this reconstruction, there are two energetically different adsorption sites for adsorbates, such as water. Here, we present an atomic force microscopy (AFM) study in which the diffusion of individual water molecules on the calcite (10.4) surface was investigated under UHV conditions at a temperature of 140 K. The positions of individual water molecules could be precisely determined in several consecutive atomically resolved images, allowing the diffusion of the water molecules to be observed. We found that the AFM tip has an influence on the diffusion of the water molecules, but that diffusion only occurs between one type of adsorption positions.

O 5.3 Mon 11:15 HSZ/0403

Nanoscopic insights on ice nucleation on microcline (001) — •Florian Schneider[1], Rasmus Väinö Erik Nilsson[2], Ralf Bechstein[1], Bernhard Reischl[2], Thomas Koop[1], Angelika Kühnle[1], and Tobias Dickbreder[3] — [1]Bielefeld University, Bielefeld, Germany — [2]University of Helsinki, Helsinki, Finland — [3]University of Vienna, Vienna, Austria

Heterogeneous ice nucleation plays a crucial role in various environmental and technological processes. An in-depth understanding of the nucleation at the atomic scale can greatly enhance our capability to create materials with particular ice-nucleating properties and improve our climate models. In the atmosphere, a particularly active ice nucleating particle is dust from the feldspar mineral microcline [1]. However, why microcline outperforms other mineral dust particles in its ice-nucleating ability still remains a puzzle. Here, we present atomic force microscopy images of ice crystals growing from the vapor phase on the (001) surface of microcline at low temperature. In contrast to the prevailing view of active sites such as step edges or cracks being responsible for ice nucleation, we observe ice growth at random positions on the bare terrace. For the closely related feldspar sanidine, in contrast, ice nucleation is prevalent at step edges as expected. This comparison underscores the exceptional ice nucleating ability of microcline as it demonstrates ice nucleation even in the absence of surface defects and raises important questions regarding the different ice nucleation mechanisms on these two feldspar mineral surfaces.

[1] Harrison, A. D. *et al.*, Atmos. Chem. Phys., 16, 2016.

Invited Talk O 5.4 Mon 11:30 HSZ/0403

Machine learning exploration of water binding and ice nucleation at silicate and carbon surfaces — •Mie Andersen — Department of Physics and Astronomy, Aarhus University, Denmark

Mineral-water interfaces play a central role in environments ranging from the interstellar medium to Earth's surface and subsurface. In astrochemistry, the chemical evolution of star-forming regions is controlled by gas-grain interactions on dust grains that may be partially or fully covered by water ice. A key quantity underlying these processes is the binding energy (BE) of adsorbates, which determines desorption and diffusion rates and controls chemical kinetics.

In this contribution, we explore computational strategies to quantify BE distributions at complex, partially ice-covered mineral surfaces. Using graphene and forsterite as model grain substrates, we combine atomistic simulations with machine-learning interatomic potentials to generate realistic surface structures and to efficiently sample BEs. The modelled ice structures range from amorphous structures generated by low-temperature molecular dynamics simulations to highly stable crystalline structures generated by global structure optimization. The resulting BE distributions are analyzed in terms of surface heterogeneity, ice coverage and hydrogen bonding.

While motivated by astrochemical applications, the presented methodology is broadly transferable to mineral-water interfaces under terrestrial conditions. The approach offers a general framework for linking molecular-scale interfacial structure to macroscopic transport and reaction models across disciplines.

O 5.5 Mon 12:00 HSZ/0403

Chiral water structures on dolomite(104) surfaces — •Jonas Heggemann[1], Paul Laubrock[1], Jie Huang[2], Adam S. Foster[2,3], and Philipp Rahe[1] — [1]Institute of Physics, Osnabrück University, Osnabrück, Germany — [2]Department of Applied Physics, Aalto University, Helsinki, Finland — [3]Nano Life Science Institute (WPI NanoLSI), Kanazawa University, Kanazawa, Japan

The formation mechanisms of dolomite ($CaMg(CO_3)_2$), an abundant rock-forming carbonate mineral with rhombohedral structure [1], are still poorly understood in the earth's crust [2]. The lack of replicating mineral growth under geological conditions in the laboratory is a further characteristic of the "dolomite problem" [2]. Consensus could be reached that dolomite formation only occurs in the presence of water [3] and it is further known that (104) is the most stable surface [4]. Here, we unravel a chiral character of dolomite(104) surfaces from non-contact atomic force microscopy data acquired with CO terminated tips. Backed by density functional theory and probe-particle model calculations, the presence of two surface enantiomers is identified. We further investigate water adsorption, with coverage ranging from single molecules to a full monolayer. Preferred water adsorption is found at calcium and magnesium surface sites; yet, the geometries carry a clear chiral property.

[1] L. S. Land, AAPG **24**, 1 (1982)
[2] J. A. Roberts, Nature Geoscience **17**, 716 (2024)
[3] S. E. Kaczmarek *et al.*, Sedimentology **61**, 1862 (2014)
[4] N. H. De Leeuw, Am. Mineral. **87**, 679 (2002)

O 5.6 Mon 12:15 HSZ/0403

Atomically Resolved Imaging of the Gypsum (010) surface — •David Kugler, Andrea Conti, Tun Sinner, Florian Mittendorfer, Michael Schmid, Gareth S. Parkinson, Ulrike Diebold, and Jan Balajka — Institute of Applied Physics, TU Wien, Vienna, Austria

Gypsum ($CaSO_4\cdot 2H_2O$), the dihydrate of calcium sulfate, is the most abundant sulfate mineral in Earth′s crust and it is widely used as a fertilizer and as a construction material. Its bulk crystal structure consists of alternating calcium sulfate bilayers and bilayers of crystal water. While the water in the bulk has been extensively studied, a comprehensive understanding of surface processes is still missing. Water is, however, present on all surfaces in ambient environment and influences surface chemistry. Because the adjacent layers are linked only by hydrogen bonds, gypsum cleaves readily along the (010) plane, exposing large, atomically flat terraces. In this work, noncontact atomic force microscopy (nc-AFM) with a qPlus sensor was used to resolve the atomic structure of the cleaved gypsum (010) surface and to visualize the configuration of adsorbed water. Our results indicate that one of the surface crystal water molecules rotates into a lower energy orientation, forming a hydrogen bond with the second crystal water molecule within the unit cell. Preliminary ab-initio modeling suggests that the first adsorbed water layer preserves the periodicity of the bulk structure by forming hydrogen bonds with the surface crystal water.

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

Time: Monday 10:30–12:30 Location: TRE/PHYS

O 6.1 Mon 10:30 TRE/PHYS

Support-dependent reactivity of Fe-DCA 2D Metal-Organic Frameworks — •Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Tadeáš Lesovský[2], Ayesha Jabeen[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Purkyňova 123, Brno 61200, Czechia — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno 61200, Czechia

2D Metal-Organic Frameworks (2D MOFs) are promising materials for applications in catalysis, sensing and spintronics. 2D MOFs based on 9,10-dicyanoanthracene (DCA) linker molecules are particularly intriguing due to their recently demonstrated magnetic and topological properties. Here, we study the reactivity of Fe-DCA supported on two weakly-interacting supports: graphene/Ir(111) and Au(111). Using Scanning Tunneling Microscopy (STM), X-Ray Photoemission Spectroscopy (XPS) and Low-Energy Electron Microscopy/Diffraction (LEEM/LEED), we test how the Fe-DCA reacts with carbon monoxide and molecular oxygen. When the Fe-DCA is supported on graphene, the CO adsorbs on the Fe-sites at temperatures below 200 K, while O2 exposure causes structural collapse of the 2D MOF at room temperature. In contrast, when the Fe-DCA is supported on Au(111), it appears inert to CO adsorption. Overall, our results show how the chemical reactivity of 2D MOFs depends on the supporting surface, providing critical insights for the potential integration of MOFs into functional devices.

O 6.2 Mon 10:45 TRE/PHYS

LT-STM investigation of azulene-based molecular architectures on metal surfaces — •Suchetana Sarkar[1,4], Natasha Khera[1], Kwan Ho Au-Yeung[1,5], Renxiang Liu[1,2,3], Ji Ma[1,2,3], Xinliang Feng[1,2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Chair of Molecular Functional Materials and Faculty of Chemistry & Food Chemistry, TU Dresden, 01062 Dresden, Germany — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, Halle, Germany — [4]Present address: Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany — [5]Present address: Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

Azulene-based molecules offer a unique platform for probing on-surface self-assembly and electronic structure due to their non-benzenoid topology and intrinsic dipole. Presented here are the investigations of two related systems: a cyclopenta[cd]azulene trimer (CPAT) and a phenyl-functionalized analogue (CPAT-Ph), using low-temperature scanning tunneling microscopy and spectroscopy. CPAT forms well-ordered homochiral domains on Au(111), whereas CPAT-Ph exhibits weak adsorption and high mobility on Au(111) and shows no ordered phases on Cu(110). Spectroscopy reveals clear electronic differences between the molecules and substrate-induced shifts for CPAT-Ph. Finally, the results of thermally induced ring-closing reactions are also shown, discussing routes toward on-surface synthesis of non-benzenoid nanographenes.

O 6.3 Mon 11:00 TRE/PHYS

Surface study of heteromolecular layers for charge injection: deprotonated carboxylic acids mixed with pentacene — •Jakub Planer[1], Veronika Stará[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Institute of Physical Engineering, Brno University of Technology, Czech Republic

Heteromolecular organic films represent promising candidates for efficient charge-injection layers in organic optoelectronic devices. Using surface-science experiments together with ab-initio modeling, we investigate the structural and electronic properties of intermixed layers composed of fully deprotonated carboxylic acids and pentacene (PEN) on Ag(100) and Ag(111) substrates. Our work demonstrates that these molecules form blends capable of modulating the electrode work function by up to 0.5 eV, depending on the mixing ratio, while remaining stable during subsequent organic-semiconductor deposition. These findings underline the potential of mixed carboxylate–PEN layers as practical, robust charge-injection modifiers and show that various carboxylic acids can be effectively used in such heteromolecular interfaces [1,2].

[1] Stará, Veronika, et al. *Tunable Energy-Level Alignment in Multilayers of Carboxylic Acids on Silver.* Physical Review Applied, **18**, (2022)

[2] Krajňák, T. et al. *Robust Dipolar Layers between Organic Semiconductors and Silver for Energy-Level Alignment.* ACS Appl. Mater. Interfaces, **16**, (2024)

O 6.4 Mon 11:15 TRE/PHYS

Orientational Order of Phenyl Rotors on Triangular Platforms on Ag and Au(111) — Richard Berndt[1], Richard Berndt[2], Richard Berndt[2], Richard Berndt[3], and •Richard

Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, CAU Kiel, Germany — [3]Centro de Física de Materiales, Donostia-San Sebastián, Spain

We investigated trioxatriangulenium functionalized with phenyl on Ag(111) and Au(111) using low-temperature scanning tunneling microscopy (STM). On Ag, the molecules form hexagonal arrays and the orientations of the phenyl moieties are resolved. Moreover, STM images suggest a dimerization of the molecules. Density functional theory calculations reproduce the experimental data. Van der Waals interaction is the dominant binding mechanism. The apparent dimerization results from an asymmetry of the phenyl wavefunction, which reflects intramolecular hydrogen bonding between the ligand and an oxygen atom of the triangulenium platform. Direct long-range interaction between phenyl moieties across molecules and the intramolecular H bonding are decisive for the orientations of the phenyl moieties. Similar experimental results were obtained on Au(111).

O 6.5 Mon 11:30 TRE/PHYS

Adsorption and Isomerization of Azobenzene Tetramers on Au(111) — •Natasha Khera[1], Ebru Cihan[1], Franz Plate[1], Soyoung Park[2], Ningwei Sun[2], Dmitry A. Ryndyk[1,2], Franziska Lissel[2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Leibniz Institute of Polymer Research Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, 21073 Hamburg, Germany

This work investigates the manipulation and voltage-induced switching of star-shaped azobenzene tetramers [1] on Au(111) using low-temperature ultra-high vacuum scanning tunneling microscopy (LT-UHV STM) to study their adsorption behavior and cis-trans isomerization. On terraces, molecules in the trans state are highly mobile and difficult to image stably, whereas voltage induced switching to the cis state makes them immobile for reliable measurement. The study also utilizes step-edge sites where trans molecules are more stable and can be addressed without prior switching. Voltage pulses with the STM tip produces reproducible switching between high-contrast and low-contrast STM signatures, consistent with the cis-trans isomerization of the azobenzene core. Electric-field-dependent measurements are also performed by retracting the STM tip and recording tip-height vs bias characteristics, providing insight into the electric-field driven response of the molecules.

[1]. M. Baroncini, et al. Nature Chemistry 7, 634-640, (2015)

O 6.6 Mon 11:45 TRE/PHYS

Steering interfacial molecular self-assembly by substrate-molecule charge transfer — •Benjamin Achatz, Matthias Zeilerbauer, Marco Thaler, and Laerte Patera — Department of Physical Chemistry, University of Innsbruck, Innsbruck, 6020, Austria

Scanning probe microscopy studies of organic molecules on metal substrates have furthered our understanding of substrate-molecule charge transfer processes [1]. On surface self-assembly of the electron acceptor C_{60} is driven by an interplay of short-range attractive Van der Waals forces and long-range repulsive electrostatic interactions [2]. Here we report the formation of an intermixed phase composed of C_{60} and Zn(II)-5,10,15,20-tetrakis(4-aminophenyl)porphyrin (ZnTAPP) molecules on Ag(111). An approach combining scanning tunneling spectroscopy (STS) and Kelvin probe force microscopy (KPFM) was used to investigate the degree of substrate-molecule charge transfer for C_{60} in close-packed islands and a row-like intermixed structure. Analysis of our tunneling and force spectroscopy measurements revealed that mitigation of the coulomb repulsion drives the formation of the intermixed phase and promotes additional charge transfer to the C_{60} molecules. These results demonstrate that controlling long-range Coulomb interactions can steer the formation of distinct self-assembled structures on metal substrates, offering insights for the design of new charge-optimized molecular nanostructures.

[1] R. Otero et al., Surf. Sci. Rep. 72, 105 (2017).

[2] M. Švec et al., Phys. Rev. B 86, 121407 (2012).

O 6.7 Mon 12:00 TRE/PHYS

Nanostructuring of organic radicals on cobalt surfaces — •Arkaprava Das and M. Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Organic radicals are potential candidates for groundbreaking applications like energy storage, quantum computing, and spintronics. To investigate the nature of the adsorption of the radical derivative molecules on cobalt surfaces, we investigate their electronic structure and morphology. The electronic structure at the interface is investigated by using X-ray photoelectron spectroscopy (XPS), and the morphology is studied with scanning electron microscopy. The radical/Co interface interactions have resulted in different nanostructures crucial for device fabrication, whereas changes in line shape of core level spectra confer direct evidence of changed electronic properties at the interface. Considering ecological requirements, we also endeavour to minimize the materials consumption by making the Co substrate reusable, which is in line with the principles of closed-loop circular economy.

O 6.8 Mon 12:15 TRE/PHYS

Competition between dative bonds and aromatic gains — •Jonas Brandhoff[1], Richard Berger[2], Felix Otto[1], Maximilian Schaal[1], Lorenz Brill[1], Oliver T. Hofmann[2], Peter Puschnig[3], Torsten Fritz[1], and Roman Forker[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Solid State Physics, Technical University Graz, Petersgasse 16, 8010 Graz, Austria — [3]Institute of Physics, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Upon molecular adsorption on a surface, a variety of interactions can occur. Identifying which mechanisms dominate this complex quantum-mechanical landscape is crucial for understanding molecule – surface coupling. One key factor in many π-conjugated systems is aromaticity – a fundamental concept in chemistry describing the energetic stabilization that arises from particular π-electron arrangements. To investigate how aromaticity competes with other adsorption-driven interactions, we study 5,7,12,14-pentacenetetrone (P4O) on different metal surfaces as a model system. P4O is a prototypical molecule expected to undergo aromatic stabilization upon adsorption, where charge transfer from the substrate modifies the topology of the occupied π-system and leads to a more energetically favorable configuration. Using photoemission orbital tomography measurements combined with density functional theory calculations, we show how hybridization with the surface can outweigh a potential aromatic stabilization, *not* necessarily maximizing the latter. We reveal a mechanism in which the unoccupied π-system of the molecule forms dative bonds with the substrate.

O 7: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

Invited Talk O 7.1 Mon 10:30 TRE/MATH

Magnetic Order in 2D Materials Beyond Bulk Constraints — •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln

Even though exfoliated microflakes remain widely used in 2D magnetism research, their bulk origin restricts access to many potentially interesting phases, an obstacle that molecular beam epitaxy (MBE) can overcome. MBE enables the controlled synthesis of single-layer materials directly related to, yet often distinct from, their bulk counterparts.

In my talk, I will present structural characterization and discuss the mechanisms behind the formation of such novel 2D materials grown via MBE on graphene. [1-2] The emerging magnetic properties of these new 2D materials will be exemplified with two cases: Cr_2S_3-2D and Fe_2S_2-2D. Cr_2S_3 forms a covalently bonded NiAs-type structure without van der Waals gaps. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD), we show that it hosts ferromagnetic coupling within the plane with magnetic moments pointing out-of-plane, combined with A-type antiferromagnetic coupling between different Cr planes. Fe_2S_2 exhibits a unique hexagonal phase, in which Fe atoms occupy tetragonally coordinated sites. Spin-polarized STM reveals that the moments are noncollinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming a Néel state and a 2Q state.

[1] Knispel et al. Small, 2025 21, 2408044.

[2] Safeer et al. Adv. Funct. Mater. 2025, 202500907.

O 7.2 Mon 11:00 TRE/MATH

Ab initio modeling of magnons and magnon-phonon coupling in 2D magnetic materials — Ali Esquembre-Kucukalic1[1], Khoa Le[2], Hsiao-Yi Chen[3], Ivan Maliyov[2], Jin-Jian Zhou[4], Davide Sangalli[5], and •Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Valencia, Spain — [2]CALTECH, California, USA — [3]Tohoku University, Japan — [4]Beijing Institute of Technology, Beijing, China — [5]ISM-CNR, Roma, Italy

Understanding spin-wave excitations in two-dimensional magnetic materials is essential for advancing spintronic and quantum information technologies. Chromium trihalides and related 2D magnets provide a platform where the choice of halide influences on the magnetic behavior, yet its impact on magnon properties is not completely understood. We present first-principles calculations of magnon dispersions and wave functions in monolayer Cr trihalides using the Bethe-Salpeter equation (BSE), resolving key features such as the topological gap at the Dirac point. The BSE analysis reveals that magnons originate from electronic transitions spanning a wider energy range than excitons, offering new insight magnon character and enabling the extraction of Heisenberg exchange parameters. Building on this framework, we develop an ab initio description of mag-ph coupling by deriving BSE-based mag-ph interaction matrices and applying them to monolayer CrI3 and hydrogenated graphene. We show that mag-ph and electron-phonon couplings differ markedly, identifying specific phonon modes that dominate magnon scattering.

O 7.3 Mon 11:15 TRE/MATH

Electron-phonon interaction in transition-metal dichalcogenides — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We developed a generally applicable ab-initio implementation on top of density functional theory using a basis set of localized Gaussian orbitals. It combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation [1], which are usually neglected.

In addition to the renormalization of the electronic bands, electron-phonon interaction introduces a line broadening due to finite-lifetime effects, which have recently been incorporated into our implementation. In this presentation, we discuss our results, including those with finite-lifetime effects, for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

O 7.4 Mon 11:30 TRE/MATH

Surface-state engineering for nonlinear charge and spin photocurrent generation — •Javier Sivianes[1], Peio Garcia-Goiricelaya[2], Daniel Hernangómez-Pérez[3], and Julen Ibañez-Azpiroz[1,4,5] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Leioa, Spain — [3]CIC nanoGUNE BRTA, San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [5]Donostia International Physics Center (DIPC), Donostia, Spain

We systematically explore the generation of nonlinear charge and spin photocurrents using spin-orbit-split surface states. This mechanism enables net DC flow along the surface plane even in centrosymmetric bulk environments like the Rashba prototype Au(111), where we characterize the main quadratic contributions by combining model predictions with density functional calculations. We further identify the Tl/Si(111) surface as a prime scenario for experimental verification; with slight doping, it develops metallic surface states featuring remarkable relativistic properties deviating from the Rashba paradigm, while the bulk remains semiconducting. Its nonlinear charge photocurrent reveals a distinct angular signature and a magnitude comparable to bulk ferroelectrics, highlighting the potential of surface-state photocurrents for low-bias optoelectronic applications. Moreover, the nontrivial spin texture of its surface states enables the generation of pure out-of-plane spin-polarized currents, offering a highly versatile nonlinear spin-filtering functionality beyond the conventional spin Hall effect.

O 7.5 Mon 11:45 TRE/MATH

Influence of Vanadium Doping on WSe_2, as seen through ARPES — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kallåne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics offers a compelling, energy-efficient alternative to traditional electronics with potential applications in communications, sensing, and information processing. The vanadium-doped layered transition metal dichalcogenide $2H$-WSe_2 is particularly promising as a room-temperature magnetic semiconductor with gate-tunable transport properties. Here, we use a combination of 11 eV laser, 21.2 eV He-lamp, and soft X-ray synchrotron ARPES to highlight the influence of a fairly small vanadium doping on the electronic structure of WSe_2. Both the pristine and doped compounds were grown by chemical vapor transport in our own laboratory.

O 7.6 Mon 12:00 TRE/MATH

Engineering sulfur vacancy dimers in monolayer WS_2 — •Daniel Jansen[1], Guangyao Miao[1], Jan Keienburg[1], Jeison Fischer[1], Thomas Michely[1], Hannu-Pekka Komsa[2], and Wouter Jolie[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Sulfur vacancies [1] and sulfur vacancy dimers in nearest-neighbor distance [2] in monolayer WS_2 have been experimentally proven to yield bright and stable photon emission, thus holding promises for the development of quantum technologies.

Here we investigate dimers of sulfur vacancies in different configurations in monolayer WS_2 created with the tip of a scanning tunneling microscope [3]. Scanning tunneling spectroscopy reveals strong hybridization of the sulfur vacancy electronic in-gap states, validated by density functional theory calculations. For dimers in nearest-neighbor configuration we find that inelastically tunneling electrons can induce sulfur atom migration, resulting in a rotary motion of the dimer. This motion is studied in detail by analyzing the emerging telegraph noise in the junction. Lastly, we elaborate on scenarios to make use of the dimer motion for the design of vacancy structures and lattices.

[1] Schuler et al., Sci. Adv. **6**, 38 (2020)
[2] Sun et al., Nature Commun. **15**, 9476 (2024)
[3] Jansen et al., Phys. Rev. B **109**, 195430 (2024)

O 7.7 Mon 12:15 TRE/MATH

Alkali-metal doped transition metal chlorides confined in bilayer graphene: Insights from first-principles calculations — •Munawar Ali[1], Arkady V. Krasheninnikov[2], Giovanni Cantele[1], and Mahdi Ghorbani-Asl[2] — [1]Università degli Studi di Napoli "Federico II," Dipartimento di Fisica "Ettore Pancini," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The intercalation of atomic and molecular species into layered materials has emerged as a powerful strategy for synthesizing novel two-dimensional systems with tunable electronic, magnetic, and energy-storage properties. Encapsulating transition-metal halides into bilayer graphene has proven effective for stabilizing 2D magnetic phases that are otherwise thermodynamically unstable. Using density functional theory, we systematically investigate the intercalation of metal chlorides (TCl_3, T = Fe, Cu, Mo, Al) doped with alkali metals (Li, Na, K, Rb, Cs) across a range of concentrations. Li- and Na-doped $FeCl_3$, $CuCl_3$, and $MoCl_3$ monolayers exhibit the highest thermodynamic stability, whereas $AlCl_3$ remains unstable even under doping. Bader charge analyses reveal substantial charge transfer from the graphene host to the intercalated layers, particularly in the case of $CuCl_3$, which also shows the strongest binding. These findings provide a theoretical framework for understanding the stability of these heterostructures and highlight alkali-metal-intercalated graphene systems as a platform for engineering tunable 2D magnetic materials.

O 8: Nanostructures at surfaces:1D, 2D, networks I

Time: Monday 10:30–12:30 Location: WILL/A317

O 8.1 Mon 10:30 WILL/A317

Quantum confinement of excited states in a two-dimension metal-organic coordinated network — •Lu Lyu[1], Martin Anstett[2], Wei Yao[3], Tobias Eul[1], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [3]Institute of Advanced Light Source Facilities, Shenzhen 518107, China

Quantum confinement effects of surface electrons in two-dimensional metal-organic coordinated networks (2D-MOCNs) provide a highly tunable platform for exploring the laws of quantum mechanics in condensed matter systems. Here, we focus on a porous network formed by coordinating pyridine-functionalized T4PT molecules with Co atoms on Au(111). One-photon photoemission (1PPE) experiments reveal a substantial energy shift of the Shockley surface state (SS) that is indicative of a hybridization with Co centers. This hybridization is responsible for a leaky channel for electrons between adjacent pores, which prevents the quantum confinement of SS electrons. In contrast, excited electrons into the unoccupied image potential states (IPS) reveal clear signatures of a substantial quantum confinement in a two-photon photoemission (2PPE) experiment. These contrasting observations of SS and IPS can be attributed to the 3D nature of the quantum well potential of the 2D-MOCNs and the distinct surface-perpendicular wave function distribution in the SS and the IPS.

O 8.2 Mon 10:45 WILL/A317

On-surface prepared 2D MOFs as models of single-atom catalysts: Fe-N$_3$ vs. Fe-N$_4$ — •Zdeněk Jakub[1], Jakub Planer[1], Dominik Hrůza[1], Ayesha Jabeen[1], Tadeáš Lesovský[1], and Jan Čechal[1,2] — [1]CEITEC, Brno University of Technology, Brno, Czechia — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czechia

What defines the reactivity of the so-called single-atom catalysts? Here, we utilize 2D Metal-Organic Frameworks (MOFs) synthesized on an inert graphene support to address this fundamental question. By temperature-dependent scanning tunneling microscopy and density functional theory, we quantify the CO adsorption strengths on threefold-coordinated (Fe-N$_3$) and fourfold-coordinated (Fe-N$_4$) iron sites embedded within Fe-DCA and Fe-TCNQ 2D MOFs. A significant 0.5 eV difference in CO binding strengths is found, despite the fact that the electronic parameters like Fe oxidation state, spin configuration, occupancy of the individual d-orbitals and their positions with respect to Fermi level are almost identical prior to CO adsorption. We trace the origin of the different reactivity to the higher structural flexibility of the Fe-N$_3$ sites compared to Fe-N$_4$. These results highlight the key role of local coordination and demonstrate that reactivity cannot be reliably predicted from electronic structure parameters alone.

Invited Talk O 8.3 Mon 11:00 WILL/A317

Controlling nanostructures on surfaces via intermolecular interactions — •Yunjun Cao — Physical Chemistry I, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Synthesizing sophisticated nanostructures on surfaces requires precise control over intermolecular interactions ranging from strong covalent bonds to weak van der Waals interactions. In the first part of the talk, I will present an irreversible, multi-step covalent coupling strategy for reactive molecules. By precisely controlling the reaction sequence, we synthesize highly branched nanostructures on a metal surface [1]. As a complementary approach, I will then introduce a reversible, multi-step self-assembly protocol for sterically crowded molecules, highlighting how intermolecular van der Waals interactions steer the formation of well-separated cyclic nanostructures with an unprecedented high yield [2]. Finally, I will turn to the single-molecule level and discuss how to control via van der Waals interactions the configuration of individual molecules [3] and the potential energy landscape of a dynamic chirality switch [4]. Our studies highlight how tunable intermolecular interaction strengths control the synthesis of tailored nanostructures on surfaces.

[1] Y. Cao et al., Nat. Commun. in press (2025). [2] Y. Cao et al., ACS Nano 19, 21942 (2025). [3] Y. Cao et al., Phys. Rev. B 111, 115426 (2025). [4] Y. Cao et al., Nat. Commun. 14, 4500 (2023).

O 8.4 Mon 11:30 WILL/A317

Autonomous Nanoworld: Building Nanostructure Without Human Intervention — •Bernhard Ramsauer[1], Qigang Zhong[2], Stefan Pranger[3], Bettina Könghofer[3], and Oliver T. Hofmann[1] — [1]nstitute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, 8010, Austria — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, 215006, China — [3]Institute of Applied Information Processing and Communications, Graz University of Technology, Graz, 8010, Austria

In this contribution, we present atomically precise molecular nanostructures fabricated without human intervention. We demonstrate that simultaneous control of molecular position and orientation is attainable - both are prerequisites for constructing covalently bonded nanostructures in the future. We employ deep reinforcement learning agents to learn the complex tip-molecule-surface interactions by determining the optimal manipulation parameters for moving and rotating molecules. Because exhaustive sampling of all possible manipulation parameters is impossible, we generate a simulation based on selected experiments. This simulation allows us to train robust agents that even generalize to unseen adsorption conditions and arbitrary nanostructures. With this strategy, we autonomously assemble molecular building blocks into arbitrary geometries, establishing a reliable platform for automated molecular assembly.

O 8.5 Mon 11:45 WILL/A317

The Tale of a Band Melting in a Low-Dimensional Nanostructure — •Lenart Dudy[1,2], Julian Aulbach[2], Joerg Schaefer[2], Ralph Claessen[2], Victor Rogalev[2,3], and Piotr Chudzinski[4,5] — [1]Synchrotron SOLEIL, France — [2]U Würzburg, Germany — [3]Diamond Light Source, UK — [4]Queen's U Belfast, UK — [5]Polish Academy of Sciences, Poland

We explore the unusual phenomenon of “band melting” in the quasi-one-dimensional nanostructure Si(553)-Au. Using angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STM), we observe a striking disappearance of a well-defined electronic band upon increasing temperature, while the atomic structure remains unchanged. Such dramatic temperature-driven changes are rare and typically associated with strongly correlated systems like Kondo or Mott phases.

Our findings point to electronic disorder and suppressed quantum coherence along one dimension. Supported by theoretical insights, we interpret this behavior within a phenomenological framework involving Luttinger-liquid physics and frustrated (pseudo-)spin interactions. This work sheds light on the interplay between dimensionality, correlations, and disorder in low-dimensional materials, opening new perspectives for understanding emergent electronic phases in nanostructures.

O 8.6 Mon 12:00 WILL/A317

Iron-porphyrin coordination network with surface-bound dysprosium adatoms: implications for long-range magnetic ordering — •Pierre Josse[1,2], Massine Kelai[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], and Fabio Donati[1,3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Ordering spins on surfaces offers significant promise for spintronic, magnetic, magnetoelectric, and magneto-optic technologies. One effective approach is to employ spin-active centers embedded within molecular frameworks capable of self-organizing on surfaces. Porphyrins, with their exceptional chemical versatility and tunability, stand out as particularly suitable candidates for this purpose. Various strategies can be used to achieve such spin ordering, including molecular self-assembly, metal-ligand coordination, and on-surface synthesis involving the formation of C-C bonds. In this work, we present the specific strategies we use to organize spins on surfaces and examine how these methods influence long-range magnetic ordering.

O 8.7 Mon 12:15 WILL/A317

On-Surface Synthesis on Oxide — •Sonja Bohl[1], Kassandra Zoltner[1], Leonard Neuhaus[1], Stefan R. Kachel[1], Agustina Heredia[2], Cissie Slopianka[1], Sophie Schäfer[1], Lisa Arnold[1], Doris Grumelli[2], Sabine Wenzel[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Universität Marburg — [2]INIFTA, Universidad Nacional de La Plata

Oxide surfaces offer the advantage of weak molecule-substrate interactions, enabling a more direct and undistorted probing of the properties of adsorbed molecules compared to metal substrates. However, the reduced adsorption energies represent a central challenge for on-surface synthesis, requiring adjusted precursor strategies to prevent premature desorption from the oxide substrates. In this work, we explore approaches to enable on-surface reactions on thin-film oxides and well-defined bulk oxides. While various nano-carbon structures have previously been synthesized on metal surfaces, we investigate whether analogous processes can be realized on oxides. Furthermore, we examine how metal-organic nanostructures interact with bulk oxide surfaces and whether the substrate can induce changes in their coordination environment. Our methodology combines on-surface synthesis with scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and temperature-programmed desorption (TPD).

O 9: Organic molecules on inorganic substrates: electronic, optical and other properties I

Time: Monday 15:00–18:00 Location: HSZ/0201

O 9.1 Mon 15:00 HSZ/0201

Adsorption-induced chirality of an otherwise highly-symmetrical molecule — •Jannis Lessmeister[1], Chetana Badala Viswanatha[1], Andreas Windischbacher[2], Christian S. Kern[2], Lu Lyu[3], Vitaliy Feyer[4], Iulia Cojocariu[4], Daniel Baranowski[4], Martin Aeschlimann[1], Peter Puschnig[2], and Benjamin Stadtmüller[3] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Graz, 8010 Graz, Austria — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [4]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany

Chirality is a fundamental concept with far-reaching implications across chemistry, biology and materials science. In condensed matter, interest has grown around the chiral-induced spin selectivity (CISS) effect, which promises spin-dependent functionality in chiral molecules without magnetic or heavy-metal components. So far, however, the role of the interface for CISS remains unclear.

To illuminate the interactions at chiral metal-molecular interfaces, we explore how the highly-symmetrical molecule pentacene adsorbes on a naturally chiral copper surface. Employing momentum microscopy we identify changes of the emission pattern of the frontier molecular orbitals of pentacene adsorbed on chiral Cu(643) versus achiral Cu(110). In conjunction with density functional theory calculations, we can attribute these observations to a twisting of pentacene and thus to an adsorption-induced chirality of the otherwise symmetric molecule.

O 9.2 Mon 15:15 HSZ/0201

Explaining Principles of Tip-Enhanced Raman Images with Ab Initio Modeling — •Krystof Brezina[1], Yair Litman[2], and Mariana Rossi[1] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

Tip-enhanced Raman spectroscopy (TERS) is an emerging method for imaging vibrational motion and chemically characterizing surface-bound molecular adsorbates. Existing approaches to TERS simulation often build on strong approximations, including a simplification or neglect of the underlying metallic substrate, often leading to discrepancies with experiments. In this work, we present a new, *ab initio* finite-field formulation of a TERS simulation framework [1] that can efficiently address large-scale, realistic systems under periodic boundary conditions [2]. This treatment is essential as it eliminates known artifacts in simulated TERS images stemming from substrate approximations, as shown by our benchmarks on adsorbates and surface defects, and allows for simulations directly comparable to experiments. In this direction, our simulations of Mg(II)-porphine on Ag(100) correctly explain the spatial intensity variation of experimental TERS images and provide an insight into the fundamental principles that define substrate contribution to the scattering cross section in TERS. Our infrastructure is generally applicable to any solid substrate, is computationally efficient and available within the FHI-aims electronic structure code.

[1] Litman Y. et al. *J. Phys. Chem. Lett.*, 14, 6850–6859 (2023)
[2] Brezina K., Litman Y. and Rossi M. *arXiv:2509.13075* (2025)

O 9.3 Mon 15:30 HSZ/0201

Periodic Potential Engineering of 2D Superlattices for Enhanced Photocatalysis — •Qun Yang — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Atomically thin semiconductors hold great promise for photocatalytic solar energy conversion, yet often face key challenges such as rapid electron-hole recombination, inappropriate band gaps, and misaligned energy levels to redox potentials. We introduce a general design strategy based on symmetry-defined periodic potentials for 2D photocatalyst engineering. These long-range modulations reshape the band structure and induce robust electron-hole separation without altering the material lattice. Applied to a monolayer InSe photocatalyst, we show that experimentally achievable moiré patterns, such as those formed with twisted hBN, enable miniband formation and tunable spatial charge separation. Moreover, the periodic potential modulates local adsorption energetics, providing a new handle to enhance catalytic activity for both photocatalytic hydrogen and oxygen evolution reactions. Our results provide a path toward the realization of high-efficiency solar-to-chemical energy conversion in a broad range of 2D materials.

O 9.4 Mon 15:45 HSZ/0201

Supramolecular organisation of thermolabile $TbPc_2$ derivatives at surfaces — •Patrick Lawes[1], Joachim Reichert[1], Anthoula C. Papageorgiou[1,3], Joe Komeda[4], Svetlana

Klyatskaya[4], Andreas Walz[1,2], Annette Huettig[1,2], Hartmut Schlichting[1,2], Rochio Sánchez-de-Armas[6], Nicolas Montenegro-Pohlhammer[6,7], Carmen J. Calzado[6], Jean-Pierre Bucher[5], Johannes V. Barth[1], and Mario Ruben[4,8] — [1]TU Münich, DE — [2]pureions GmbH, Gilching, DE — [3]National and Kapodistrian University of Athens, GR — [4]Karlsruhe Insitute of Technology, DE — [5]IPCMS Université de Strasbourg FR — [6]Universidad de Sevilla, ES — [7]DIC, CIBQA, Universidad Bernardo OHiggins, CL — [8]CESQ, ISIS, Université de Strasbourg, FR

Creation and study of novel materials towards the goal of quantum information processing, involves sophisticated chemistry integrated into useful architectures. The self-organization of single-molecule magnets, is widely studied and reported. Utilizing electrospray ion beam deposition permits the study of thermolabile, functionalised bis(phthalocyaninato) terbium complexes on surfaces. This work aims to tailor the lattices of spin centres. Complex ligand tuned structures were characterised by scanning tunneling microscopy allowing for potential study into quantum criticality and quantum technologies.

O 9.5 Mon 16:00 HSZ/0201

Orbitals of Artificial Atoms in a Gapped Two-Dimensional Vacuum — Mong-Wen Gu[1,2], Aizhan Sabitova[1,2], Taner Esat[1,2], Christian Wagner[1,2], F. Stefan Tautz[1,2,3], Aleksandr Rodin[4,5], and •Ruslan Temirov[1,2,6] — [1]PGI-3, Forschungszentrum Jülich, Germany — [2]JARA, Fundamentals of Future Information Technology, Germany — [3]RWTH Aachen, Germany — [4]NUS, Singapore — [5]Yale-NUS College, Singapore — [6]University of Cologne, Germany

Artificial atoms–engineered nanostructures that confine electronic states–offer a route toward atom-by-atom design of electronic functionality. In this work, we use low-temperature STM and STS to study single-molecule vacancies in a commensurate PTCDA/Ag(111) monolayer, which act as attractive potentials for the two-dimensional interface-state electrons.

Using feature-detection STS [1,2], we directly image the vacancy-induced bound states and identify artificial analogues of s- and p-orbitals that split from the parabolic band minimum and hybridise when two vacancies are brought into proximity. Beyond these conventional orbital analogues, the periodically corrugated interface-state band hosts partial band gaps that support additional quasi-localised states with no counterparts in natural atoms. Tight-binding simulations reproduce these high-energy states and reveal their origin in the gap regions of the 2D dispersion.

[1] A. Sabitova, et. al., PRB 98, 205429 (2018), [2] J. Martinez-Castro, Commun. Mater. 3, 57 (2022)

O 9.6 Mon 16:15 HSZ/0201

Thermal and photo-induced one-dimensional switching of azobenzene derivatives on a graphite surface — •Thiruvancheril Gopakumar[1], Hariom Birla[1], Showkat H. Mir[1], Khushboo Yadav[1], Thomas Halbritter[2], Alexander Heckel[2], and Jayant K. Singh[3] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt, Max-von-Laue-Str. 9, 60438 Frankfurt, Germany — [3]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India

In this presentation we demonstrate an unusual one-dimensional (1D) cascade effect in the thermal- and photo-induced switching of azobenzene derivatives deposited on graphite surface. Upon thermal- and photo-induction, molecules switch between their geometric states (trans and cis) along a selected lattice within the assembly up to several hundreds of nanometres. Generally, such directionality is observed only for a length scale of few nanometres. It is revealed that the strong intermolecular interaction along one of the lattices compared to the other is at the origin of the 1D cascading effect. Harnessing cooperative switching opens possibilities for engineering the responses of molecular film to external trigger and provides opportunities to control the directionality of switching/reactions, and novel nanostructures.

O 9.7 Mon 16:30 HSZ/0201

Accessing Energetically Restricted Optical Transitions in a Single Free-Base Porphyrin Molecule — •Eve Ammerman, Nils Krane, and Bruno Schuler — Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Charge transfer between a single molecule and the electrodes of an STM leads to a series of excitation and relaxation processes, including radiative relaxation from the molecule's optically active excited states. Utilizing the STM tunnel junction in electroluminescence experiments enables optical characterization on sub-molecular lengthscales. However, the electroluminescence phenomenon is constrained by the alignment of ionization and optical state energies. Here, we show how positive ion resonance energy of a free-base tetrabenzoporphyrin (H2TBP) can be tuned relative to the optical emission energy through local gating by the STM tunnel junction or by work function engineering. The tuning of the energy level alignment allows us to produce optical emission from H2TBP on Ag(111), where electroluminescence is energetically restricted, or on Ag(110) where the molecule becomes bright.

O 9.8 Mon 16:45 HSZ/0201

Optical characterisation of single chlorophyll molecules at the sub-nanometre scale — Thiago G. L. Brito[1], •Daniel Arribas[1], Myriam Wadsack[1], Claudia Leticia Gómez Flores[1], Victor Feitosa[1], Klaus Kuhnke[1], Klaus Kern[1,2], Kelvin Anggara[1], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

As one of the main biomolecules harvesting light in photosynthetic organisms, chlorophyll plays a crucial role in biological systems, ultimately sustaining life on Earth. Therefore, the fundamental understanding of its optical properties has attracted widespread interest from the scientific community. However, traditional spectroscopic experiments, often probing complexes, only provide an averaged understanding of the rich photophysics of chlorophyll, where the effects of each possible molecular configuration and the local environment are smeared out. In this work, we address this by exploiting the sub-nm resolution of scanning tunnelling microscopy and the highly-localised plasmonic enhancement of the picocavity in the tunnelling junction. We characterise individual chlorophyll molecules, deposited by electrospray ion beam deposition on a Ag(111) surface with NaCl islands as decoupling layer. By analysing the fluorescence emission excited by the tunnelling electrons, we observe the structural dependency of the molecular opto-electronic properties. Our investigation opens new opportunities for the fundamental understanding of light-harvesting during photosynthesis with unprecedented sub-molecular resolution.

O 9.9 Mon 17:00 HSZ/0201

Polaronic transport through a molecular system with scanning probe microscopy — •Laëtitia Farinacci[1,2,3], Gaël Reecht[3], Christian Lotze[3], and Katharina Franke[3] — [1]University of Wuerzburg, Wuerzburg, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Stuttgart, Germany — [3]Freie Universitaet Berlin, Berlin, Germany

Polarons are quasi-particles in which electron excitations couple to distortions of the local ions network surrounding them. Typically, they are studied in metal oxides where they heavily influence charge transport and thereby often are key to understand and characterize the materials' properties. Here, we use scanning tunneling microscopy and atomic force microscopy to study the properties of Fe-porphine-chloride (FeP-Cl) molecules adsorbed on Pb(111). We observe distinct properties in the dI/dV signal that are indicative of polaronic transport.

More precisely, we find that the FeP molecules form islands in which Cl adatoms are trapped between the molecules. This leads to an effective gating of the molecules by local electric fields that stabilize either of two electronic configurations. Some FeP molecules display sharp peaks in their dI/dV reminiscent of vibrational modes. Importantly, the mapping of these peaks in dI/dV reveal the key role of the electric field and the necessity to account for charge transport through the island. These ingredients are the fundaments of polaron formation and will provide complementary understanding of the fundamental phenomena at the origin their formation in organic/inorganic interfaces.

O 9.10 Mon 17:15 HSZ/0201

Debromination and π-radical formation by single-electron injection on an insulator — •Ye Liu[1], Felix Giselbrecht[1], Lucía Gómez-Rodrigo[2], Manuel Vilas-Varela[2], Tzu-Chao Hung[1], Diego Peña[2], and Jascha Repp[1] — [1]University of Regensburg, Germany. — [2]Universidade de Santiago de Compostela, Spain.

The creation of π-radicals in nanostructures offers promising opportunities in spintronics and quantum technologies1,2, yet their controlled formation on an insulator remains challenging3. Here, we investigated the charge-induced reaction of 11-bromo-11H-benzo[b]fluorene on thick NaCl films (> 20 monolayers) using non-contact atomic force microscopy. The injection of only one electron from the microscope's tip induces debromination, which yield an open-shell structure and a bromide anion. In contrast, removal of an electron from the precursor results in a cation without bond cleavage. The voltage threshold for debromination depends on the molecular adsorption geometry, specifically on whether the bromine atom points upward or downward, reflecting opposite orientations of the molecular dipole moment. We present a feasible tip-induced synthesis strategy for generating a π-radical in molecule on an insulator, offering a promising route toward constructing larger open-shell nanostructure with multiple π-radicals on such surfaces.

O 9.11 Mon 17:30 HSZ/0201

Intramolecular cyclization of helicenes towards non-benzenoid nanographenes via formation of radicals — •Daniel Rothhardt[1], Ming-Lun Pan[2], Christian Wäckerlin[3,4], Hans Josef Hug[1], Yao-Ting Wu[2], Karl-Heinz Ernst[1,5,6], and Miloš Baljozović[1] — [1]Empa, Dübendorf, Switzerland — [2]National Cheng Kung University, Tainan, Taiwan — [3]PSI, Villigen PSI, Switzerland — [4]EPFL, Lausanne, Switzerland — [5]The Czech Academy of Sciences, Prague, Czech Republic — [6]University of Zurich, Zurich, Switzerland

On-surface synthesis has recently become a leading tool for controllable C-C bond formation that would otherwise hardly be accessible by conventional solution chemistry. The advancement of on-surface synthesis gave rise to a novel class of magnetic materials, namely open-shell magnetic nanographenes. The magnetism here mostly stems from the formation of unpaired electrons (radicals) due to a sublattice imbalance, topological frustration or aromatic stabilization. Such carbon-based spin systems are often considered promising candidates for spintronics applications due to their weak spin-orbit coupling and hyperfine interaction, allowing for long spin-lifetime and spin diffusion lengths. Here we demonstrate that the radical formation within the non-planar hydrocarbons such as helicenes leads to intramolecular bond formation and reorganization on Au(111) substrate resulting in non-benzenoid nanographenes. The products are identified using ToF-SIMS, STM and nc-AFM, corroborating the proposed radical-induced cyclization mechanism.

O 9.12 Mon 17:45 HSZ/0201

A Molecule with Half-Möbius Topology — Igor Roncevic[1,2], Fabian Paschke[3], Yueze Gao[2], Leonard-Alexander Lieske[3], Lene A. Gödde[2], Jascha Repp[4], Florian Albrecht[3], Harry L. Anderson[2], and •Leo Gross[3] — [1]Department of Chemistry, The University of Manchester, Oxford Road, Manchester, United Kingdom — [2]Department of Chemistry, Oxford University, Chemistry Research Laboratory, Oxford, United Kingdom — [3]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [4]Institute of Experimental and Applied Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, Regensburg, Germany

Stereoisomers of $C_{13}Cl_2$ exhibiting helical orbitals around a ring of carbon atoms were synthesized by atom manipulation on bilayer NaCl on Au(111). We resolved the enantiomeric geometries of the closed-shell singlet states by atomic force microscopy and mapped their helical orbital densities by scanning tunnelling microscopy. A π-orbital basis of the helical, non-planar singlets that twists by 90° in one circulation is consistent with a half-Möbius topology. In such a topology, the π-orbital basis changes sign with respect to two circumnavigations and is periodic with respect to four circumnavigations. This is in contrast to a topologically trivial Hückel basis, which shows no twist, and a Möbius basis, which twist by 180° in one circulation. We demonstrate reversible switching of the topology, between the two singlets of oppositely threaded half-Möbius topology, and the planar, topologically trivial, triplet state.

O 10: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

O 10.1 Mon 15:00 HSZ/0204

A virtual super-moiré: $MnBr_2$ on graphene on Ir(110) — Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], •Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

$MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of Gr/$MnBr_2$/Ir(110) is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice – two lattices not in contact with each other. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110), and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110). Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2$/Gr/Ir(110) super-moiré.

O 10.2 Mon 15:15 HSZ/0204

Magnetism of monolayers of $FeCl_2$ and $FeBr_2$ Epitaxially Grown on Bi_2Se_3 — •Sebastien E. Hadjadj[1], Weibin Li[2], Pierluigi Gargiani[2], Cinthia Piamonteze[3], Oleksandr Stetsovych[4], Pavel Jelínek[4], Maxim Ilyn[1], and Celia Rogero[1] — [1]Materials Physics Center(MPC - CFM), Donostia, Spain — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Two-dimensional transition metal dihalides exhibit novel magnetic and electronic properties. By combining 2D magnetic semiconductors with topological insulators (TIs) novel quantum and spintronic phenomena can be investigated. Here, we report the uniform and epitaxial growth of monolayer $FeCl_2$ and $FeBr_2$ on the TI Bi_2Se_3. Structural and electronic characterization via LEED, STM, and STS measurements revealed a material-specific moiré pattern resulting from lattice mismatch, as well as a position-independent bandgap of 4 eV. Synchrotron-radiation-based XAS and XMCD measurements confirm robust ferromagnetic order down to the monolayer limit, with an intrinsic reduction of the effective spin magnetic moment by 40-50%. These magnetic vdW heterostructures provide a platform for investigating magnetic proximity effects and moiré-induced modifications of topological surface states. [1] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847*9856,(2023) [2] S. Kerschbaumer et al., Adv. Science, e08262,(2025)

O 10.3 Mon 15:30 HSZ/0204

Rise and fall of 1T-TaS_2: Epitaxial growth of monolayer TaS_2 on Au(111) — •Lars Buss[1], Cathy Sulaiman[1], Raquel Sánchez-Barquilla[1], Iulia Cojocariu[2], Marcin Szpytma[3], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy — [3]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland — [4]Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional TaS_2 has attracted extensive research interest due to its ability to exhibit electron correlation effects, including charge density waves (CDWs). In particular, 1T-TaS_2 is of interest as it shows a CDW at room temperature. However, when grown on metal substrates, only 2H-TaS_2 has been reported. To elucidate the reasons for the apparent lack of 1T-TaS_2 growth in the literature, we have investigated the growth of TaS_2 on Au(111) employing *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED) as well as X-ray photoemission electron microscopy (XPEEM) [1]. We show that at elevated temperatures TaS_2 nucleates and grows in the metastable 1T-TaS_2 phase, which transforms into the stable 2H-TaS_2 phase via a temperature-activated process and then continues to grow at a considerably lower rate. Furthermore, we observe CDW-like ordering in 1T-TaS_2/Au(111), though it is suppressed in 2H-TaS_2/Au(111).

[1] L. Buß et al. Phys. Rev. Materials **9**, 074006 (2025).

O 10.4 Mon 15:45 HSZ/0204

Band-Like Transport and its Modulation by Nitrogen Doping in Transferable Semi-Conducting 2D-imine Covalent Organic Framework — •Vijay Bahadur Yadav, Diksha Srivastava, Satya Veer Singh, Itu Pandey, Manabendra Chandra, and Thiruvancheril G. Gopakumar — Indian Institute of Technology Kanpur

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are promising semiconductors for thin-film electronics and sensing due to their extended in-plane π-conjugation, enabling efficient charge transport. Here, we investigate two highly crystalline 2D imine COF films synthesised via quasi-equilibrium Schiff base condensation. By selecting molecular precursors, we tuned the nitrogen content, producing COFs with ten and six nitrogen atoms per unit cell (10N-COF and 6N-COF). The films are chemically stable in organic solvents and water, mechanically robust, and transferable onto various substrates, allowing fabrication over areas of tens of square centimeters. Electrical measurements using silver electrode arrays show linear current*voltage behaviour, indicating band-like transport, with consistent responses across multiple regions. The conductivity of 10N-COF is ˜36 times higher than that of 6N-COF. Density functional theory calculations reveal similar band gaps but enhanced band dispersion near the Fermi level in 10N-COF, improving charge carrier mobility. Nitrogen incorporation thus effectively tunes charge transport in 2D COFs.

O 10.5 Mon 16:00 HSZ/0204

Co_2S_2: a new 2D material and its phase transitions — •Abdallah Karaka, Max Wolfertz, Affan Safeer, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra high vacuum conditions, 2D materials can be synthesized under conditions far from equilibrium for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: P$\bar{3}$m1 trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing with a lattice constant of 3.66 ± 0.05 Å and a height of 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.52 ± 0.05 Å and a height of 11.7 Å. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase.

O 10.6 Mon 16:15 HSZ/0204

Tailored growth of 2D alloy transition metal dichalcogenides with tunable optical and electrical properties using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Nhat Lam Duong[1], Julian Picker[1], Rahul Sharma[1], Christof Neumann[1], Mona Sedighi[2], Johannes Biskupek[2], Muhammad Sufyan Ramzan[1], Caterina Cocchi[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Doping or alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) provides a promising route to tune the optical, magnetic, and electronic properties. Here, we present a liquid-precursor-based chemical vapor deposition (CVD) for the controlled growth of large-area monolayer $(V_xW_zMo_{1\text{-}x\text{-}y})S_2$ alloys with tunable optical and electrical properties. Comprehensive characterization using atomic force microscopy, transmission electron microscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy, and ab initio calculations confirms the structural and optical quality. Notably, PL shows a noticeable defect exciton peak at room temperature in the V-doped monolayer. Furthermore, by adjusting the composition, we modulate the carrier type of these monolayers from n-type to p-type or even make the monolayers metallic for high vanadium concentrations, which is deduced from electrical transport measurements and density functional theory calculations. This work demonstrates high potential of liquid-precursor CVD as a platform for the tailored growth of complex 2D TMD alloys for next-generation optoelectronic devices.

O 10.7 Mon 16:30 HSZ/0204

CVD growth and characterization of WSe_2 monolayers on Au(111) and their conversion to Janus SeWS — •Julian Picker[1], Jonas Brandhoff[2], Maximilian Schaal[2], Felix Otto[2], Christof Neumann[1], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) exhibit distinctive optical and electronic properties in the two-dimensional monolayer limit. Recently, Janus TMDs have attracted significant attention because their asymmetric chalcogen composition breaks the out-of-plane symmetry and enables properties not attainable in conventional TMDs. In this work, we initially investigate the structural and electronic characteristics of WSe_2 monolayers grown on Au(111) via ambient-pressure chemical vapor deposition (CVD). Surface-sensitive techniques - including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and angle-resolved photoelectron spectroscopy (ARPES) - were employed to characterize the properties of these monolayers. Subsequently, the WSe_2 monolayers were transformed into Janus SeWS monolayers through selective chalcogen replacement at the WSe_2/Au interface. A comparative analysis reveals the structural and electronic differences between the two systems.

O 10.8 Mon 16:45 HSZ/0204

Controlling polymorphism in the growth of 2D manganese sulfide on graphene via substrate interaction — •Max Wolfertz, Abdallah Karaka, Nicolas Georgopoulos, Oktay Güleryüz, Affan Safeer, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide on graphene/Ir substrates grown via molecular beam epitaxy. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and - spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: manganese sulfide in trigonal CuI-structure (space group P-3m1) and MnS in thin platelets of a cubic rock-salt structure (space group Fm-3m). Their in-plane lattice parameters are 4.16 Å, and 3.63 Å respectively. We show that the substrate exerts a strong influence on the phase selected. While the growth on Gr/Ir(111) results in a large share of cubic MnS, the Gr/Ir(110) substrate favors the formation of single layer trigonal manganese sulfide. Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

O 10.9 Mon 17:00 HSZ/0204

Low Temperature MOCVD Growth of two-dimensional InSe and InSe/WS2 Heterostructures — •Robin Guenkel, Nils Langlotz, Matvei Kislitsyn, Juergen Belz, and Kerstin Volz — mar.quest|Marburg Center for Quantum Materials and Sustainable Technologies, Philipps University Marburg, Germany

Two-dimensional van der Waals heterostructures offer powerful opportunities for engineered optoelectronic functionality, particularly when type-II band alignment enables efficient charge separation and interlayer transitions. InSe and WS* are especially promising in this regard because their band structures allow for the formation of a type-II interface at the Γ point, which avoids momentum mismatch. This is an essential requirement for robust radiative processes in 2D stacks. This talk presents a low-temperature metal-organic chemical vapor deposition (MOCVD) approach for synthesizing high-quality InSe and vertically integrated InSe/WS2 heterostructures. Using DTBSe and TMIn at 350 °C, we synthesize homogeneous, single-phase InSe films on 2-inch sapphire substrates and extend the process to directly grow on monolayer WS2. Atomic force microscopy, Raman spectroscopy, and energy-dispersive X-ray spectroscopy provide insight into the morphology, crystallinity, and composition of the films, offering a detailed understanding of the growth behavior and the influence of the substrate surface chemistry.

O 10.10 Mon 17:15 HSZ/0204

Synthesis of Vertically Stacked 2D-hBN/Borophene Het-

erostructures on Ir(111) via Intrinsic Segregation — •Marko Kriegel, Karim Omambac, Smruti Mohanty, Birk Finke, Frank-J. Meyer zu Heringdorf, and Michael Horn-von Hoegen — University Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Lotharstr. 1, 47057 Duisburg, Germany

Research efforts on 2D materials increasingly target complex architectures built from high-quality heterostructures. A key challenge remains the reliable and scalable in-situ fabrication of such systems. In this work, we use high-resolution spot-profile analysis LEED (SPA-LEED) and -microscopy (LEEM) to investigate a synthesis route for an hBN/borophene heterostructure on Ir(111) based on *intrinsic segregation*. At elevated temperatures, boron dissolves into the Ir subsurface region during exposure to the borazine precursor $B_3N_3H_6$ in a CVD process [1], thereby creating a boron reservoir. Increasing the precursor pressure drives the chemical balance toward formation of a complete hBN layer across the Ir surface [2]. Upon cooldown, the decreasing boron solubility induces segregation, resulting in the growth of a continuous borophene layer beneath the hBN overlayer. This one-step CVD approach establishes a promising, scalable pathway for the controlled synthesis of high-quality 2D heterostructures. [1] K. Omambac et al., ACS Nano **15** (2021) 7421 [2] K. Omambac et al., ACS Nano **17** (2023) 17946

O 10.11 Mon 17:30 HSZ/0204

MBE growth and characterization of high-quality monolayer MoS2 on stepped Au surface — •Sayan Debnath, Ram Prakash Pandeya, Konstantin Shchukin, Patrik Staudenmayer, and Alexander Grüneis — Optoelektronische Materialien Institut für Festkörperelektronik, TU Wien, 1040 Wien, Austria

In the present work, we investigate the growth of sub-monolayer MoS2 on Au(788) and Au(111), using molecular beam epitaxy. Sample growth quality is characterized using low-energy electron diffraction, X-ray photoemission spectroscopy, and scanning electron microscopy. Furthermore, a comparative study of the electronic properties was performed by studying the band structure using angle-resolved photoemission spectroscopy (ARPES), and the vibrational properties were measured by angle-resolved polarized Raman (ARPR) spectroscopy.

Our study reveals superior crystalline quality, with fewer S deficiencies, and better azimuthal order of MoS2 grown on the stepped Au(788) substrate compared to the Au(111). In the case of ARPES, we observed more resolved band dispersion on MoS2/Au (788), confirmed by probing the spin-orbit splitting at the Brillouin zone boundary (K point). On the other hand, ARPR of the first Raman mode E2g on MoS2/Au (788) deviates from the symmetry of freestanding MoS2, suggesting the effect of the stepped surface on the vibrational properties. We discuss the role of increased catalytic activity at step edges in promoting the growth of high-quality TMDCs, such as MoS2 and WS2, on stepped surfaces.

O 11: Metal & Semiconductor substrates: Adsorption and reaction of small molecules II

Time: Monday 15:00–17:00 Location: HSZ/0401

O 11.1 Mon 15:00 HSZ/0401

Ethylene on Si(001) revisited: New insights from XPS, STM, and Monte Carlo Simulations — •Jannick A. Peters, Sophie Göbel, and Michael Dürr — Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

The adsorption of ethylene - the smallest organic molecule with a C=C double bond - on Si(001) seems straightforward and is widely used as reference, e.g., for the determination of absolute surface coverage. On the other hand, there is ongoing discussion about adsorption configurations, coverage dependence, and in particular the site-selective adsorption based on strongly reduced reactivity on the partially covered surface, leading to two-step adsorption kinetics. In this study, the adsorption of ethylene on Si(001) was investigated at 300 K by means of XPS and STM with special focus on the coverage dependence, and was further modelled by means of Monte Carlo simulations. We can show that the first step of the two-step adsorption kinetics results in a saturation coverage of 0.7 ML, which is significantly higher than the commonly referenced coverage of 0.5 ML. STM measurements show that this behaviour is caused by a combination of adsorption statistics, nearest-neighbour interactions, and site-selective hindrance. Higher coverage up to 1 ML is then reached with a significantly higher dose due to the reduced reactivity of the remaining surface sites. Monte Carlo simulations taking into account a limited set of reaction channels accurately describe the complete coverage dependence as well as the local order of the adsorbates on the surface.

O 11.2 Mon 15:15 HSZ/0401

The Influence of Doping on Inelastic H Atom Scattering from Silicon — •Malte Opfermann, Kerstin Krüger, Sophia Tödter, and Oliver Bünermann — Institut für physikalische Chemie, Georg- August-Universität Göttingen, Tammannstraße 6, 37077 Göttingen

Inelastic H atom scattering experiments on the semiconducting Ge(111)c(2x8) surface have revealed a bimodal energy-loss distribution consisting of a narrow low energy-loss component and a broad high energy-loss component with an onset equal to the surface band gap. Theoretical calculations attribute the low energy-loss component to an adiabatic scattering mechanism at the adatom. The high energy-loss component is explained by a non-adiabatic scattering mechanism involving electron transfer across the surface band gap from the rest atom to the adatom.

Recently, we extended our studies to scattering experiments from the Si(100)2x1 surface. Although the experimental energy loss distributions resemble the bimodal behavior of Ge(111)c(2x8), the first component is broader, and the second exhibits a visible but less well-defined onset at the surface band gap. To gain further insight, we carried out scattering experiments from n-doped and p-doped surfaces. The first component shifts to lower energy losses for n-type doping and to higher energy losses for p-type doping, whereas the second component remains essentially unaffected. Based on the theoretical results for Ge(111)c(2x8), we propose a scattering mechanism for the Si(100)2x1 surface.

O 11.3 Mon 15:30 HSZ/0401

***Ab initio* insights into the OER activity of pristine and metal-supported Co_3O_4(111)** — •Muhammad Munawar[1,2] and Rossitza Pentcheva[1] — [1]Department of Physics and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]IMPRS SusMet, Max Planck Institute for Sustainable Materials GmbH, Max Planck-Straße 1, 40237, Düsseldorf, Germany

Co_3O_4 is a promising anode material for the oxygen evolution reaction (OER), yet the role of metallic supports on its electronic properties and performance remains elusive. Here, we employ density functional theory with a Hubbard U term (DFT+U) to investigate the structural, electronic, and catalytic properties of pristine Co_3O_4(111) and Co_3O_4(111) grown on Pt(111). Using *ab-initio* thermodynamics, we determine that the Co tetrahedral termination is the most stable Co_3O_4(111) surface across a broad range of oxygen chemical potentials. Our results reveal that a built-in electric field emerges when Co_3O_4(111) is grown on a metallic substrate like Pt(111), that shifts the valence band maximum in the surface layer toward the Fermi level. Moreover, the work function increases monotonically with applied strain. Furthermore, we compare the OER activity of the pristine Co_3O_4(111) and Co_3O_4(111)/Pt(111) surface. These results provide atomic scale insight into structure-property relationships at oxide and oxide/metal interface, offering guidance for the rational design of next generation oxide-based electrocatalysts.

O 11.4 Mon 15:45 HSZ/0401

Through Stronger Hinderance to Higher Reactivity: Influence of the Alkyl Chains on the Activation Energy of Ether Cleavage on Silicon — Timo Glaser[1], Gustav F. Nolte[1], Tamam Bohamud[1], Philip Keller[1], Mathieu G. Silly[2], Hendrik Weiske[3], Ralf Tonner-Zech[3], and •Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Synchrotron SOLEIL, Gif sur Yvette, France — [3]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany

Reactivity in surface chemistry is often discussed in terms of the interaction between surface states and the functional groups of the reacting molecule. Herein we demonstrate that for finite submonolayer coverage, i.e., surface coverage at which the molecular adsorbates cannot be treated as isolated molecules anymore, the seemingly innocent side chains of the adsorbate can also play a decisive role. For the example of ether cleavage on Si(001), which represents the surface analogue of an $\mathrm{S_N}2$-type reaction, we show both experimentally by means of real-time XPS as well as based on ab-initio calculations that steric hindrance by the side chains determines the activation energy for C-O dissociation into the final state. In contrast to a simple expectation, the *stronger* steric hindrance of the butyl group in butyl methyl ether leads to a *lower* activation energy for ether cleavage on Si(001) when compared to diethyl ether. This effect was traced back to different degrees of destabilization of the precursor and the transition state [1].
[1] T. Glaser, et al., Angew. Chem. Int. Ed. e19990 (2025).

O 11.5 Mon 16:00 HSZ/0401

Frontier Orbitals Control Adsorbate Bonding to Stepped Transition Metal Surfaces — •Florian Nitz[1], Stefan Hörandl[1], Dmitriy Borodin[2], and Alec Wodtke[1] — [1]Institute for Physical Chemistry, Georg-August University of Goettingen, Tammannstraße 6, 37077 Goettingen, Germany — [2]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, South Korea

Developing intuitive models of bonding and reactivity lies at the heart of physical chemistry. While such models have been developed for atoms and molecules, we still lack concepts to explain bonding and reactivity in the solid state, including surface chemistry and catalysis. Here, we address this gap and present a model of covalent bonding between molecular orbitals of an adsorbate and symmetry-specific bands on a metal surface atom, analogous to frontier orbital theory in molecular chemistry. We apply the model to the adsorption of three molecules–CO, NO, and NH_3–on stepped platinum surfaces of varying step density and compare its predictions to experimental adsorption energies. The experiment reveals that the adsorption energies vary systematically with step density, an unexpected phenomenon that can only be explained by the frontier orbital model. Correlations of the adsorbate bond strength with the mean energy of the metal d-electrons or with surface strain fail to describe the experimental observations. This highlights frontier orbitals as a powerful concept to rationalize bonding and reactivity in condensed-phase systems.

O 11.6 Mon 16:15 HSZ/0401

Memory friction and zero-point motion in hydrogen surface diffusion — •George Trenins and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

By virtue of their small mass, hydrogen atoms readily manifest quantum dynamical effects under typical experimental conditions. In particular, hydrogen diffusion on metal surfaces is strongly influenced by nonadiabatic interactions with the conduction electrons. Such "electronic friction" is incorporated into numerical simulations via the generalized Langevin equation (GLE). Additionally, hydrogen possesses substantial zero-point energy and can undergo quantum tunnelling. This is accurately described by "ring-polymer molecular dynamics" (RPMD), an atomistic simulation approach rooted in the path-integral formulation of quantum mechanics. Using a rigorous combination of the GLE and RPMD frameworks, we show that a combination of zero-point motion and non-Markovian (memory) friction are key to the temperature dependence of H-atom diffusion on copper surfaces [1]. In a limited temperature range, the two effects happen to mask each other almost perfectly, creating the appearance of classical, memoryless dynamics. Outside this range, the experiment displays non-Arrhenius behaviour that is not captured by classical dynamics but is readily explained when quantum effects are taken into account. [1] G. Trenins, M. Rossi, Phys. Rev. Lett. **134**, 226201 (2025).

O 11.7 Mon 16:30 HSZ/0401

When plasma meets surfaces - Nitrogen plasma-induced surface transformations on copper — •Ester Perez Penco and Roland Bliem — ARCNL, Amsterdam , The Netherlands

Inside EUVL setups, materials are exposed to challenging conditions, most importantly a plasma generated by the interaction of EUV radiation with the main background gas, hydrogen, and trace elements such as nitrogen. The reactive nature of plasma environments causes even trace gases to significantly influence material properties and affect the condition of surfaces. Copper is widely used in semiconductor technology, including applications as functional parts of the latest generation of chip manufacturing tools using extreme ultraviolet lithography (EUVL), therefore, it is relevant to study its behaviour in such reactive environment.

In this surface science study, we investigate the interaction of plasma-activated nitrogen with Cu(111) surfaces using in situ X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). By systematically comparing the effects of molecular nitrogen, neutral atoms, ions, and nitrogen plasma, we provide detailed insights into how individual plasma species modify the copper surface. Our findings reveal that while radicals modify the very surface layer, higher energy species are required to induce structural disorder and incorporate into deeper layers. The results presented in this study aid in the prediction of plasma-induced changes and the role of trace elements in the EUVL environment.

O 11.8 Mon 16:45 HSZ/0401

From Gold to Copper: N-heterocyclic Carbene Self-Assembly for Area-Selective Deposition — •Franz Thiemann[1], Patrick Melix[1], Emmett Desroche[2], Francesco Tumino[2], Cathleen Crudden[2], and Ralf Tonner-Zech[1] — [1]Wilhelm-Ostwald Institute, Universität Leipzig, Germany — [2]Carbon to Metal Coating Institute, Queen's University, Kingston, Canada

N-heterocyclic carbenes (NHCs) are promising small-molecule inhibitors for area-selective atomic layer deposition (ASD) due to their strong, selective binding to metal surfaces. Using density functional theory with PBE-D4 functionals and periodic surface slabs, this study investigates NHC adsorption on a Cu(111) surface and compares it with previously studied Au(111) systems. In both cases, experimentally observed overlayer formation could be reproduced by DFT calculations and verified using STM images, revealing a distinctive dimer pattern in which NHCs bind to extracted copper adatoms at high density (1.8 NHC/nm^2) with a tilted molecular orientation. Energy decomposition analysis for extended systems revealed the origin of the stable overlayer: strong σ-donation to the surface and π-backdonation, combined with dispersion interactions between the NHC backbones, result in a highly stable blocking layer. [1] Furlan et al. Chem. Mater., 5753, 37 (2025). [2] DesRoche et al., in Preparation. [3] Raupach et al. J. Chem. Phys., 194105, 142 (2015).

O 12: Scanning probe microscopy: light matter interaction at atomic scales

Time: Monday 15:00–17:45 Location: HSZ/0403

O 12.1 Mon 15:00 HSZ/0403

Upconversion electroluminescence in VOPc via adsorption-induced interaction of unpaired spin — •Lukas Gerhard[1], Vibhuti Rai[1], Christof Holzer[1], Carsten Rockstuhl[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany

Molecules with unpaired spins (radicals) promise favourable spin statistics in their electroluminescence. Here, we combine scanning tunneling microscopy induced luminescence and density functional theory to study single vanadyl phthalocyanine molecules, which are stable neutral radicals. Two distinct adsorption geometries of the molecule on NaCl/Au(111) lead to a difference in the interaction of the unpaired electron with the substrate, which in turn allows us to investigate its effects on the light emission process [1]. Remarkably, we observe that up-conversion electroluminescence is gated by the adsorption geometry of the molecule, an effect we attribute to a reordering of excited states and enhanced excited state transition probabilities. The profound influence of the unpaired electron via state reordering opens new possibilities for tuning not only molecular electroluminescence but also many other spin dependent phenomena.

[1] V. N. Rai, C. Holzer, C. Rockstuhl, W. Wulfhekel, and L. Gerhard, arXiv:2508.11501.

O 12.2 Mon 15:15 HSZ/0403

Machine Learning for Atomic-Scale Molecular Discovery from Tip-Enhanced Raman Spectroscopy — Harshit Sethi[1], Markus Juntilla[1], •Orlando J Silveira[1], and Adam S Foster[1,2] — [1]Aalto University, Espoo, Finland — [2]Kanazawa University, Kanazawa, Japan

Tip-enhanced Raman spectroscopy (TERS) combines the nanoscale spatial resolution of scanning probe microscopy with the chemical specificity of Raman spectroscopy, offering a powerful tool for resolving both molecular structure and composition. However, extracting precise atomic-scale information from complex TERS hyperspectral data remains a significant challenge. In this work, we address this gap by developing an automated machine learning framework to decode simulated TERS images for molecular structure discovery. Our approach uses convolutional neural networks (CNNs) to analyze hyperspectral datasets generated by modeling the plasmonic enhancement at a probe tip and the vibrational properties of planar molecules via density functional theory. To handle varying numbers of vibrational modes, we introduce a spectral binning procedure that standardizes the input for network training. This model provides a foundational proof of concept for the autonomous identification of molecular structures from TERS data, advancing the development of automated platforms for atomic-scale materials characterization and discovery.

O 12.3 Mon 15:30 HSZ/0403

THz-induced bilayer stacking dynamics in 1T-TaS$_2$ — Shaoxiang Sheng[1,2], Yang Yang[3], Mohamad Abdo[1], Li Chen[4], Peize Lin[5], •Kurt Lichtenberg[1], Xinguo Ren[3,5], Sheng Meng[3,5], Susanne Baumann[1], and Sebastian Loth[1,6] — [1]University of Stuttgart, Inst. for Functional Matter and Quantum Technologies — [2]Tsientang Inst. for Advanced Study — [3]IOP, Chinese Academy of Sciences — [4]Songshan Lake Materials Laboratory — [5]Inst. of Light Resources and Environmental Science, Henan Academy of Sciences — [6]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart

The electronic properties of layered materials change dramatically with variations in the interlayer coupling and the stacking order [1]. We employ terahertz pump-probe spectroscopy in conjunction with scanning tunneling microscopy (STM) to investigate the role of stacking order dynamics and of domain structures in layered 1T-TaS2 at the atomic scale. TaS2 exhibits diverse charge-density wave (CDW) phases and an insulating ground state at low temperatures [2]. We show that terahertz pulses can induce insulator-to-metal transitions (IMTs) and reveal hidden electronic phases in 1T-TaS2 by manipulating the bilayer stacking at femtosecond time and atomic length scales. This tunability promises unprecedented ultrafast control over the electronic phases also in other layered materials, suggesting applications in reconfigurable quantum devices and neuromorphic computing.

[1]: S.-H. Lee, PRL 122, 106404 (2019) [2]: V Petkov, J. Phys.: Cond. Matt. 34 345401 (2022)

O 12.4 Mon 15:45 HSZ/0403

Coherent coupling between molecular dipoles probed with STML — •Quentin Stein[1], Jakob Kuhlke[3], Song Jiang[1], Tomas Neuman[2], Michelangelo Romeo[1], Fabrice Scheurer[1], Katharina Kaiser[3], and Guillaume Schull[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR7504, F-67000 Strasbourg, France — [2]Institute of Physics, Czech Academy of Sciences Cukrovarnick'a 10, Prague, 16200, Czech Republic — [3]Georg-August-Universität Göttingen, Physikalishes Institut, 37077 Göttingen, Germany

The clustering of chromophores allows their excited states to hybridize, enabling the formation of coherently coupled dipoles spanning multiple molecules. This is of key importance for optical processes occurring in both artificial and natural molecular assemblies.

Probing these coherently coupled dipoles with atomic-scale precision cannot be achieved through conventional optical techniques because of the diffraction limit set by Abbe's law. This difficulty has recently been overcome by scanning tunneling microscopy induced luminescence (STML), which relies on the extreme confinement of the electromagnetic field in the plasmonic picocavity formed at the apex of a metallic STM-tip. The radiative decay rate of a molecular exciton placed in such a cavity is greatly increased, allowing for the detection of states that are typically optically dark. It also provides nanometer-resolved maps of molecular transition dipole moments, revealing the spatial character of the excitonic states with atomic precision. In this work, we used this approach to investigate the fluorescence of coherently coupled dipoles within simple molecular assemblies.

O 12.5 Mon 16:00 HSZ/0403

Continuous-wave all-optical microscopy at the atomic scale — •Valentin Bergbauer[1], Felix Schiegl[1], Svenja Nerreter[1], Valentin Giessibl[1], Fabian Sandner[1], Franz J. Giessibl[1], Yaroslav A. Gerasimenko[1], Tom Siday[2], Markus A. Huber[1], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93040 Regensburg, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, U.K.

Exploring matter at the most fundamental level demands optical microscopy with ever-improving spatial resolution. By confining light to the apex of a sharp metallic tip, scanning near-field optical microscopy (SNOM) circumvents the diffraction limit, though its spatial resolution is still limited by the mesoscopic tip shape, inhibiting atomic resolution. Here, we observe atomically confined optical signals with Ångström-scale lateral modulations using continuous-wave mid-infrared radiation. These signals, characterized by a picometric vertical decay and a distinct optical phase shift, are consistent with emission from lightwave-driven tunnelling currents, a mechanism recently discovered using intense THz pulses. Observing near-field optical tunnelling emission (NOTE) under continuous-wave illumination is surprising, as strong-field effects such as coherent electron driving typically require ultrafast or free-electron lasers. Demonstrating the accessibility of this tunneling-mediated contrast mechanism with standard optical setups paves the way towards routine optical imaging with atomic-scale resolution.

O 12.6 Mon 16:15 HSZ/0403

Tuning Molecular Light Emission Through Atomic-scale Control of the Local Environment — •Thiago G. L. Brito[1], Daniel Arribas[1], Sofia Canola[2], Klaus Kuhnke[1], Tomáš Neuman[2], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institute of Physics, Czech Academy of Sciences, 16200 Prague, Czech Republic

Intermolecular distances, adsorption sites, and configurations define a molecule's local environment, but their combined effect on single-molecule emission across different excitation pathways remains unclear. In this study, we measure the singlet emission of zinc phthalocyanine (ZnPc) on NaCl/Ag(111) and introduce platinum phthalocyanine (PtPc) as both a controlled perturbation of the local environment and a probe of ZnPc emission via resonant energy transfer (RET). All measurements were performed using scanning tunneling microscopy induced luminescence (STML) and tip-enhanced photoluminescence (TEPL). By systematically tuning intermolecular distances, restricting molecular rotational motion, and comparing direct electrical excitation with RET-driven and photon excitations, we reveal previously inaccessible regimes of ZnPc singlet emission, including neutral exciton-libron coupling. We further disentangle the environmental factors that influence emission spectra, demonstrating how the local environment actively shapes the optical response of single molecules.

O 12.7 Mon 16:30 HSZ/0403

Dipole-dipole coupling in assembled ZnPc-molecule clusters — •Jakob Kuhlke[1], Quentin Stein[2], Song Jiang[2], Georg Traeger[1], Fabrice Scheurer[2], Tomáš Neuman[3], Katharina Kaiser[1], and Guillaume Schull[2] — [1]Georg-August University Göttingen, IV. Physical Institute, Göttingen — [2]CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, Département Surfaces et Interfaces, Strasbourg — [3]Institute of Physics, Czech Academy of Sciences Cukrovarnická 10, Prague, 16200, Czech Republic

Dipole-coupled molecules provide a promising platform to build functional structures with tailored optical properties. We use ZnPc molecules as building blocks to investigate the coupling of molecular dipoles in different molecular assemblies.

In contrast to ZnPc monomers, dimers and chains of ZnPc molecules exhibit sharper and red-shifted emission peaks, a phenomenon known as superradiance [1], [2], [3]. Here, we extend this approach to more arbitrary clusters. We use scanning tunneling microscopy-induced luminescence (STML) to study the optical properties of several cluster configurations on the nanometer scale.

[1] L. Yang, et al. Physical Review Letters 122.23 (2019)
[2] Z. Yang, et al. Nature 531.7596 : 623-627 (2016).
[3] J. Dolezal, et al. ACS nano 16.1 : 1082-1088 (2021).

O 12.8 Mon 16:45 HSZ/0403

Selectivity in tautomerization reaction pathways triggered in single molecules on ultrashort time scales — •Niklas Friedrich, Carmen Roelcke, Tzu-Chao Hung, Yaroslav Gerasimenko, Rupert Huber, and Jascha Repp — Institute of Experimental and Applied Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, and Halle-Berlin-Regensburg Cluster of Excellence CCE, Germany

Lightwave-driven scanning tunnelling microscopy (LW-STM) is a powerful technique allowing to unravel dynamics of quantum systems on their intrinsic energy, spatial and temporal scales [1,2]. In LW-STM, the electric-field transient of ultrashort laser pulses focused into the junction of a tunnelling microscope acts as a bias-voltage transient and thereby controls tunnelling on ultrashort timescales.

Here, we explore a chemical reaction triggered on ultrashort timescales. We study free-base naphthalocyanine molecules (H2Nc) on 2ML NaCl on Cu(100). In DC-biased experiments, this system switches between different tautomers upon injection of high-energy tunnelling electrons [3]. We find that the same reaction is facilitated by ultrashort voltage transients in LW-STM for transients far exceeding the voltage of the lowest unoccupied molecular orbital. Furthermore, we observe different selectivities in the tautomerization reaction depending on the energy of the tunnelling electron that we tentatively assign to the orbital structure of H2Nc.

[1] Nat. Photon. 18, 595-602 (2024) [2] arXiv:2507.10206 (2025) [3] Science 317, 1203-1206 (2007)

O 12.9 Mon 17:00 HSZ/0403

Atomic-scale excitonic luminescence nanoscopy of moiré superlattices in van der Waals heterostructures — •Manas Pratim Biswas[1], Fábio J. R. Costa[1], Elise Jouaiti[1], Arnaud Gloppe[1], Katharina Kaiser[1,2], Fabrice Scheurer[1], Stéphane Berciaud[1], and Guillaume Schull[1] — [1]Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), Université de Strasbourg (CNRS, UMR 7504), Strasbourg, France — [2]4th Physical Institute-Solids and Nanostructures, Georg-August-Universität Göttingen, Göttingen, Germany

Atomically thin two-dimensional materials are susceptible to their environment, and stacking them into van der Waals heterostructures allows precise control of their electronic and optical properties. In semiconducting transition metal dichalogenides, excitons dominate the optical response whose properties can be tuned through interfacial interactions. Twisted and/or lattice-mismatched bilayers form a moiré superlattice that periodically modulates the electronic landscape. However, diffraction-limited optical methods average over micrometer scales, concealing these nanoscale effects. To overcome this, we employ cryogenic scanning tunneling microscope-induced luminescence[1] (STML, <7K, ultra-high vacuum) to probe exciton-moiré interplay in near-aligned WSe_2/WS_2 heterobilayers[2,3]. STML enables simultaneous atomic-scale imaging and local optical readout, with the ultimate aim of demonstrating nano-optical probing of moiré-modulated systems. References: 1. Nat. Mat. 22, 482 (2023) 2. Nat. Phys. 19, 1286 (2023) 3. Nat. Mat. 20, 945 (2021)

O 12.10 Mon 17:15 HSZ/0403

Tracing vibrational anharmonicity at the submolecular level with tip-enhanced Raman spectroscopy — •Youngwook Park[1], Ikutaro Hamada[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]The University of Osaka, Suita, Japan

Tip-enhanced Raman spectroscopy (TERS) can achieve atomic-scale vibrational imaging, yet overtones and combination bands remain difficult to access due to weak transition strengths. We show that point-contact TERS enables submolecular-resolution detection of intense overtones and combination bands from a single asymmetric perylene derivative on silicon. A 10-times signal increase upon tip–molecule contact allows us to resolve both mechanical and electrical anharmonicities with Å-level spatial contrast. The mapped mechanical anharmonicity reveals a site-specific vibrational energy exchange pathway, demonstrating TERS as a powerful tool for real-space tracking of intramolecular vibrational energy redistribution.

O 12.11 Mon 17:30 HSZ/0403

Orbital-resolved imaging of coherent femtosecond exciton dynamics in single molecules — •Caiyun Chen — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart

Understanding and controlling excitonic wavepackets is fundamental to uncovering mechanisms underlying energy conversion dynamics in organic molecular systems. We present orbital-resolved imaging of coherent exciton dynamics in single metal-centered naphthalocyanine (MNc) molecules*CoNc, CuNc, and ZnNc*adsorbed on NaCl/Ag(111). Using femtosecond scanning tunneling microscopy, we directly observe time-resolved photocurrent signals and spectroscopic signatures of coherent excitons, enabling selective excitation and control of excitons in isolated and coupled molecules. In single CuNc molecules, we measure a decoherence time (~70 fs), which decreases in dimers due to intermolecular interactions. Time-resolved measurements and photocurrent imaging reveal how central metal atoms in different naphthalocyanine molecules influence decoherence dynamics of the excited electronic state. Notably, a ZnNc molecule has longer decoherence time (~ 300 fs) compared to the CuNc and CoNc (~ 30 fs). Unpaired electrons on Co in CoNc molecule leads to distinct photocurrent imaging contrasts with the closed shell ZnNc and CuNc molecules. The origin of faster decoherence times of the excited states in CoNc and CuNc molecules is linked to conical intersections. These findings underscore the applications of ultrafast STM to probe quantum coherence and energy transfer dynamics at the single-molecule level with atomic-scale spatial resolution.

O 13: Solid-liquid interfaces: Reactions and electrochemistry I

Time: Monday 15:00–18:00 Location: TRE/PHYS

O 13.1 Mon 15:00 TRE/PHYS

The Weak Spots of IrO_2: Sampling Defect Landscapes at Operation Conditions — •Jimiben V. Patel, Nikhil Bapat, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Under the harsh oxidative potentials required for the oxygen evolution reaction, rutile IrO_2 surfaces undergo restructuring that leads to Ir dissolution and undermines catalyst durability, eventually impacting device performance. To mitigate the catalyst degradation via robust design principles, a fundamental atomistic understanding of how surface reconstructions initiate and propagate dissolution is urgently needed. Since high-resolution *operando* characterization remains challenging, atomistic simulations are essential for uncovering the underlying microscopic mechanisms. However, achieving realistic insight requires approaches that go well beyond conventional, idealized modeling frameworks. In this work, we employ machine-learned interatomic potentials trained on density-functional theory to systematically sample vacancy formation across a wide range of electrochemical environments. This allows us to resolve how surface defects nucleate, interact, and evolve under relevant oxidizing conditions. We find that vacancy formation becomes increasingly favorable at higher potentials, with isolated defects stabilizing and subsequently coalescing into larger surface pits – structures that likely act as precursors for accelerated dissolution. These findings provide a first link between applied potential and defect thermodynamics, offering predictive insight into potential-dependent degradation pathways of IrO_2.

O 13.2 Mon 15:15 TRE/PHYS

Electrochemical Free Energy Barriers at Constant Potential — •Elias Diesen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Simulating barriers for electrocatalytic reactions is methodologically very challenging due to the intricate dynamics at the electrified solid/liquid interface. In addition, standard atomistic simulations based on periodic density-functional theory (DFT) keep the charge of the simulation cell constant instead of allowing it to fluctuate during the reaction in order to maintain a (fixed) electrode potential. Here, we introduce a method to compute electrochemical free energy barriers under well-defined potential conditions. Our approach relies on umbrella sampling on top of DFT-based molecular dynamics to access the free energy of activation, including both enthalpic and entropic contributions [1]. By carefully sampling the work function along the reaction coordinate, a Legendre transformation of the resulting canonical (constant-charge) energetics is then used to obtain grand canonical (constant-potential) results [2]. The method is demonstrated for proton deposition over Au(111). We extract potential-dependent barriers and examine kinetic scaling relations as well as use our results to benchmark common approximations in the recent literature. This work paves the way for systematic studies under realistic electrochemical conditions at e.g. varying temperatures or considering different proton-donating species.

[1] E. Diesen *et al.*, ACS Catal. **15**, 5403 (2025).

[2] S.D. Beinlich *et al.*, J. Chem. Theory Comput. **19**, 8323 (2023).

O 13.3 Mon 15:30 TRE/PHYS

Customizable Electrostatic Potentials in DFT Supercell Calculations: Implementation and Application to Electrified Interfaces — •Samuel Mattoso[1], Jing Yang[1], Florian Florian Deissenbeck[1], Ahmed Abdelkawy[1], Christoph Freysoldt[1], Stefan Wippermann[1,2], Mira Todorova[1], and Jörg Neugebauer Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

Electric fields drive reactions, reshape surfaces, guide protein folding and dictate selectivity in chemistry and materials science. While Density Functional Theory (DFT) is a standard tool for modelling such phenomena, introducing user-defined customizable electrostatic potentials usually requires invasive code modifications and deep coding expertise. We will present a lightweight, Python-based implementation that allows adding external electric fields to supercell DFT calculations via a new VASP-Python interface. We outline the necessary energy- and force-corrections, describe the computational setup, and provide a streamlined workflow that works entirely within VASP without altering the source code. The method's versatility is demonstrated on several case studies: molecular adsorption on charged surfaces, field-ion microscopy, electrochemical solid-water interfaces, and implicit solvent models. This approach offers a simple, flexible route for researchers to incorporate external fields into DFT simulations, enabling exploration of field-dependent phenomena across chemistry and materials science.

O 13.4 Mon 15:45 TRE/PHYS

Ion-specific charge transfer and capacitance in the compact double layer of solvated cations at metal electrodes — •Fabiola Dominguez Flores, Axel Gross, and Wolfgang Schmickler — Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany

A molecular-scale understanding of the compact double layer is essential for fundamental electrochemistry. Using density-functional theory with a hybrid implicit-explicit solvation model, we investigate the adsorption of solvated cations (K^+, Na^+, Ca^{2+}, Mg^{2+}) on metal electrodes. This approach captures the local hydration structure while modeling a dilute electrolyte where no diffuse layer forms. Our results reveal two distinct physical regimes: alkali ions retain their unit charge, while divalent ions exhibit substantial partial charge transfer, directly quantified by Bader analysis. This charge transfer governs the interfacial capacitance, which we calculate to be 10-20 μF cm^{-2}, in excellent agreement with experiment. We demonstrate that the electrosorption valency equals the negative of this partial charge. Interpreting these results with a parallel-plate model yields an effective dielectric constant dictated by the polarizabilities of the metal and the water layer. This work provides fundamental microscopic insight into how ion-specific electronic interactions control the properties of the electrochemical double layer.

O 13.5 Mon 16:00 TRE/PHYS

Electrokinetic spectroscopy of ion dynamics near charged surfaces using modulated surface acoustic waves — •Ofer Manor, Li Yifan, and Sudeepthi Aremanda — Technion, Haifa, Israel

We use MHz-level frequency-modulated surface acoustic waves (SAWs) to study the dynamics of ions in the electrical double layer (EDL) to appear near the charged glass/electrolyte interface. The SAW travels in the solid; the EDL exists in the electrolyte; both phenomena are entangled through a field effect, a mechanical evanescent wave, which is invoked in the electrolyte by the SAW and vibrates ions in the EDL to result in the leakage of an electrical field off the glass/electrolyte interface. We show measured spectra of electrolyte comprising different types and concentrations of salts and salt mixtures. This is a spectroscopy of ion dynamics in isolated and unique EDLs.

EDLs are nanometer-thick clouds of ions that appear at the charged interface between a substrate and an electrolyte solution and determines its electrical properties. Ions migrate through the EDL within micro- to nano-seconds: These are the EDL relaxation-times for charging and discharging, which are a product of the EDL structure and ion species therein.

Ion relaxation-times similar to the SAW periodic time result in an ion electro-mechanical synchronization, which maximizes ion vibration and the leakage of electrical fields off the EDL. The leakage identifies ion relaxation-time spectra for different electrolytes and the presence of ions and the intrinsic rate by which they charge and discharge EDLs.

O 13.6 Mon 16:15 TRE/PHYS

Impact of the Negative Dielectric Responses on Solvation and Adsorption at Electrified Interfaces — •Zhenyu Wang[1], Mira Todorova[1], Christoph Freysoldt[1], Stefan Wippermann[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Department of Physics, Philipps-Universität Marburg, Marburg, Germany

Understanding processes at electrified solid-liquid interfaces is central to electrocatalysis, corrosion, and water-splitting, yet the dielectric response of interfacial water remains poorly understood. Using a capacitor geometry in which water is confined between oppositely charged electrodes, we perform several hundred nanoseconds-long molecular dynamics simulations to probe both the dielectric behaviour of neat water and the solvation of ions under bias. The simulations reveal pronounced oscillations in the screening of interfacial water, giving rise to regions in which the local dielectric constant becomes negative. This dielectric response gives rise to weakly bound adsorption states. By correlating the computed potential profiles with the evolution of Na$^+$ and Cl$^-$ solvation shells, we demonstrate that the rate-limiting step is not related to the charge transfer barrier but originates from the reorganization of the ion solvation shell when transferring through the negative-dielectric regions. This insight bridges atomistic dielectric anomalies with macroscopic electrochemical behaviour and provides a quantitative basis to describe ion migration in the vicinity of the electrified interface.

O 13.7 Mon 16:30 TRE/PHYS

Selectivity in Electrochemical Oxidation Reactions: Challenges in Ethylene Epoxidation — •Pauline Schütt and Alexander Bagger — Department of Physics, Technical University of Denmark

Electrochemical technologies play a central role in the sustainable production of fuels and chemicals, but their applications remain limited due to significant overpotentials and challenges in controlling selectivity. Alternative oxidation reactions could potentially generate value-added products on the anode side of electrochemical cells, but typically suffer from competition with the oxygen evolution reaction (OER).[1] Density functional theory (DFT) predictions and concepts from computational catalysis provide useful tools to systematically analyze selectivity and establish trends across different catalyst and reaction systems.[2] We here discuss key challenges restricting such alternative oxidation reactions and their competition with the OER, with a focus on ethylene epoxidation.

[1] L. F. T. Novaes *et al.* Chemical Society Reviews **50**(14), 7941-8002 (2021).

[2] P. Schütt, L. Karlsson and A. Bagger, in preparation, (2026).

O 13.8 Mon 16:45 TRE/PHYS

Bias, Barriers, and Beyond: Perturbative Insights into Electrochemical Reactivity — •Nicolas G. Hörmann and Karsten Reuter — Fritz-Haber-Institut der MPG

Electrochemical processes at solid-liquid interfaces are strongly shaped by the applied potential, yet capturing these effects efficiently remains a central challenge for atomistic modelling. In this talk, I will provide an overview of recent advances made in our group, focusing on perturbative and response-based approaches for electrochemical energetics and kinetics. Building on a rigorous connection between the constant-charge and constant-potential ensembles, we establish general connections between computational formalisms and clarify how potential-dependent properties emerge.

These insights enable efficient Taylor-expanded descriptions of energetics that avoid explicit simulations at different applied biases and allow analytical assessments of non-Nernstian shifts in hydrogen underpotential deposition, potential-dependent symmetry factors and potentiostat-free barrier calculations. Implementing them into bias-aware ML potentials opens the door to long-timescale molecular dynamics and accelerated exploration of electrochemical reaction pathways.

O 13.9 Mon 17:00 TRE/PHYS

Electro-osmotic Flow in Nano-capillaries via Optical Imaging and I/V Measurements: Influence of different salts and concentrations — •Aleksei Overchenko[1], Simon Brauburger[2], Frank Cichos[1], and Ulrich Keyser[2] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig — [2]University of Cambridge, Cavendish Laboratory, JJ Thomson Ave

Electro-osmotic flow (EOF) is of great interest in solid-state nanopores (SSNPs) due to its ability to pump, mix, and separate fluids in micro- and nanofluidic devices without mechanical components. However, EOF remains insufficiently explored at the nanoscale. Although KCl, NaCl, and LiCl are the most commonly used salts for driving matter through nanopores, no systematic qualitative or quantitative study has yet evaluated how different ions and concentrations affect EOF magnitude in nanopores.

We investigated the influence of various salts and their concentrations (10 mM to 1 M) on EOF behavior in 100 nm SiO2 glass capillaries. Flow visualization was performed using dark-field optical microscopy with simultaneous I/V measurements via a custom-designed flow cell. Tracer particles included 250 nm polystyrene and AuNPs.

This study provides higher spatial resolution and more detailed characterization of EOF than previously reported, offering new insights into nanoscale behavior. Understanding EOF under different ionic conditions is essential for future applications, including controlled manipulation of single DNA molecules and proteins.

O 13.10 Mon 17:15 TRE/PHYS

Facet-dependent restructuring and catalytic activity of Cu single crystals during CO electro-oxidation — Matthias Leitner, Francesc Valls Mascaro, •Andrea Auer, and Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, Austria

Understanding how surface structure relates to catalytic activity is essential for designing efficient electrocatalysts. Copper (Cu) is known to restructure under reaction conditions, yet the precise impact of this dynamic behavior on activity remains largely unclear. Here, we combine electrochemistry with in situ electrochemical scanning tunneling microscopy (EC-STM) to investigate CO electro-oxidation on Cu(111) and Cu(100) single crystals and correlate activity with facet-specific structural changes. Both surfaces undergo nanometer-scale restructuring, forming undercoordinated Cu adatoms that act as active sites. Their evolution, however, differs significantly: Cu(111) shows dynamic, reversible restructuring that maintains a high density of adatom nanoclusters, whereas Cu(100) forms clusters that evolve less reversibly, with a gradual reduction in density. Interestingly, the evolution of clusters and their density does not directly correlate with the observed catalytic activity for either facet. Instead, we propose that the differences in activity stem primarily from variations in the effective density of the catalytically active Cu adatoms and their distinct interaction with reactants, rather than from different structural motifs. These results underscore the crucial role of dynamic restructuring in guiding the design of Cu-based electrocatalysts.

O 13.11 Mon 17:30 TRE/PHYS

In-situ magneto-optical tracking of redox reactions in NiFe electrocatalysts — •Sandhya Chandola[1,2], Karuppasamy Dharmaraj[2], Jörg Rappich[2], and Norbert Esser[1] — [1]Institut für Festkörperphysik,TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 8, 12489 Berlin, Germany

Nickel/Iron (NiFe)-based electrocatalysts are known to be efficient catalysts for the oxygen evolution reaction (OER), involved in water splitting. By using a polarization sensitive optical spectroscopy technique, Reflection Anisotropy Spectroscopy (RAS), at near normal incidence, we show how the polarization state of the reflected light can be directly correlated with the oxidation state changes of NiFe catalysts via two entangled magnetic effects, which are the magneto-optical Kerr effect (MOKE) at the surface of the NiFe layer and Faraday rotation within the layer. The polarization state can be used to monitor phase transitions which are not observed in unpolarized absorption spectra.

Increasing amounts of Fe in the NiFe films correspond to greater changes in the RAS/MOKE intensities, up to the solubility limit of ~ 25% Fe, after which the spectra do not show any more changes. RAS/MOKE is shown to be a valuable spectroscopic technique which can probe changes in the redox states for different NiFe ratios, due to the indirect influence of magneto-optical effects with the implied role of ferromagnetic ordering in enhancing catalytic activity.

O 13.12 Mon 17:45 TRE/PHYS

Size Dependent Stability of Pt-supported Ceria Nanoparticles in Alkaline Electrolyte — Lukáš Fusek[1], Pankaj Kumar Samal[1], Jiří Keresteš[1], Ivan Khalakhan[1], Viktor Johánek[1], Yaroslava Lykhach[2], Jörg Libuda[2], Olaf Brummel[2], and •Josef Mysliveček[1] — [1]Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, 180 00 Praha 8, Czech Republic — [2]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Ceria nanoparticles find applications in electrocatalysis as co-catalysts for alcohol and CO oxidation, and for fuel cell and water electrolysis reactions. Synergistic effects of ceria are expected to critically depend on the cerium phases established under electrochemical conditions.

We perform a combined surface science and electrochemical study of CeO2(111) nanoparticles on Pt(111). Under electrochemical operation conditions, large ceria nanoparticles exhibit a stable redox behavior, while nanoparticles smaller than 5 nm destabilize and convert to a fully hydrated phase. Both types of nanoparticles block OH adsorption and H evolution on Pt(111), but do not block H adsorption, indicating H intercalation.

Our results reveal the nature of the electrocatalytically active cerium phases [10.1039/d3cp03831a] and underline the relevance of combined surface science and electrochemical experiments [10.1021/acs.jpclett.5c01465] for obtaining in-operando information on model electrocatalyst systems.

O 14: Ultrafast electron dynamics at surface and interfaces I

Time: Monday 15:00–18:00 Location: TRE/MATH

Invited Talk O 14.1 Mon 15:00 TRE/MATH

Spin and time-resolved ARPES and the orbital angular momentum of light — Pierre Nonnon[1,2], Romain Géneaux[1], Karol Hricovini[1,2], Christine Richter[1,2], David Bresteau[1], and •Mauro Fanciulli[1,2] — [1]Cergy Paris University, France — [2]LIDYL CEA Saclay, France

I will present the recently developed Panoramix beamline at Attolab, open to users, which allows for spin, time and angle-resolved photoemission spectroscopy (STARPES) experiments. The combination of a high harmonic generation (HHG) setup with tunable repetition rate and pulse duration, and a hemispherical analyzer with a 3D spin detector, permits to study charge and spin ultrafast dynamics in material surfaces. As an example, I will compare the observation of chiroptical resonant control of spin polarized excitons in bulk 2H-WSe2, to how the spin polarization changes for electrons pumped beyond bandgap resonance in the unoccupied conduction band. In the search of ever-increasing multidimensional spectroscopic techniques, I will conclude on the possibility to further include exotic light pulses with azimuthally varying phase or polarization, and how they might affect the photoemission process.

O 14.2 Mon 15:30 TRE/MATH

Disentangling exciton resonances in 2D materials by time-resolved XUV-ARPES — •Gregor Zinke[1,2], Antonius Naujok[1], Franz Spartz[1], Sebastian Hedwig[1], Tobias Eul[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern - Landau, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, 86159 Augsburg

Ultrafast and coherent electron dynamics in 2D materials and their heterostructures are governed by the complex energy landscape of various excitons. These quasi-particles are often separated only by tens of meV, making them difficult to distinguish in conventional time-resolved experiments due to the spectral linewidth of ultrashort pulses. Although interferometric photoemission experiments have shown potential in resolving (coherent) excitation pathways and absorption resonances, they depend mostly on optical pulses, limiting the observable momentum space, leaving high-symmetry points of 2D materials inaccessible. To address these limitations, we present a modified version of interferometric trARPES that employs two active, phase-stabilized IR pump pulses and a fs-XUV probe pulse for photoionization. We demonstrate the capability of our approach by examining the well-known A-exciton transition energies in WSe_2 at different frequencies of our pump spectrum, showing how temporal Fourier analysis of the entire ARPES spectrum allows linking distinct transition energies to congruent excitation paths within the WSe_2 electronic band structure.

O 14.3 Mon 15:45 TRE/MATH

Multi-mode momentum microscopy for studying light-induced metastable states — •Junde Liu[1], Bent van Wingerden[1], Hashima Marukara[1], Paul Werner[1], Daniel Steil[1], G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Jan Philipp Bange[1], Olena Tkach[2], Gerd Schönhense[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Johannes Gutenberg-Universität Mainz, Germany

Light-induced ultrafast phase transitions characterized by domain competition involving interlayer ordering, chirality, and topological defects are attracting growing interest [1]. This calls for time-resolved momentum microscopy, which offers simultaneous spatiotemporal resolution and direct access to band structures [2]. However, conventional high-field setups near the sample are prone to field-emission and space-charge effects, particularly in the case of cleaved crystal surfaces.

Here, using cleaved bulk TaS_2 as an exemplary system, we employ a momentum microscope with a newly designed lens system [3] that minimizes the electric field at the sample in the gap-lens mode to suppress field emission, or applies a retarding field in the repeller mode to remove slow electrons and thereby mitigates space-charge effects. This development paves the way to study cleaved crystals and enables dark-field imaging capabilities of domain-resolved electronic structure, nonequilibrium pathways, and the microscopic mechanisms of light-driven phase transitions. [1] Liu et al., *arxiv:2405.02831* (2024); [2] Reutzel, Jansen, Mathias, *Adv. in Phys. X* 9, 2378722 (2024); [3] Tkach & Schönhense, *Ultramicroscopy* 276, 114167 (2025).

O 14.4 Mon 16:00 TRE/MATH

Tracking ultrafast exciton-polariton propagation and coherent energy exchange in thin WSe_2 films — •Tobias Eul[1,2], Kai Rossnagel[2,3,4], and Michael Bauer[2,3] — [1]Institute of Physics, University of Augsburg — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University — [3]Institute of Experimental and Applied Physics, Kiel University — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg

Efficient charge transfer of electrons and holes after photogeneration is fundamental for light-induced energy conversion. The propagation of bound electron-hole pairs, i.e., excitons, can enhance this efficiency by reducing non-radiative losses before charge separation and extraction. A promising approach to improve exciton propagation is via exciton-polaritons, quasiparticles formed by the strong coupling of excitons and photons. In these hybrid states, the excitation coherently oscillates between exciton and photon character, enabling the photonic component to transport energy over extended distances. Using photoemission electron microscopy, we visualize the propagation of exciton-polaritons in a thin WSe2 film by observing the ultrafast energy exchange between excitons and photons.

O 14.5 Mon 16:15 TRE/MATH

Probing On-Chip THz Generation by Momentum Streaking in Photoelectron Emission Microscopy — •David Huber, Wolfgang Hoppe, Georg Woltersdorf, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg

THz electromagnetic radiation provides ultrafast electric fields on the femtosecond timescale. Using THz radiation as a pump in time-resolved photoemission experiments enables sub-cycle probing of induced dynamics e.g. charge and spin currents. The momentum and energy streaking of electrons in vacuum – i.e., their acceleration due to the Coulomb force – has long been shown to reliably probe electric fields and THz radiation.

In a spintronic THz emitter, we generate a spin current through the ultrafast demagnetization of a 3 nm ferromagnetic thin film, which results in a surface charge current in an adjacent 3 nm platinum film due to the inverse spin Hall effect. Similar to dipole radiation, the charge current emits THz radiation into the vacuum. By time-resolved inplane momentum streaking of photoemitted electrons, we probe the single-cycle THz electric field in front of the surface and deduce the electric surface current. We verify our findings using simulated THz radiation and streaking.

O 14.6 Mon 16:30 TRE/MATH

Interplay between intraband acceleration and interband excitation in Bi_2Te_3 by subcycle time-resolved THz-ARPES — •Tim Bergmeier[1,2], Suguru Ito[1], Jens Güdde[1], and Ulrich Höfer[2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fachbereich Physik, Universität Regensburg, Germany

Angle-resolved photoemission spectroscopy (ARPES) using THz driving fields with subcycle temporal resolution offers unique capabilities to investigate the dynamics of lateral Dirac currents in the surface state of topological insulators. Whereas low THz-frequencies result in pure intraband accelerations within the surface state [1], additional interband excitations become possible at higher frequencies [2,3].

Here, we present subcycle-resolved THz-ARPES measurements with 2D momentum imaging resolving the full Dirac cone of Bi_2Te_3. For this purpose, we generate frequency-tunable two-cycle MIR pulses (20-40

THz) with electric field strengths up to MV/cm at the sample surface, combined with an ultrashort 400 nm two-photon probe (<15 fs), at a repetition rate of 200 kHz. For a frequency of 25 THz, we show that the momentum distribution of the field-driven intraband acceleration is strongly influenced by the Dirac cones hexagonal warping, while being superimposed with resonant interband excitations that are only possible in the materials $\overline{\Gamma M}$ direction.

[1] J. Reimann et al., Nature 562, 396 (2018).
[2] S. Ito et al., Nature 616, 696 (2023).
[3] C.P. Schmid et al., Nature 593, 385 (2021).

O 14.7 Mon 16:45 TRE/MATH

Realistic nuclear ensembles for electronic excitation dynamics — •Hannah Bertschi, George Trenins, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Understanding how large-amplitude anharmonic nuclear motion influences electronic excitations is essential for explaining related phenomena in weakly-bound systems. To model charge transfer and vibronic spectra, we employ real-time time-dependent density functional theory coupled to multitrajectory Ehrenfest dynamics. In this approach, nuclear anharmonicity is incorporated through the sampling of initial conditions. In contrast to more conventional methods, we generate nuclear configurations and momenta using quantum thermostat molecular dynamics [1]. The resulting distributions of nuclear positions and momenta agree well with exact quantum references obtained from path-integral molecular dynamics, even for systems with large-amplitude motion such as the water dimer. However, the quantum thermostat does not perfectly capture the anharmonic zero-point energy of every degree of freedom, which can be mitigated by carefully choosing the parametrization of the thermostat. We show that the initial nuclear conditions of a water dimer on phenanthrene have a strong impact on both the direction and magnitude of charge transfer. Moreover, the nonadiabatic dynamics can even reverse the direction of the transfer. [1] M. Ceriotti et al., Phys. Rev. Lett. 103, 030603 (2009).

O 14.8 Mon 17:00 TRE/MATH

Laser-induced anisotropic electronic response and inverse Faraday effect in hexagonal boron nitride from real-time time-dependent density functional theory — •Cheng Wang, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The ultrafast electronic response of hexagonal boron nitride (h-BN) is investigated using real-time time-dependent density functional theory (RT-TDDFT) within an all-electron LAPW framework of the Elk code. We vary the light polarization (in-plane vs out-of-plane), dimensionality (monolayer, bilayer, bulk) and photon energy, and resolve the time-dependent projected density of states into orbital channels and identify the microscopic pathways of carrier injection. For out-of-plane linearly polarized light, the charge transfer is suppressed in the monolayer, weak in the bilayer, and strong in the bulk. Under in-plane polarization and a photon energy slightly above the DFT band gap, we identify a direct interband excitation pathway from the N p_z to B p_z orbitals. At higher photon energy, the bulk response is dominated by a local charge redistribution within N p_x-orbitals. Circularly polarized light induces a notable orbital angular momentum, while spin contributions remain negligible.

Funding by DFG within CRC1242 (project C02) and computational time on the MagnitUDE and AmplitUDE supercomputers at the University of Duisburg-Essen are gratefully acknowledged.

O 14.9 Mon 17:15 TRE/MATH

Theory of resonantly enhanced light-induced superconducting pairing in K_3C_{60} — •Juan I. Aranzadi[1], Joseph Tindall[2], Paul Fadler[1], and Michael A. Sentef[1,3] — [1]Institute for Theoretical Physics, University of Bremen/ BCCMS — [2]Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA — [3]MPSD, CFEL, Hamburg

K_3C_{60} exhibits unconventional s-wave superconductivity with a critical temperature of approximately 20K, where the superconducting state emerges from a balance between strong electronic correlations and Jahn-Teller phonon-mediated pairing [1].

Recent pump-probe measurements have shown that optical excitation induces optical signatures reminiscent of the equilibrium superconducting state at temperatures higher than Tc [2, 3]. Notably, a 10 THz resonance was observed to trigger metastable superconducting-like properties that persist for temperatures up to 300 K [4].

The mechanism underlying this non-equilibrium superconducting state remains poorly understood. To address this question, we investigate a driven three-orbital Hubbard-Kanamori model which serves as a minimal model for equilibrium superconductivity in K_3C_{60} using numerical techniques including exact diagonalization and tensor networks.

[1] Nomura, Y., et al. (2015). *Science Advances*, **1**
[2] Mitrano, M. et al. (2016). *Nature*, **530**, 461–464.
[3] Budden, M. et al. (2021). *Nature Physics*, **17**, 611–618.
[4] Rowe, E. et al. (2023). *Nature Physics*, **19**, 1821–1826.

O 14.10 Mon 17:30 TRE/MATH

Ultrafast table-top three-dimensional photoemission orbital tomography — •G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Thi Lan Dinh[2], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Lennart Weinhagen[1], Bent van Wingerden[1], Fabio Frassetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russell Luke[2], and Stefan Mathias[1] — [1]University of Göttingen, I. Physikalisches Institut, Göttingen, Germany — [2]University of Göttingen, Institute of Numerical and Applied Mathematics, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, 35131 Padova, Italy

In photoemission orbital tomography (POT), molecular orbitals can be imaged with femtosecond resolution. Also, when combined with photon-energy-dependent measurements, POT is, so far, the only method that can probe the orbitals of adsorbed molecules in 3D. However, the study of, e.g., hybridization in organic/inorganic heterostructures [Bennecke *et al.*, arXiv:2411.14993 (2024)] by 3D-POT is extremely challenging due to the demanding nature of the experiment. Here, we present a table-top approach for 3D POT: By combining a photoelectron momentum microscope with a pulse-preserving monochromator for laser-generated extreme ultraviolet light, we speed up data acquisition. Moreover, we developed a new reconstruction algorithm that reduces the sampling requirements by about an order of magnitude [Dinh *et al.*, New J. Phys. 26 043024 (2024)]. Our first results achieved on PTCDA/Ag(110) highlight the potential for ultrafast femtosecond time-resolved 3D-POT.

O 14.11 Mon 17:45 TRE/MATH

Temporal Advancement of Photoelectrons emitted via Evanescent Waves — •Luis Maschmann, Andreas Gebauer, Tillmann Schabbehard, and Walter Pfeiffer — Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

Photoelectron emission dynamics in solids is governed both by propagating and evanescent wave components. Here we employ a one-dimensional Kronig-Penney model to investigate the role of evanescent waves on the photoelectron wave packet dynamics based on time-reversed LEED states within one-step theory and time-dependent Schrödinger equation simulations. Using a Kronig-Penney potential with a large bandgap, we can clearly distinguish the dynamics for evanescent and propagating photoelectron emission channels. For emission via evanescent states, i.e., within the final state bandgap, the photoelectron appears temporally advanced and seemingly originates from the bulk-vacuum interface, although the emitter well is located well below the interface. Our results establish a direct analogy to the temporal evolution of a wave packet undergoing quantum mechanical tunneling through a potential barrier and significantly influence the interpretation of attosecond time-resolved photoemission delays.

O 15: Spins on surfaces at the atomic scale I

Time: Monday 15:00–18:00 Location: WILL/A317

Invited Talk O 15.1 Mon 15:00 WILL/A317

Tuning Spin-1/2 Interactions in Graphene: From Long-Range Coupling to Altermagnetic Order — •Beatriz Viña-Bausá[1], Manuel A. García-Blázquez[1], Antonio T. Costa[2], Joao C. G. Henriques[2], Roberto Carrasco[1], Eva Cortés-del Río[1], Diego Expósito[1], Pierre Mallet[3], Jean-Yves Veuillen[3], Joaquín Fernandez-Rossier[2], Juan J. Palacios[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]International Iberian Nanotechnology Laboratory, Portugal — [3]Université Grenoble Alpes, France

Here, we demonstrate that graphene, functionalized with H atoms, serves as a versatile platform for engineering and investigating long-range magnetic interactions. Through scanning tunneling microscopy, we manipulate spin-1/2 moments induced by single H atoms on graphene and quantify their coupling via spin excitations using inelastic electron tunneling spectroscopy[1]. Our measurements reveal robust ferromagnetic and antiferromagnetic exchange interactions in H pairs, extending over nanometer-scale distances. Additionally, guided by symmetry selection, we realize unconventional magnetic phases in our system, namely altermagnets and Lieb ferrimagnets[2]. Our results, supported by mean-field Hubbard and density functional theory calculations put forward hydrogenated graphene as a promising material for simulating exotic spin systems.

[1] B. Viña-Bausá, et al., arXiv:2511.06887 (2025)

[2] B. Viña-Bausá, et al., Nano Letters 25,11554-11561 (2025)

O 15.2 Mon 15:30 WILL/A317

versatile building blocks for molecular qubits on surfaces — •Saba Taherpour[1,2], Corina Urdaniz[1,3], Jisoo Yu[1,3], Jose Reina-Galvez[1,3,4], Kevin Lizárraga[1,3], and Christoph Wolf[1,3] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Korea — [3]Ewha Womans University, Seoul 03760, Korea — [4]University of Konstanz, 78457 Konstanz, Germany

Electron spins are natural quantum objects. Molecules that host an electron spin S=1/2 can therefore be considered qubit candidates provided they have reasonable coherence times. In this work, I will show based on first-principles calculations how the charge transfer across an Ag/MgO interface can be utilized to change the charge and spin state of 3d transition-metal phthalocyanine molecules. Iron(II) phthalocyanine (FePc) emerges as a promising qubit candidate. We present density functional theory calculations and nonequilibrium quantum transport simulations based on recent developments of all electrical electron spin resonance in atomic scale magnetic transport junctions. Our results indicate that FePc on the Ag/MgO substrate can be used as molecular building block of on-surface qubit architectures.

O 15.3 Mon 15:45 WILL/A317

Creating multi-well energy landscapes from coupled orbital memory states — •Kira Junghans, Niek M. M. Aarts, Hermann Osterhage, Julián D. Rojas-Castillo, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The interaction between atomic spins on surfaces is usually dictated by the exchange interaction. Its short-range nature strongly favors spin orientations that are either ferro- or antiferromagnetic. Recently, it was shown that memory can be created from an atomic spin using its valency [1]. Unlike the exchange interaction, it was shown that the interactions between orbital memory elements are long-range. This can lead to complex stochastic dynamics often needed in computational schemes based on theoretical neuroscience [2]. Exploiting this new functionality requires a deeper understanding of the nature of the interaction as well as the uniqueness of this material system.

Here, we study the stochastic dynamics of Co and Fe atoms on black phosphorus with scanning tunneling microscopy and spectroscopy. We quantify how the state favorability and lifetimes are influenced in dimers at different distances and by the neighboring atoms' state. We find that heterogenous dimers can also lead to complex stochastic noise, analogous to multi-well behavior. Furthermore, we investigate the dynamics of multiple coupled atoms and show that the state favorabilities can be tuned by the states of all surrounding atoms.

[1] B. Kiraly et al., Nat. Comm. 9, 3904 (2018).

[2] B. Kiraly et al., Nat. Nanotechn. 16, 414 (2021).

O 15.4 Mon 16:00 WILL/A317

Single spin control of atomic defects in monolayer MoS_2 — •Kwan Ho Au-Yeung[1,3], Wantong Huang[1,3], Johanna Matusche[1,3], Paul Greule[1,3], Jonas Arnold[1,3], Lovis Hardeweg[1,3], Máté Stark[1,3], Luise Renz[1,3], Affan Safeer[2], Daniel Jansen[2], Jeison Fischer[2], Thomas Michely[2], Wolfgang Wernsdorfer[1,3], Christoph Sürgers[1,3], Johannes Schwenk[1,3], Wouter Jolie[2], and Philip Willke[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe — [2]II. Physikalisches Institut, Universität zu Köln, Köln — [3]Center for Integrated Quantum Science and Technology, Karlsruhe Institute of Technology, Karlsruhe

Point defects in two-dimensional (2D) semiconductors host localized quantum states that can function as sensors, single-photon emitters, and qubits, but their controlled realization and individual addressability in atomically thin hosts remain challenging. Here we combine scanning tunneling microscopy with electron spin resonance (ESR-STM) to achieve single-spin control of atomic defect in a monolayer transition-metal dichalcogenide. Using STM manipulation, we create individual point defects, including sulfur vacancies and substitutional impurities in monolayer MoS_2 on graphene/Ir(111). Scanning tunneling spectroscopy and ESR measurements reveal their electronic structures and magnetic properties respectively, while pulsed ESR schemes enable quantum control of their spin states at the atomic scale. Our results demonstrate that monolayer MoS_2 provides a solid-state quantum platform that directly links 2D materials engineering with atomic-scale spin initialization, control, and readout.

O 15.5 Mon 16:15 WILL/A317

Imaging 2D ferromagnetic order with a single nickelocene molecule — •Leonard Edens[1], Trisha Sai[1], Divya Jyoti[1], Stefano Trivini[1], Fabian Schulz[1], and Nacho Pascual[1,2] — [1]CIC nanoGUNE BRTA, 20018 Donostia - San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Lanthanide intermetallic compounds formed on coinage metal (111) surfaces exhibit ferromagnetic ground states with moments robustly aligned towards a polarization axis, even in the single monolayer limit. Characteristic of these 2D magnetic systems is the intricate dependence of the easy axis on 4f occupancy, and the formation of a moiré-induced superstructure with the support, which causes an inhomogeneous local magnetization [1]. Here, we study two representative alloys of this family of materials, $GdAu_2$ and $TbAu_2$, which respectively magnetize in- and out-of-plane. To sense their magnetic state, we employ a single nickelocene molecule adsorbed on the tip of a scanning tunnelling microscope. By quantifying the directional exchange field atom-by-atom, we characterize incommensurate order and local perturbations to the moiré-congruent magnetic texture. Further insight into the nature of the exchange field is gained by studying its dependence on vertical separation and externally applied magnetic fields.

[1] Edens et al. Advanced Materials (2025). `https://doi.org/10.1002/adma.202510753`

O 15.6 Mon 16:30 WILL/A317

Two-photon transition in an Er-Ti atomic spin pair — •Dasom Choi[1,2], Yaowu Liu[1,2], Stefano Reale[2,3], Jeongmin Oh[1,2], Lei Fang[1,2], We-hyo Seo[1,2], Andreas Heinrich[1,2], Fabio Donati[1,2], and Soo-hyon Phark[1,2] — [1]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [2]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul, Republic of Korea — [3]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Multi-photon process becomes a key ingredient in quantum information science, offering a promising route to nonlinear quantum transitions and entanglement generation. Extending this to atomic spin qubits on surfaces is of great interest, yet has not been demonstrated. In this work, we investigate a spin-pair of Er and Ti atoms adsorbed on a MgO/Ag(100) surface using a scanning tunneling microscope (STM). By applying pulsed electron spin resonance in the STM, we realize two-photon resonant transitions corresponding to an angular momentum change of $\Delta m = \pm 2$ of the spin-pair, a phenomenon beyond the conventional single-photon processes as shown at the single atom level. Our work demonstrates the ability to coherently control higher-order quantum transitions at the single spin level, which provides a novel pathway towards implementing multi-quantum gate operations in atomic spin qubits, highlighting the potential of single atomic lanthanides on a surface for quantum information processing.

O 15.7 Mon 16:45 WILL/A317

Landau-Zener transitions of multilevel atomic spins — •Lukas Veldman[1,2], Henrik Lichtl[1,2], Nicolaj Betz[1,2], Johannes Schust[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Susanne Baumann[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart — [3]Carl Zeiss Stiftung Center for Quantum Photonics — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna, Tenerife, Spain

The ability to perform Landau-Zener (LZ) transitions is a powerful and relatively unexplored tool to study and control spins on the nanoscale. LZ transitions provide spectroscopic information about energy level crossings, state populations and can even be used as a driving mechanism for coherent control over quantum spin states. In an idealized picture of a two level system (TLS), these qualities can be relatively easily understood via the LZ model. Here, we show LZ transitions on antiferromagnetic Fe chains on Cu2N/Cu(100) induced by ramping the magnetic field emanating from the tip of a scanning tunneling microscope (STM). Using real time measurement of the spin state we distinguish between classical and quantum tunneling transition processes. We find that avoided level crossings in higher excited states play a significant role in the dynamics between the ground states, showcasing the necessity to go beyond the TLS approximation used in the standard LZ model.

O 15.8 Mon 17:00 WILL/A317

Robustness of zero-energy edge states to disorder in bottom-up designed Fe chains on a superconducting Rashba alloy — •Harim Jang[1], Daniel Crawford[2], Jens Wiebe[1], Stephan Rachel[3], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics and Nanoscience Center, University of Jyväskylä, Finland — [3]School of Physics, University of Melbourne, Parkville, Australia

In this talk, we report on the role of disorder for the observation of Majorana zero modes (MMs) and a topological gap in a tailored 1D magnet-superconductor hybrid (MSH) system, showing the robustness of MMs to disorder, even in cases for which the topological gap is fully suppressed. We constructed 1D spin chains from Fe atoms on the Rashba surface alloy BiAg2/Ag(111) with proximity-induced superconductivity from a Nb(110) substrate. While the Fe chains have perfect crystalline order by design, the BiAg2/Ag(111) film exhibits nanoscale potential disorder, observed by scanning tunneling microscopy. However, this doesn't prevent the emergence of zero-energy states at the Fe chain's ends, in agreement with tight-binding calculations which show that they only appear in the topologically non-trivial regime [1]. This may not only explain earlier observations of MMs in disordered MSH systems, but also provides novel perspectives for the realization of robust Majorana qubits. [1] H. Jang et al., arXiv:2506.17414 (2025)

O 15.9 Mon 17:15 WILL/A317

Coherent control of a single 4f electron spin — •Yaowu Liu[1,2], Dasom Choi[1,2,3], Stefano Reale[1,2], Jeongmin Oh[1,2,3], Lei Fang[1,2], We-hyon Soe[1,2], Andreas Heinrich[1,2,3], Soo-hyon Phark[1,2], and Fabio Donati[1,2,3] — [1]IBS Center for Quantum Nanoscience (QNS) — [2]Ewha Womans University, Seoul 03760, Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Electron spins on surface provide an atomic scale qubit platform for quantum information science using scanning tunneling microscopy (STM). Lanthanide atoms, with their strongly localized 4f electrons, can be potential candidates for single atom qubits with a long quantum coherence. However, STM tunneling current can strongly reduce the coherence time of surface atoms if they are probed directly. To circumvent this issue, it is possible to use an alternative scheme where a Ti ($S = 1/2$) atom located in a position within a 1 nm distance from a single Er atom on MgO surface can sense the quantum spin states of its 4f electron shells. In this work, we performed pulsed electron spin resonance (ESR) on the Er atom and demonstrated coherent control of 4f-electron spin of a single Er atom. Moreover, we observed a tenfold enhancement of Rabi rate compared to the direct drive of Ti atom from the tip, which is ascribed to the anisotropy of exchange interaction between the two spins.

O 15.10 Mon 17:30 WILL/A317

Kondo physics of composite molecular spins made from coupled nanographenes — •David Jacob — Department of Physics, University of Alicante, Spain

Open-shell nanographenes can now be fabricated by on-surface synthesis (OSS) and stabilized on metallic substrates, enabling access to their intrinsic (multi)radical character. Scanning-tunneling spectroscopy (STS) reveals clear Kondo signatures, demonstrating that these nanographenes host quantum spins whose magnitude reflects their degree of radicality [1]. By covalently linking such magnetic nanographenes, coupled spin systems can be engineered in controlled geometries–including dimers [2], hexagons [3], chains [4], and other topologies–allowing quantum magnetism to be probed at the atomic scale. Here we investigate coupled nanographenes whose constituent units have different spin magnitudes. We show that the composite nature of the resulting effective molecular spin leads to a rich spectrum of spin excitations and to unconventional Kondo behavior.

References:

[1] *JACS Au* **3**, 1358 (2023); *Phys. Rev. Res.* **6**, L022061 (2024).

[2] *Phys. Rev. B* **106**, 205405 (2022); *Nano Lett.* **23**, 9353 (2023).

[3] *Angew. Chem. Int. Ed.* **60**, 25224 (2021).

[4] *Nature* 588, **287** (2022).

O 15.11 Mon 17:45 WILL/A317

Site-Specific magnetism of Ho atoms on MgO — •Andrés Pinar Solé[1,2], Merve Ercelik[1,2], Jungseok Chae[1,2], Fabio Donati[3], Dmitriy Borodin[1,2], and Andreas Heinrich[3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS) — [2]Ewha Womans University — [3]Department of Physics, Ewha Womans University

Holmium (Ho) atoms on ultrathin MgO films are model systems for single-atom magnetism, where spin stability and relaxation strongly depend on the local crystal field and adsorption site. Isolated Ho atoms on oxygen sites of Ag(100)/MgO exhibit magnetic bistability but lack clear inelastic spin-excitation features; nevertheless, their magnetic states can be switched and read electrically through spin-polarized tunneling.

By extending to Ho dimers, additional spin-flip excitations become accessible, providing deeper insight into the electronic and magnetic states of Ho on MgO. The magnetic behavior of Ho dimers reflects the intra-atomic exchange coupling between the highly localized 4f moment and the outer valence-shell spins. Certain Ho dimers exhibit pronounced inelastic conductance steps, revealing strong magnetic interactions both between the atoms and with the surrounding MgO crystal field. Using STM-based atom manipulation, we precisely assemble Ho dimers on bridge and oxygen sites and probe their magnetic and electronic properties via Kelvin probe force microscopy (KPFM) and inelastic electron tunneling spectroscopy (IETS) in a combined STM/AFM UHV setup.

O 16: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Monday 18:00–20:00 Location: P2

O 16.1 Mon 18:00 P2

Ab initio study of water clusters and thin film adsorption on Bi(111) surfaces — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth, as a semimetal with strong spin-orbit coupling, plays an important role in many electrochemical applications, including electrocatalysis, electrode materials, and seawater desalination [1]. In these environments, interaction between Bi surfaces and water is unavoidable. The Bi(111) surface is both the natural cleavage plane of bulk Bi and the preferred growth surface in epitaxial processes, and is therefore suitable for studying water adsorption. While the atomic and electronic structures of Bi(111) surfaces have been well characterized, understanding of the water-Bi interface remains incomplete, and existing theoretical studies report partially conflicting results [2,3].

In this work, we employ density functional theory (DFT) to systematically investigate the adsorption behavior of isolated water molecules, molecular clusters, and thin water films on Bi(111). We examine the interplay between water-water and water-metal interactions and determine energetically favorable adsorption sites and configurations for water clusters and ultrathin films.

[1] V. Jovanovski, *et al.*, Curr. Opin. Electrochem. **3**, 114-122 (2017).
[2] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).
[3] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 16.2 Mon 18:00 P2

Structure and Dynamics of Na^+ and Cs^+ adsorbed on Cu(111) and solvated by D_2O molecules — Florian Denizer[1], Jayita Patwari[1,2], John Thomas[1], Inga Langguth[2], Karina Morgenstern[2], and •Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Phys. Chemie I, Ruhr-Univ. Bochum

Alkali cations in liquid water represent widely studied model systems of solvation science in which the water-water interaction competes with the local water-cation coupling. On electrode surfaces additional interactions become relevant. In our investigation using time-resolved two-photon photoemission and low-temperature scanning tunneling microscopy we compare Na^+ and Cs^+ on Cu(111) coadsorbed with individual D_2O molecules. $D_2O/Na^+/Cu(111)$ forms 10 nm wide, flat-lying aggregates. We observe a linear increase of the electronic lifetime of the $3s$ electron transfer resonance at the Cu(111)-Na^+ interface as a function of the number n of adsorbed D_2O molecules per ion combined with a maximal energy transfer to solvent modes ΔE of 0.6 eV at $n = 6 - 7$ [1]. On $D_2O/Cs^+/Cu(111)$ we find exclusively one or three D_2O attached to Cs^+. This leads to a stepwise increase in the corresponding $6s$ electron lifetime with n. ΔE is half that of $Na^+/Cu(111)$ which we associate with difference in ion core diameter and modified interactions with Cu(111) [2]. Comparing both systems we identify pronounced differences rooted in the microscopic connection between structure and dynamics.

[1] Kühne et al., JPC C **129**, 2054 (2025). [2] Thomas et al., JPC C **127**, 23467 (2023).

O 17: Spins on surfaces at the atomic scale – Poster

Time: Monday 18:00–20:00 Location: P2

O 17.1 Mon 18:00 P2

Conformational Control of Spin Lifetimes of a Single Molecule Magnet on a Metal Surface — •Sufyan Shehada[1], Corina Urdaniz[2], Manuel dos Santos Dias[3], Christoph Wolf[2], Dmitriy Borodin[2], Andreas Heinrich[2], Ruslan Temirov[1], Jeongmin Oh[1], Yujeong Bae[2], F. Stefan Tautz[1], Taner Esat[1], and Samir Lounis[4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]IBS Center for Quantum Nanoscience (QNS), South Korea — [3]Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom — [4]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

We present a first-principles study of a spin-engineered molecular nanostructure: a PTCDA molecule coordinated to two Fe atoms on an Ag(111) surface. This work complements recent STM-based quantum sensing experiments, where upright molecules were assembled on metallic pedestals to enable precise spin manipulation and nanoscale magnetic field detection using electron spin resonance [1-3]. Using density functional theory (DFT), we investigate how adsorption geometry influences exchange interactions and magnetic anisotropy energy in both standing and lying conformations. Incorporating DFT-derived parameters and experimental input, we developed a spin model to simulate spin relaxation dynamics [4-6]. This reveals how conformational control can regulate spin lifetimes at the single-molecule level.

[1] Esat et al., Nature '18. [2] Esat et al., PRR '23.[3] Esat et al., Nat. Nanotechnol. '24. [4] Khajetoorians et al., Science '13.[5] Delgado et al., Surf. Sci. '14.[6] Hermenau et al., Nat. Commun. '17.

O 17.2 Mon 18:00 P2

Towards faster dynamics of magnons in atomic spin chains — Christina Mier[1], Alexandra Meerovici Goryn[1], •Michael Schelchshorn[1], Lukas Veldman[2], and Sander Otte[1] — [1]Delft University of Technology, Delft, The Netherlands. — [2]University of Stuttgart, Stuttgart, Germany.

The coherent free evolution of coupled atomic spins [1] as well as electron and nuclear spins within a single atom [2] has previously been demonstrated using ESR-STM. Extending this approach to atomically assembled spin chains, provides a tunable platform for investigating magnon transport and interactions; by exploiting the spectral resolution of ESR-STM, we achieve controlled excitation and tuning of coherent spin-wave modes while pump-probe techniques allow us to directly map their dynamics on a nanosecond time scale. In particular, by engineering stronger exchange coupling both within the chain itself and to the readout atom, we observe many more oscillations within the coherence times, demonstrating dynamical timescales significantly faster than those reported by Veldman et al. [1]. This work addresses the coherent magnon dynamics within precisely engineered atomic spin chains and paves the way for probing more complex collective excitations in larger spin systems.

[1] Veldman, L.M., et al., Science, 2021. 372(6545): p. 964-968.
[2] Veldman, L.M., et al., Nature Communications, 2024. 15(1): p. 7951.

O 17.3 Mon 18:00 P2

Development of Time-Resolved Pump-probe SP-STS for Ultrafast Spin Dynamics in SAM — •Yannick Noettger[1] and Artem Odobesko[2] — [1]Wuerzburg University — [2]Wuerzburg University

Achieving coherent control of Single Atom Magnets (SAMs) is necessary for their use in quantum technologies and requires fundamental understanding of their spin dynamics on the atomic scale. Scanning tunneling microscopy (STM) provides a unique platform for probing and manipulating SAMs with atomic precision. One major challenge is minimizing coupling of the SAM to the surrounding as substrate-mediated relaxation strongly limits coherence and lifetime. Usually this is done by placing the SAM on a thin insulating layer on a metal substrate. We used an extended approach by combining the decoupling layer with a superconducting substrate, potentially enabling enhanced lifetimes due to the gap in the SC density of states. We investigate NaCl/Cu(111)/NbOx heterostructures grown by e-beam evaporation, which exhibit substrate induced superconductivity within the Cu(111)-layer up to a film thickness of 3ML. NaCl deposition on Cu(111)/NbOx was achieved, however showing very different growth characteristics than on bare Cu(111). Furthermore we implemented an all-electrical pump-probe spectroscopy scheme into our existing STM setup demonstrating functionalization and precise synchronization with the Lock-In Amplifier, although pump-probe measurements on single Fe atoms on Cu2N/Cu(001) did not yield any measurable lifetimes, highlighting limitations of our current STM setup.

O 17.4 Mon 18:00 P2

Structural characterization of Sc$_3$N@C$_{80}$ on Ag(111) with scanning probe microscopy — •Caroline Hommel[1,2], Seong-Hyun Hong[1,4], Andrés Pinar Solé[1,2], Merve Ercelik[1,3], Robert Ranecki[1,2], Shinjae Nam[1,2], Dmitriy Borodin[1,2], Andreas Heinrich[1,3], and Lukas Spree[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [4]Department of Physics, Korea University, Seoul 03760, Republic of Korea

Endohedral fullerenes are a fascinating class of compounds, that consist of a number of atoms trapped inside a fullerene cage structure. Among them, the Nitride Cluster Fullerenes (NCF) stand out for their stability and relatively high production yield. Sc$_3$N@I_h-C$_{80}$ is the most abundant species in this class. Its electronic structure and the relatively free rotation of the internal cluster make it a promising candidate for molecular electronics.

In the presented work, we use STM and AFM with a CO functionalized tip to characterize individual Sc$_3$N@I_h-C$_{80}$ molecules on Ag(111). This allows us to resolve their adsorption configuration and study the interaction of cage, cluster, and substrate in highest detail.

Studying Sc$_3$N@I_h-C$_{80}$ at the single molecule level provides direct access to its geometric and electronic characteristics, which are often hidden in bulk measurements.

O 17.5 Mon 18:00 P2

Study of correlated spin interactions in bottom-up assembled molecular structures — •Lars Pütz[1,2,3], Daria Sostina[1,2,3], Stefan Tautz[1,3,4], and Markus Ternes[1,2,3] — [1]Peter Grünberg Institut (PGI-3); Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Experimentalphysik II B, RWTH Aachen University, 52072 Aachen, Germany — [3]Jülich Aachen Research Alliance (JARA), Fundamenatls of Future Information Technology, 52425 Jülich Germany — [4]Experimentalphysik IV A, RWTH Aachen University, 52072 Aachen, Germany

Correlated physics hosts phenomena such as unconventional superconductivity and exotic magnetic phases, yet their theoretical description is often challenging. To provide a starting point, we investigate finite correlated systems. We study NTCDA molecules deposited on an Ag(111) surface using a low-temperature scanning tunneling microscope. These molecules can receive an additional electron from the surface, which turns each of them into a spin-1/2 system. Normally, this spin is screened by the substrate through the Kondo effect. By using molecular manipulation techniques, we built small molecular structures in which the spin-exchange interaction between two neighboring molecular spins overcomes the screening from the surface. In these structures, we observe singlet-triplet excitations. Moreover, these excitations exhibit a spatially varying bias asymmetry in scanning tunneling spectroscopy, reflecting the phase pattern of the triplet wave function and thus providing experimental access to it.

O 17.6 Mon 18:00 P2

Spectra and competing correlations in coupled magnetic impurities on superconducting substrates — •Carlos Quesada Pérez and David Jacob — Departamento de Física, Universidad de Alicante, Spain

The study of magnetic impurities in superconductors is a fundamental challenge in condensed matter physics, crucial for understanding phenomena like in-gap states such as Yu-Shiba-Rusinov (YSR) states. Systems with multiple impurities can potentially host exotic ground states relevant for topological quantum applications. Accurate numerical methods like the numerical renormalization group are computationally too demanding for solving more than two impurity levels. Recently, an efficient impurity solver was proposed, based on the exact diagonalization of a single impurity connected to discretized superconducting reservoirs [1]. In this work, we extend this model to the case of two magnetic impurities coupled to BCS superconductors. By exact diagonalization of the resulting tight-binding Hamiltonian, we study the competition between the impurity-superconductor coupling and the impurity-impurity exchange to form a singlet with the bath or a singlet between the impurities themselves. The results reveal the evolution of YSR states and spin correlations, showing transitions between distinct quantum phases driven by this competition.
References:
[1] Phys. Rev. B **108**, L220506 (2023)

O 17.7 Mon 18:00 P2

Atomic-Scale Engineering of Spin Defects in Monolayer MoS$_2$ — •Johannes Schwenk[1], Wantong Huang[1], Kwan Ho Au-Yeung[1], Johanna Matusche[1], Paul Greule[1], Jonas Arnold[1], Lovis Hardeweg[1], Máté Stark[1], Luise Renz[1], Affan Safeer[2], Daniel Jansen[2], Jeison Fischer[2], Thomas Michely[2], Wolfgang Wernsdorfer[1], Christoph Sürgers[1], Wouter Jolie[2], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany

Solid-state spin defects have become a promising platform for quantum technologies, including quantum sensing, communication, and computing. However, reliably creating and addressing such defects individually remains a major challenge. Here, we create distinct defect types in monolayer MoS$_2$ using the tip of a scanning tunnelling microscope, i.e. sulphur vacancies and substitutional impurities. Moreover, we characterize their spin properties using electron spin resonance scanning tunnelling microscopy (ESR-STM) and demonstrate coherent control of the spin defects. By constructing dimers of defects, we show that their spins can be coupled via magnetic exchange, which provides a path to realize larger spin structures. These results open a new avenue to design and engineer quantum states at the atomic scale for applications in quantum sensing and simulations [Nat. Nanotech.19,1782-1788 (2024)].

O 17.8 Mon 18:00 P2

Switching properties of a spin-crossover complex on Cu(111) analyzed from time traces of the tunneling current — •Katharina Biel[1], Jasmeen Jasmeen[1], Sujoy Karan[1], Karl Ridier[2], Gael Reecht[1], and Manuel Gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]LCC, CNRS and Université de Toulouse, France

Spin-crossover molecules can be switched between two states associated with different spin, a low spin (LS) and a high spin (HS) state. The switching between these two states can be induced by tunneling electrons, among other triggers, which offer the possibility to use a scanning tunneling microscope (STM) to investigate the switching dynamics at the single molecular level.

Here we investigate the spin-crossover molecule [Fe(HB(1,2,4-trazolyl)$_3$)$_2$], which forms self-assembled islands on Cu(111) and exhibits efficient switching under electron injection. The switching is monitored via time traces of the tunneling current, exhibiting two levels corresponding to the different spin states. Statistical analysis of these traces provides a detailed view on the switching properties. In particular we studied the influence of the applied voltage and the tunneling current on the switching rate. The influence of the applied voltage and the tunneling current on the switching yield is studied in details.

O 17.9 Mon 18:00 P2

Spin-Electric Control of Individual Spins on Surfaces — Paul Greule[1], Wantong Huang[1], Máté Stark[1], Kwan Ho Au-Yeung[1], Johannes Schwenk[1], Jose Reina-Gálvez[2], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Christoph Wolf[3], and •Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Department of Physics, University of Konstanz, Konstanz, Germany — [3]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea.

Individual magnetic molecules are promising building blocks for quantum technologies because of their chemical tunability, nanoscale dimensions, and ability to self-assemble into ordered arrays. In this work, we present spin-electric coupling (SEC) for two molecular spin systems, iron phthalocyanine (FePc) and Fe-FePc complexes, adsorbed on a surface. We use electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) to locally address them with the STM tip and electrically tune them using the applied bias voltage. These measurements reveal a pronounced nonlinear voltage dependence of the resonance frequency, linked to the energic onset of other molecular orbitals. We attribute this effect to a transportmediated exchange field from the magnetic tip, providing a large, highly localized, and broadly applicable SEC mechanism. Finally, we demonstrate that the SEC enables all-electrical coherent spin control: In Rabi oscillation measurements of both single and coupled Fe-FePc complexes we show that the spin dynamics can be tuned.

O 17.10 Mon 18:00 P2

Defluorination of F_{16}Cu-Phthalocyanine on Superconducting Pb(100) — •Julian Skolaut, Biswajit Pabi, Alexander Weismann, and Richard Berndt — Institute for Experimental and Applied Physics, CAU Kiel, Germany

F_{16}Cu-phthalocyanine was investigated on a superconducting Pb(100) surface using low-temperature scanning tunneling microscopy. We achieved controllable defluorination of selected lobes. A single defluorinated lobe serves as a pivot point for rotation toward eight different azimuthal orientations. Defluorination of more than one lobe eliminates the ability to rotate. The energy of the lowest unoccupied molecular orbital depends on the degree of defluorination and is lowest when two lobes have been defluorinated. We also observed Yu-Shiba-Rusinov states, which exhibit shifts depending on the adsorption configuration and azimuthal orientation.

O 17.11 Mon 18:00 P2

Investigations of FePc molecular spins on a superconducting substrate — •Luise Renz[1], Máté Stark[1], Jonas Arnold[1], Johannes Schwenk[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], and Philip Willke[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron spin resonance (ESR) measurements performed with a scanning tunneling microscope (STM) has emerged as an excellent technique to probe quantum spin systems at the nanoscale. However, the spin lifetimes of surface spins are limited by scattering with substrate electrons[1]. This can be prevented by employing thin insulating layers[1]. Alternatively, superconducting substrates can be used for decoupling[2].
Here, we present results on FePc molecules on a superconducting substrate. First, we characterize the FePc molecules on the new substrate by investigating the Zeeman splitting and the molecular orbitals. Our findings show that FePc resembles a spin-1/2 system, and that the molecular orbitals exhibit a similar pattern as was previously reported on MgO/Ag(001)[3]. Additionally, we perform all electric pump-probe measurements on single FePc molecules. By adjusting the external magnetic field, we can switch between the normal conducting and superconducting state and investigate the influence of the superconductor on the T_1 time of the FePc molecules. [1] Nat. Phys. 13, 403 (2017) [2] Nat. Phys. 9, 765 (2013) [3] Nat Commun 16, 5208 (2025)

O 17.12 Mon 18:00 P2

Spin Screening in MoS_2 Mirror Twin Boundaries on Graphene/Ir(110) — •Kuber Vyas, Tfyeche Tounsi, Jeison Fischer, Affan Safeer, Thomas Michely, and Wouter Jolie — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Mirror twin boundaries (MTBs) are line defects that host confined states in the bandgap of monolayer MoS_2(1). The confined states closest to the Fermi energy splits into a singly and a doubly occupied level separated by the Coulomb repulsion U, forming a spin-1/2 system. The spin of the singly occupied state is then screened by the electron bath present in the substrate below, giving rise to a Kondo resonance pinned to the Fermi energy.

In this work, we investigate spin screening in MoS_2 MTBs grown on graphene/Ir(110) using low-temperature scanning tunnelling microscopy and spectroscopy. STS spectra recorded along the boundaries show two pronounced impurity peaks separated by the Coulomb energy U, together with a zero-bias feature which can be attributed to the Kondo resonance. MTBs on Gr/Ir(110) exhibit significantly broadened impurity-level widths, indicating strong hybridization γ with the electron bath provided by the graphene/Ir(110) substrate. This enhanced hybridization results in a Kondo temperature T_K comparable to the measurement temperature (7 K), enabling us to study the phase transition between the Kondo singlet phase below and the magnetic phase above the Kondo temperature. [1] C. van Efferen et al, Nat. Phys. 20, 82-87 (2024)

O 18: New methods: Theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 18.1 Mon 18:00 P2

Cost-Efficient Approach for Training MACE Potentials — •Antonia Gerstenberg[1,2], Thomas Bligaard[2], and Andreas Lynge Vishart[2] — [1]currently: Fritz-Haber-Institut der MPG, Berlin, Germany — [2]DTU, Department of Energy Conversion and Storage, Denmark

Machine learning interatomic potentials (MLIPs) such as MACE offer near DFT accuracy at a fraction of the computational cost. However, a limiting factor is the cost of generating high-quality training data. This project investigates the development of a systematic and cost-efficient approach to training robust MACE models. It is therefore explored to what extent models trained on the cheapest available structures (e.g., dimers and trimers) can extrapolate to larger structures such as nanoparticles and vice versa.

To test this, an active learning workflow was implemented, iteratively adding structures with increasing numbers of atoms. The results show that widely used training strategies, including standard active learning workflows, fail to reliably extrapolate to out-of-distribution structures. The results highlight the importance of structural diversity and weight restriction from the outset.

O 18.2 Mon 18:00 P2

The application of classical DFT for describing small molecules diffusion in porous materials. — •Mikhail Suetin and Michael te Vrugt — Institute of Physics, Johannes Gutenberg Universität-Mainz, Staudingerweg 9, 55128, Mainz, Germany.

Metal-Organic Frameworks (MOFs) are relatively new, but promising materials potentially suitable for separation of hydrocarbon molecules for chemical industry aiming reaching the Net-Zero targets. Thousands of MOFs have been obtained experimentally, and about a million computationally. In this study, we conducted computational screening of the CoRE MOF database. Classical molecular dynamics simulations are employed for considering separation via diffusion. More importantly, classical density functional theory (cDFT) approach was employed to dramatically accelerate calculations of diffusion coefficients.

O 18.3 Mon 18:00 P2

Increasing the Transferability of Machine Learning Potentials by Learning Atomic Properties — •Johann Richard

Springborn[1,2], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces of complex systems. While they significantly speed up the evaluation of the energy and forces in comparison to ab-initio methods, they require high-quality reference data for training. Depending on the systems to be studied, generating this training data can become the computational bottleneck. Therefore it is of high interest to reduce the number and complexity of structures to be computed. We propose to achieve this goal by training MLPs on atomic properties instead of global quantities such as the system's total energy. This approach aims to increase the transferability of the resulting MLPs to more complicated systems while still utilizing easily accessible reference data.

O 18.4 Mon 18:00 P2

Radial Dirac-Fock solver using integral equation method — •Ernests Lazdans, Janis Užulis, and Andris Gulans — University of Latvia, Riga, Latvia

We present a relativistic generalized Kohn-Sham solver for spherically symmetric atoms. It follows the approach introduced in a multiwavelet code [1] where the Dirac equation is represented in the integral form. The solver supports local and hybrid exchange-correlation functionals and various nuclear distributions (point-like, Gaussian, and spherical). In validation test, we find that it yields Hartree-Fock energies in full agreement for all ten digits given by Visscher *et al.* [2]. However, our numerical tests show that numerical errors in our obtained atomic energies are below 10 nHa, *i.e.*, our solver's precision exceeds that of previously published data. We use the solver for testing performance of multiple exchange-correlation functionals for predicting electron removal energies from core and valence shells in noble gas atoms. The future applications of this tool include integrating it into a linearised augmented plane wave code.

[1] Anderson J. *et al.*, J. Chem. Phys. **151**, 234112 (2019)

[2] L. Visscher *et al.*, Atomic Data and Nuclear Data Tables **67**, 207-224 (1997)

O 18.5 Mon 18:00 P2

Towards Efficient Time-Dependent Density-Functional Theory through Hubbard On- and Inter-Site Corrections — •Lydia Fichte, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Density-functional theory (DFT) with a Hubbard correction (DFT+U) can mitigate self-interaction errors in a manner similar to hybrid functionals, but at significantly lower computational cost. This makes extending DFT+U to the time-dependent regime particularly attractive, as it allows for accurate simulations of electron dynamics at reduced computational expense. However, the on-site subspace defined by DFT+U can be too rigid to describe phenomena involving strong orbital hybridization or charge transfer between sites, necessitating a more flexible definition of the correlated subspace. To address this, we are incorporating inter-site interactions through the $+V$ correction to enable a more complete and adaptable description. We implement this as an efficient real-time time-dependent DFT+U+V framework in the all-electron electronic-structure code FHI-aims, enabling accurate and scalable simulations of correlated electron dynamics. We discuss the current status of the implementation and highlight the pitfalls and intricacies encountered when working with a numeric atom-centered orbital basis, both in the ground state and in time-dependent simulations.

O 18.6 Mon 18:00 P2

Calculating surface energy using machine learning interatomic potentials — •Friedrich Neumann[1], Tom Barnowsky[2,3], Rico Friedrich[2,3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg — [2]Technische Universität Dresden - Theoretische Chemie, 01062 Dresden — [3]Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

The surface energy of a material is a fundamental property that governs the behaviour of solid interfaces in a wide range of phenomena. While density functional theory (DFT) provides highly accurate values, its computational scaling limits its applicability for large systems and systematic surface-energy screening. In this work, a workflow was developed to estimate surface energies using machine-learning interatomic potentials (ML-IAPs). Atomic Cluster Expansion (ACE) models were fitted to DFT-based molecular-dynamics data for Al, Pt, and Au, and effective two-body contributions were extracted from the resulting potentials. These were combined with a bond-counting approach to compute surface energies and Wulff constructions. Although in our present ACE model the absolute magnitudes of the pair interactions are influenced by many-body interaction, preventing quantitative reproduction of surface energies, the approach still captures general trends and identifies the dominant facets in the Wulff constructions. In this specific formulation, the results illustrate how many-body interaction can affect the apparent pair contribution.

O 19: Vacuum Science & Technology: Theory and Applications – Poster

Time: Monday 18:00–20:00 Location: P2

O 19.1 Mon 18:00 P2

Contact-Separation phenomenon at the Silica-Gold interface: AFM and ToF-SIMS insights — •Nisha Ranjan, Tolga Acartürk, Kathrin Küster, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Contact-Separation (CS) electrification at solid interfaces constitutes a fundamental phenomenon. However, it often exhibits uncertainties and irreproducibility [1,2]. The silica-gold contact pair is a model example of a dielectric-metal system with a similar elastic modulus that shows a significant variation in charging properties such as polarity reversal among CS surfaces [3]. We aim to understand the phenomenon with interfacial interactions and chemical composition using direct microscale measurements under ultra-high vacuum conditions at the silica-gold interface. We use Atomic Force Microscope/Force Spectroscopy (AFM/FS) to quantify interfacial interactions, such as electrostatic force, van der Waals interaction, contact area, contact pressure, and deformation. Repeated approach-retraction cycles enabled the correlation of mechanical response with charge accumulation and compositional change. We use Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) for surface composition mapping to assess mechanochemistry. Our finding demonstrates that the magnitude of the force is significantly influenced by the charge accumulation. Concurrently, a change in surface composition was also observed. [1] I. Jimidar and J. Méndez Harper, Physics Today 78(8), 54 (2025). [2] D.J. Lacks, Angew. Chem. Int. Ed. 51, 6822 (2012). [3] G. Fatti et al., PRL 131, 166201 (2023).

O 19.2 Mon 18:00 P2

Simulation-Guided GIXPS: Planning faster (HA)XPS measurements while enabling depth-sensitivity — •David Capalbo[1], Oliver Rehm[1], Endrit Kusari[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]DESY, Hamburg, Germany — [3]FZ Jülich GmbH, PGI-6, Jülich, Germany

(Hard) X-Ray Photoelectron Spectroscopy ((HA)XPS) is an established method for characterizing surfaces, interfaces, and the bulk material properties of thin films, multilayers, and devices. Such measurements, when performed at a synchrotron-based setup, can produce faster and better resolved data compared to a laboratory setup, but beamtime is limited and highly competed for. We present a simulation-based approach that enables faster and more efficient measurements by exploiting grazing-incidence (GI) angle geometries (0.3°-2°). At these GI angles, tunable depth-selective photoelectron emission becomes possible while increasing the signal by up to two orders of magnitude at characteristic angles. In our approach, an additional damping term is added to an already existing simulation model, which enables the user to simulate an accurate GI(HA)XPS response before the beamtime. This enables them to identify and prioritise configurations of interest, reduce the required aquisition time, all while keeping the expected advantages of standard (HA)XPS measurements. O.Rehm *et* *al.*

O 19.3 Mon 18:00 P2

Electrospray Ion Beam Deposition for Atomic Resolution Native Protein Structure Investigation at Surfaces — •Stephan Rauschenbach — University of Oxford, Kavli Institute for Nanoscience Discovery, Department of Chemistry, Sherringdon Road, Oxford

Electrospray ion beam deposition (ESIBD) enables controlled deposition of intact biomolecules from solution onto surfaces under ultra-high vacuum conditions. We present ESIBD as a sample preparation method for cryo-EM, scanning probe, and holography applications, bridging native electrospray ionisation mass spectrometry with surface-based structural characterisation techniques.

The method combines mass-selective soft landing with controlled ice growth embedding protocols. Proteins maintain their native conformations during the gentle electrospray process and deposition. For cryoEM Ice matrix formation occurs post-deposition minimising mechanical stress and denaturation.

Here we discuss the state of the art implementation of this method on commercial and self-built platforms and demonstrate atomic resolution imaging of soluble and membrane proteins deposited on surfaces in vacuum.

O 19.4 Mon 18:00 P2

Analysis of the charge distribution of an insulating sphere in contact electrification processes — •Andre Mölleken, Hermann Nienhaus, and Rolf Möller — Experimental Physics, University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE)

While the mechanisms of contact electrification between metals are well established, non-conductive materials present a more complex scenario due to the emergence of nonuniform surface charge distributions. This study investigates how such charge inhomogeneities on an insulating sphere like Al2O3 or quartz influence the subsequent charge transfer during contact with a planar metal or insulator electrode. We employ a redesigned experimental setup based on an established parallel-plate capacitor concept [1], enabling high-temporal-resolution measurements of induced and transferred charges as the sphere bounces on the lower electrode. By decomposing the measured signal into monopole and dipole components, we extract the net charge, quantify the dipole moment of the surface charge distribution, and determine the rotational frequency of the bouncing sphere. This approach reveals how initial charge patterns evolve dynamically and modulate the efficiency and direction of charge transfer upon impact. The new setup allows controlled manipulation of the sphere's initial surface charge distribution prior to each experiment. The results offer a novel way to study how the charge distribution on the surface influences the contact electrification process. [1] M. Kaponig, A. Mölleken, H. Nienhaus, R. Möller, Dynamics of contact electrification, Sci. Adv. 2021, 7 (22), eabg7595.

O 19.5 Mon 18:00 P2

Contact electrification between Au and hydrogen-passivated Si(111) surfaces — •Christian Gruber, Andre Mölleken, Tobias Prost, Hermann Nienhaus, and Rolf Möller — Experimental Physics, University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE)

The charge of 1mm Au spheres bouncing on a hydrogen-passivated Si(111) surface under vacuum conditions is measured in a parallel-plate capacitor setup with fC charge sensitivity and microsecond time resolution [1]. The transferred charge between metal and semiconductor is determined as a function of impact velocity ranging from 1 to 0 m/s, of doping and of surface condition after preparation. Light exposure to the semiconductor surfaces during experiments shows no significant influence on the results. On p-doped samples the Au spheres collect a charge of typical a few 100fC with each contact. The dependence on the preparation is not as clear as on n-doped samples, on which the quality of the surface preparation clearly causes a polarity change. On n-doped samples the Au spheres collect a typical charge of a few 100 fC to over 1000 fC. However, in the limit of zero impact velocity the variations between the different samples become negligible and Au is found to be charged negative. The results are compared with predicted charge transfer between Au and Si in static Schottky diode models.

[1] M. Kaponig, A. Mölleken, H. Nienhaus, R. Möller, Dynamics of contact electrification, Sci. Adv. 2021, 7 (22), eabg7595.

O 19.6 Mon 18:00 P2

Towards nanoscale EUV spectroscopy of 2D heterostructures using interferometric coherent diffractive imaging — •Hannah Strauch, Jan Mädrich, Daniel Steil, Stefan Mathias, and G. S. Matthijs Jansen — University of Göttingen, 1st Institute of Physics, Göttingen, Germany

Time-resolved spectroscopy in the extreme ultraviolet (EUV) energy range provides element-specific insight into electronic and structural dynamics. Particularly, EUV spectroscopy of nanoscale 2D material heterostructures enables to identify the individual layer contributions due to its element-specificity. For such systems, however, a spatially resolved probe is essential: 2D material heterostructures are both intrinsically micro-scale and highly susceptible to spatial inhomogeneities. The comprehensive understanding of ultrafast dynamics in those systems therefore requires simultaneous spatial, spectral, and temporal resolution, which is a combination that remains experimentally demanding even with state-of-the-art techniques.

We will present our progress towards such a comprehensive measurement approach with our table-top EUV interferometry-based setup, which enables time-resolved spectroscopy with spatial resolution through the combination of Fourier transform holography (FTH) with interferometric Fourier transform spectroscopy (FTS). The surface sensitivity required for few-layer systems is provided through measurements in reflection geometry.

O 19.7 Mon 18:00 P2

Development of a Low Temperature Two-Level System Microscope for Superconducting Quantum Circuits — •David Mazibrada[1], Johannes Schwenk[1], Jürgen Liesenfeld[1], Hannes Rotzinger[1,2], Philip Willke[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI) — [2]Institut for Quantum Materials and Technologies (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Superconducting quantum circuits are among the most advanced platforms for solid-state qubits. Their performance is perturbed, however, by parasitic two-level systems (TLS). The electric fields of the qubit interact with the electrical dipole moment of the TLS, leading to an exchange of photons between the two quantum systems. TLS are mostly of an unknown nature and position, and identifying them locally would help to improve future qubits. Since TLS couple not only to the qubit's microwave field but also to externally applied electric fields, this interaction enables us to probe and localize individual TLS.

We present a microscope combining a cryogenic atomic force microscope (AFM) and a superconducting quantum circuit. By applying a local electric field with the AFM tip and performing microwave spectroscopy, we aim to identify, characterize, and map the position of individual TLS on superconducting quantum circuits.

O 19.8 Mon 18:00 P2

Prospects of ARPES measurements in an external static magnetic field — Dmitry Usanov and •Daniil Yevtushynsky — Laboratory for Quantum Magnetism, EPFL, 1015 Lausanne, Switzeralnd

Angle-resolved photoemission spectroscopy (ARPES) has traditionally been performed in magnetically shielded environments, as external magnetic fields distort electron trajectories and worsen the momentum resolution. This limitation has prevented direct observation of many field-dependent electronic phenomena. Recent studies, however, have demonstrated that applying a strongly localized static magnetic field enables ARPES measurements under external field conditions. We propose to test a newly developed compact magnetic circuit, integrated into a standard flag-type sample holder, capable of generating a high magnetic flux density at the sample position while minimizing its effect on photoelectron trajectories. In the presentation we will discuss the optical action of the designed magnetic field and subsequent aberration corrections for different types of samples. In addition, we will provide estimations of the maximum magnetic field for ARPES in the soft X-ray and VUV ranges. At the end, we will propose different test systems, where moderate magnetic fields can tune the spin order and induce pronounced modifications of the band structure near the Fermi level. Successful implementation will establish a new experimental capability - ARPES in controlled static magnetic fields - opening pathways to study field-dependent band topology and spin-charge coupling across a broad class of quantum materials and heterostructures.

O 19.9 Mon 18:00 P2

New Electrospray Ion Beam Deposition source for well-controlled STM sample preparation — •Niclas Przibylla[1], Markus Etzkorn[1], Stephan Rauschenbach[2], and Uta

Schlickum[1] — [1]Institute of Applied Physics, TU Braunschweig, Braunschweig — [2]Kavli Institute for Nanoscience Discovery, University of Oxford, United Kingdom

High resolution imaging of complex biomolecules such as peptides, glycans, and photosynthesis building blocks are crucial for advancing their fundamental functionalities and exploring them for quantum technologies, Scanning probe microscopy techniques together with mass-selected electrospray ion beam deposition enable atomic-level structural characterization of these molecules. This project deploys a novel electrospray ion beam deposition (ESIBD) system with Python-based programmable control for depositing non-volatile molecules onto clean surfaces under ultra-high vacuum conditions. The process involves electrospray ionization, mass-to-charge filtering via quadrupole ion guides, and electrostatic focusing onto nitrogen-cooled samples. Key innovations include a modular chamber architecture allowing future expansion, alongside RF-operation using rectangular voltage waves for enhanced mass filtering precision. Frequency-asymmetric and amplitude-asymmetric waveforms will enable systematic investigation of ion stability diagram effects, advancing deposition control capabilities.

O 19.10 Mon 18:00 P2

Electronoptical Concept of ARPES and RIXS Combined in a Novel Photoelectron Microscope — O. Tkach[1], Y. Lytvynenko[1], C. Fawaz[2], T. Lacmann[3], S. Chernov[4], O. Fedchenko[1,5], H. Agarwal[1], M. Hoesch[4], J. K. Dey[4], J. Dilling[4,6], L. Bruckmeier[4,6], M. Scholz[4], J. Schunck[4,7], S. Roth[2], K. Rossnagel[4,6], M. Beye[8], M. Le Tacon[2], •G. Schönhense[1], and H.-J. Elmers[1] — [1]Univ., Mainz — [2]IQMT, KIT — [3]EPFL, Switzerland — [4]DESY, Hamburg — [5]Goethe Univ. Frankfurt — [6]CAU Kiel — [7]Univ. Hamburg — [8]AlbaNova, Sweden

The instrumentation required for ARPES and Resonant Inelastic X-ray Spectroscopy (RIXS) is usually completely different. ARPES uses electron spectrometers, primarily hemispherical ones, whereas RIXS requires high-resolution X-ray spectrometers with long optical paths to achieve the desired resolution. In a special time-of-flight photoelectron microscope, we combined photoelectron momentum microscopy (MM) - imaging of the backfocal plane of the objective lens, a powerful ARPES approach - with the concept of PAXRIXS [1]. Here, the RIXS photons are converted into photoelectrons using an ultrathin foil. The position at which a RIXS photon hit the converter is a measure for the momentum transfer. For RIXS, the converter foil is moved between the sample and the extractor with fields-of-view of >4 mm. This is facilitated by a novel type of front lens which enables various operating modes. Ultrathin Au, Ag, and Pt converter foils provide energy resolutions between 20 meV and 400 meV.

[1] Dakovski et al., J. Synchrotron Radiat. 24 (2017) 1180.

O 20: Electronic structure theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 20.1 Mon 18:00 P2

From Wannier Functions to Optimal Local Orbitals: A Systematic Approach for Accurate Wavefunction Representation — •Ann Chantal Goutier and Michael Schüler — Laboratory for Materials Simulations, Paul Scherrer Institut, Villigen PSI 5232, Switzerland

Electronic structure calculations in solids are commonly carried out using DFT algorithms with large initial basis sets. These basis sets are compressed into smaller basis sets localised around atoms to calculate quantities of interest. It is desireable to be able to do this conversion with only minimal loss of accuracy. The most common algorithm for this is Wannierisation, a unitary transformation of the Hamiltonian into a space of maximally localised wave functions. Wannierisation preserves the Hamiltonian exactly, but Wannier wave functions cannot be used to construct eigenstates explicitly.

We propose new methods to create Local Orbitals directly, building on the idea of Smart Local Orbitals (Gandus, 2020). Our methods maximise the projectability of the Local Orbital basis set onto electronic eigenstates. This can be done either by blockdiagonalisation of a projectability operator, or by singular value decomposition of the overlap. It is advantageous as less information about the system is required and the Local Orbital set can be systematically improved by adjusting projectibility cut-offs. We also showcase the impact of variationally optimising the Local Orbital basis with respect to different parameters to further improve the representation of Kohn Sham states within a minimal basis.

O 21: Surface magnetism – Poster

Time: Monday 18:00–20:00 Location: P2

O 21.1 Mon 18:00 P2

Quantum confinement of spinarons in quantum corrals. — •Raffaele Aliberti[1], Juba Bouaziz[2], Ilias Klepetsans[2], and Samir Luonis[1] — [1]Institute of Physics, Martin-Luther- University Halle-Wittenberg, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Germany

For more than two decades, cobalt atoms on noble-metal (111) surfaces have served as a paradigm for the Kondo effect in scanning tun-nelling spectroscopy (STS) experiments. However, our recent first-principles predictions, supported by high-magnetic-field STS measurements, challenge this established view. We showed that the observed transport anomalies originate instead from spin excitations of Co atoms forming a distinct many-body state, the spinaron, which is a polaronic quasiparticle arising from the interaction between an excited magnetic moment and a trapped surface electron. Here, using time-dependent DFT combined with many-body perturbation theory, we investigate quantum-confinement engineering in circular and elliptical quantum corrals hosting a single Co adatom, revisiting the celebrated experiments traditionally interpreted through the lens of the Kondo effect. We demonstrate that confined electronic states significantly modify the underlying electron*boson interactions, thereby altering the amplitude and characteristics of the spinaronic states

O 21.2 Mon 18:00 P2

Spin-polarized LEED and reflectivity in altermagnetic materials — •Sourour Ayari, Aki Pulkkinen, and Jan Minar — New Technologies Research Center, University of West Bohemia in Pilsen, Plzen Czech Republic

Altermagnetic materials exhibit a characteristic non-relativistic spin splitting arising from their unconventional spin-symmetry properties [1-3], which leads to alternating spin textures in momentum space even in the absence of a net magnetization. To probe how these textures manifest at the surface, we use theoretical calculations based on the relativistic Korringa-Kohn-Rostoker multiple scattering method [4-5] to study the spin-polarized low-energy electron diffraction and angle- and spin-resolved reflectivity of electrons. These observables are sensitive to spin-dependent scattering processes and therefore provide a direct window into the surface projections of the altermagnetic spin structure. This approach enables a detailed understanding of the spin-dependent reflectivity in altermagnets and offers deeper insight into their surface electronic and magnetic properties.

References: [1] N. Dale et al., arXiv:2402.13094 (2024). [2] L. Šmejkal et al., Nat. Phys. 18, 404-408 (2022) [3]O Fedchenko, J Minár, A Akashdeep, SW D'Souza- Science advances, 2024 [4]J Krempaský, L Šmejkal, SW D'souza, M Hajlaoui- Nature, (2024) [5] J. Minár & H. Ebert, J. Electron Spectrosc. Relat. Phenom. 190, 159-170 (2013).

O 22: Surface dynamics – Poster

Time: Monday 18:00–20:00 Location: P2

O 22.1 Mon 18:00 P2

Tracing light-induced dynamics of correlated charge order at the atomic scale — •Luis Enrique Parra Lopez[1], Alkisti Vaitsi[1], Vivien Sleziona[1], Fabian Schulz[2], Martin Wolf[1], and Melanie Müller[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]CIC nanoGUNE, Donostia-San Sebastian, Spain

Terahertz-driven scanning tunneling microscopy (THz-STM) is a versatile technique that enables the study of ultrafast dynamics in quantum materials with simultaneous nanometer spatial and femtosecond temporal resolution. Here, we use THz-STM to investigate the local ultrafast response of the charge density wave (CDW) phase in 1T-TaS2. Optical-pump THz-probe measurements reveal coherent oscillations of the THz-driven tunneling current at 2.5 THz, consistent with the amplitude mode of the CDW. In addition, we observe a previously unreported 1.3 THz mode in the vicinity of a structural defect, consistent with predictions for interlayer phonons. Beyond these ultrafast collective dynamics, our measurements uncover an additional slower effect: THz-induced long-lived changes of the local density of states (LDOS). These metastable modifications appear as LDOS peak shifts indicative of local stacking changes. They do not arise from the coherent CDW response, but from a local THz-induced perturbation of the CDW lattice. We demonstrate that these changes appear predominantly near lattice inhomogeneities and are consistent with local misalignments of the stacking configuration. Together these findings highlight THz-STM as a platform for imaging and controlling nonequilibrium quantum phases at their intrinsic spatial and temporal scales.

O 22.2 Mon 18:00 P2

Photonic Structures for Purcell-Enhanced Driving of a Structural Phase Transition — •Nandana Veena Uday[1], Florian Spickmann[1,2], Sebastian Zafra Koch[1,2], Felix Kurtz[1], Claus Ropers[1,2], and Hannes Böckmann[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Direct integration of silicon photonics with low-dimensional materials connects tailored light-matter interaction with surface-sensitive probing. Here, we explore the remote optical driving of a prototypical Peierls insulator, adsorbed on the surface of a silicon photonic waveguide. Optical gratings couple infrared light to guided modes of a silicon slab, while ultrafast low-energy electron diffraction probes the waveguide-mediated optical quench of the periodic lattice distortion in adsorbed atomic indium chains. These experiments constitute first steps towards engineering photonic environments for surface phase control using tailored lithographic fabrication techniques. Potential avenues range from Purcell-enhanced photoinduced phase transitions to driven states of matter obtained by interfacing surface structures with integrated micro-resonator cavities. [1] Böckmann, Hannes, et al. Structural Dynamics 9.4 (2022)

O 22.3 Mon 18:00 P2

Non-equilibrium phonon dynamics of the kagome metal CsV_3Sb_5 — •Felix Kurtz[1,2], Lukas Jehn[1,2], Alp Akbiyik[1,2], Matthieu Le Tacon[3], Amir-Abbas Haghighirad[3], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, D-37077 Göttingen — [2]4th Physical Institute, University of Göttingen, D-37077 Göttingen — [3]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, D-76021 Karlsruhe

Tracking the equilibration processes that follow photoexcitation in materials can reveal couplings between and among electrons and lattice degrees of freedom. Thus, a variety of femtosecond electron or X-ray diffraction techniques are used to follow non-equilibrium structural dynamics. Recently, we have introduced ultrafast low-energy electron diffuse scattering (ULEEDS), a surface-sensitive method capable of tracing momentum-dependent phonon populations with out-of-plane polarization [1]. Here, we employ ULEEDS to a second material, the kagome metal CsV_3Sb_5, and reveal non-thermal phonon occupations whose subsequent equilibration is driven by phonon-phonon scattering. Comparing these results to our previous study of $TiSe_2$, we find that while a rapid buildup near the Brillouin-zone boundary still precedes a slower emergence of zone-center acoustic modes, the relaxation times in CsV_3Sb_5 are confined to a much narrower distribution.

[1] F. Kurtz *et al.*, Nat. Mater. **23**, 890-897 (2024)

O 22.4 Mon 18:00 P2

Extending Surface Phase Diagrams to Non-Equilibrium Plasmas — •Maximilian Wünschek, Alper T. Celebi, and Markus Valtiner — Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/E134, Vienna 1040, Austria

Surface phase diagrams are widely used to visualize the stability of surface reconstructions under equilibrium gas conditions. However, many growth and treatment processes use plasmas that operate far from equilibrium, where activated and ionized species are present in substantial concentrations. Examples such as ZnO have shown that unique reconstructions can be found outside the stability range defined by conventional chemical potential axes, highlighting the need to extend surface phase diagrams to non-equilibrium regimes.

Using GaN as a model system, we compile a large dataset of reconstructions for polar GaN surfaces under hydrogen, nitrogen, and oxygen environments. Building on these results, we introduce a framework for applying surface phase diagrams to plasma conditions by incorporating non-thermal species into the chemical potential landscape. A minimal kinetic model estimates plasma composition, and thermochemical properties of the constituent species are combined into an effective plasma chemical potential.

The resulting extended diagrams show how radicals and ions shift phase boundaries and stabilize surface structures inaccessible under equilibrium. This approach provides a basis for understanding and predicting surface configurations formed during plasma-assisted processing.

O 22.5 Mon 18:00 P2

Atomic vibrations in the icosahedral quasicrystal AlPdMn studied with femtosecond electron diffraction — •Moritz Schlechtriem[1,2], Victoria C. A. Taylor[2], Hyein Jung[1,2], Ralph Ernstorfer[1,2], and Yoav William Windsor[1,2] — [1]Technische Universität Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Quasicrystals (QCs) are materials in which the atomic arrangement lacks periodicity but exhibits perfect spatial order. QCs therefore produce sharp diffraction patterns with unconventional features such as 5-fold rotational symmetry. Due to the aperiodic nature of QCs, phonons are insufficient to fully describe atomic vibrations. Phasons are quasiparticles related to atomic motion in the presence of aperiodicity, and their group velocity can exceed the speed of sound. The resulting enhanced thermal conductivity gives rise to potential applications of QCs, e.g. in nanoelectronics.

Here we use pump-probe femtosecond electron diffraction (FED) to study ultrafast atomic vibrations in QCs. This enables us to study the femtosecond evolution of photoinduced atomic motion, shedding light on the coupling mechanisms between electrons, phonons and phasons.

In this presentation we focus on the icosahedral QC alloy AlPdMn. FED results, in which different high-symmetry directions (e.g. the 5-fold rotation axis) are probed, will be presented.

O 22.6 Mon 18:00 P2

Thermo-osmotic flows at the Chemically Patterned Surfaces — •Neerdhi Goswami and Frank Cichos — Universität Leipzig Linnestr. 5 04103 Leipzig Germany

The boundary flows at a solid-liquid interface are governed by the interaction of the solid and liquid, specifically by the excess enthalpy of these interactions. Consequently, chemical modification of surfaces alters boundary flow fields. By generating spatially dependent patterns of solid-liquid interactions, we can not only shape various flow fields but also directly compare excess interaction enthalpies between modified and unmodified regions.

This study analyzes opto-thermo-osmotic flow fields at a thiol-patterned gold-water interface to provide a quantitative microscopic picture of dynamic interfacial interactions through comparative analysis. Thiol stripes were generated through micro-contact printing, creating alternating patterns of modified and unmodified gold regions. Surface plasmon resonance (SPR) imaging confirmed thiol addition by detecting the characteristic frequency shift upon adsorption.

This quantitative characterization of interfacial interactions provides fundamental insights into how surface chemistry modulates boundary flows, with implications for designing responsive microfluidic systems and optimizing interfacial processes in precision separation and manipulation applications.

O 23: Catalysis and surface reactions – Poster

Time: Monday 18:00–20:00 Location: P2

O 23.1 Mon 18:00 P2

Investigating Single Atomic Catalytic Sites within Metal- Coordinated Supramolecular Networks via Submolecular Imaging in correlation with Electrochemical Analysis — •Duong Tran[1], Philipp Wiesener[1], Ying Pan[2], Nieves López- Salas[2], and Harry Mönig[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemistry, Sustainable Materials Chemistry, Universität Paderborn, Germany

Metal-organic layers serve as an excellent platform for creating single-atom catalysts (SACs). This study focuses on a heat-induced deprotonation reaction of a melem precursor and the formation of a heptazine-based metal-organic network on an Au(111) substrate. To overcome thermal desorption challenges hindering chemisorption, we developed a vacuum reactor chamber with a high-flux evaporator for precursor deposition. The resultant heptazine-based Au-nitride network aligns with previous results on Cu(111) using the same precursors. In particular, the interaction of Au(111) atoms with dehydrogenated nitrogens results in a gold atom flexibly suspended between two nitrogen atoms, indicating promising active sites for oxygen reduction reaction (ORR). Scanning tunneling microscopy (STM), noncontact atomic force microscopy (nc-AFM) with an oxygen-terminated copper tip, and X-ray photoelectron spectroscopy (XPS) confirm the strong chemisorption and stability of the network. A comparison of the catalytic performance of heptazine-based metal-nitride networks on Au(111) and on Cu(111) under ambient conditions enhances the understanding of the ORR electrochemical applications.

O 23.2 Mon 18:00 P2

Support-Dependent Thermal Activation of Pt17 Clusters on HOPG and CeO2: For-mation of Active CO Oxidation Catalysts — Papri Chakraborty[1,2,3], •Johannes Seibel[2], Nicola Da Roit[4], Artur Böttcher[2], Ajai Raj Lakshmi Nilayam[1], Christian Kübel[1], Silke Behrens[4], and Manfred Kappes[1,2,3] — [1]Institute of Nanotechnology, KIT, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Physical Chemistry, KIT, 76131 Karlsruhe, Germany — [3]Institute of Quantum Materials and Technologies, KIT, 76344 Eggenstein-Leopoldshafen, Germany — [4]Institute of Catalysis Research and Technology, KIT, 76344 Eggenstein-Leopoldshafen, Germany

Atomically precise ligand-protected metal clusters are attractive precursors for heterogeneous catalysts, potentially allowing for the precise control of the initial active site composition. However, the transformation from the protected cluster to the active catalyst, specifically the removal of the ligand shell, remains a poorly understood process that depends heavily on the support material. Here, we present a comparative study of the thermal activation of $Pt_{17}(CO)_{12}(PPh_3)_8(NO_3)_2$ on inert graphite, on reactive ceria CeO2 surfaces and in gas phase. For this we combined thermal desorption spectroscopy with high-resolution mass and ion mobility spectrometry to map the decomposition pathway of the cluster. Additionally we probed clusters supported on CeO2 before and after CO oxidation catalysis with transmission electron microscopy. This revealed dissociation of clusters and dispersion of the Pt atoms on the oxide support under certain reaction conditions.

O 23.3 Mon 18:00 P2

From model to powder systems: Sm-doped ceria for CO_2 conversion. — •Raquel Sánchez-Barquilla[1], Sichen Liu[1], Alexander Contreras-Payares[2], Pablo G. Lustemberg[2], Dominic Guttmann[1], Carlos Morales[1], Fabian Rachow[1], Verónica Ganduglia-Pirovano[2], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology, Cottbus-Senftenberg, Germany — [2]Instituto de Catálisis y Petroleoquímica, Madrid, Spain

Reducible oxides are crucial in many heterogeneously catalyzed redox reactions because they can store and release oxygen during the catalytic cycle. Among these, cerium oxide (CeO_2) stands out due to its facile transition between the Ce^{4+} and Ce^{3+} oxidation states. Furthermore, the Ce^{3+} cations have been suggested to provide the active sites for CO_2 activation. Consequently, the catalytic performance of ceria-based catalysts may be significantly enhanced by promoting and stabilizing these sites, e. g., by alloying with trivalent rare-earth (RE) metals that also form cubic sesquioxides (RE_2O_3), such as samarium.

Here, we present a model system composed of (111)-oriented Sm-doped ceria nanoislands studied using X-ray photoelectron spectroscopy under near-ambient pressure. We show that Sm is crucial for CO_2 activation. This activation is accompanied by a charge-transfer process that modifies the measured Ce^{3+}/Ce^{4+} ratio, as explained by density functional theory calculations. Once the reaction mechanism was established, we performed *operando* absorption spectroscopy on powder catalysts with different Sm/Ce ratios to examine the effect of Sm doping under more realistic conditions.

O 23.4 Mon 18:00 P2

Digital Catalysis: Accelerated Discovery Through Human in the Loop — •Charles Pare[1], Aybike Terzi[2], Christian Kunkel[1], Frederik Rüther[2], Frederic Felsen[1], Robert Baumgarten[2], Esteban Gioria[2], Raoul Naumann d'Alnoncourt[2], Christoph Scheurer[1], Frank Rosowski[2,3], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]BasCat - UniCat BASF JointLab, Berlin — [3]BASF SE, Catalysis Research, Ludwigshafen

Catalyst promoters are often key components of stable and efficient industrial heterogeneous catalysts, yet most commercial systems rely mostly on one or two promoters and predominantly leverage their isolated rather than their synergistic effects. This limitation frequently results from the laborious empirical research needed to identify formulations with jointly acting components that enhance performance. To address this challenge, we implement an accelerated catalyst discovery approach that adaptively explores a large catalyst design space using only a limited number of experiments. Its foundation lies in an efficient Design-of-Experiment (DoE), parallelized testing, and iterative integration of experimental feedback. New and competitive promoter chemistries for the non-oxidative propane dehydrogenation to propylene over supported Pt are discovered within a constrained experimental campaign. The results demonstrate the potential of adaptive DoE strategies for directed, data-efficient knowledge generation and optimization in complex catalytic systems of both academic and industrial relevance.

O 23.5 Mon 18:00 P2

Automatic Kinetic Equation Discovery from Experimental Data — •Maryke Kouyate, Gianmarco Ducci, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Optimizing and controlling industrial catalytic processes requires effective kinetic models that are both robust and interpretable, capable of predicting how key operating variables affect reactor behavior. We introduce a model-based, adaptive design-of-experiments (DoE) framework that efficiently learns parsimonious, mechanistically meaningful rate expressions from data. At each step, it selects feed conditions to maximize expected information gain.[1,2] Profile reactors further boost per-run information by providing spatio-temporally resolved composition profiles along the reactor axis. Applied to CO oxidation on Pt, the framework automatically constructs a robust, chemically interpretable kinetic model that reproduces the characteristic mid-reactor transition in concentration profiles and reveals the need for a nonlinear term to capture the observed shift from CO poisoning to a non-poisoned regime.

[1] G. Ducci *et al.*, J. Chem. Phys. **162**, 114118 (2025).
[2] M. Kouyate *et al.*, J. Chem. Phys. (in press), DOI: 10.1063/5.0289751

O 23.6 Mon 18:00 P2

Structural development of new defective titanium carbon phosphorus hybrid composites by soft x-ray spectroscopy —

•Hesham Hamad — City of Scientific Research and Technological Applications, Alexandria, Egypt — Elettra Sincrotrone Trieste, Trieste, Italy

The discovery of "black" TiO2 nanoparticles with enhanced solar absorption in the visible and near-infrared regions has sparked growing interest in solar energy applications. However, their properties remain incompletely understood. In this work, we explore a sustainable defective titanium*carbon*phosphorous (TCPH) hybrid nanocomposite for photocatalytic applications. TCPH was synthesized and applied in the degradation of methyl orange (MO) dye, a model organic pollutant. Characterization revealed the presence of Ti3+ species, oxygen vacancies, and a core-shell structure, along with a significant increase in surface area. These features enhance charge transport and separation, leading to excellent photocatalytic activity. X-ray photoelectron spectroscopy (XPS) confirmed the Ti3+ modifications in TCPH. To further probe its properties, synchrotron-based X-ray absorption fine structure (XAFS) spectroscopy was employed. This advanced technique provides insights into unoccupied and occupied states, particularly the O 2p and Ti 3d hybrid orbitals, revealing the electronic and crystalline structures of anatase, rutile, Ti metal, and TCPH. The combination of XAFS with complementary methods, including XRD, XPS, and HRTEM, enables a comprehensive understanding of TCPH's morphology, crystallinity, and local electronic structure.

O 23.7 Mon 18:00 P2

Cooperative Co-Fe Effect on the OER Activity of $CoFe_2O_4$ (100), (001) and (111) surfaces

— Shohreh Rafiezadeh, •Aparna Chaitram, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen, Duisburg

Water splitting, a key method for green hydrogen production, is limited by the sluggish anodic half process - the oxygen evolution reaction (OER) [1]. This necessitates finding efficient and affordable electrocatalysts which can reduce the overpotential. Using density functional theory calculations with an on-site Hubbard U term, we study the OER activity of the $CoFe_2O_4$ (001), (100), and (111) surfaces, exploring a wide range of potential active sites and the effect of solvation. The lowest overpotential of 0.20 V is found for an octahedral Co at the A-layer termination of the (100) surface, which contains both Fe and Co. This is attributed to the synergistic stabilization of the *OOH intermediate by binding to a neighbouring Fe site[2]. Remarkably, sites with higher catalytic activity are found to retain bulk like oxidation states. Our results show that such bonding configurations that break the OER scaling relationships reveal new routes to designing catalysts for water splitting.

We acknowledge funding by DFG within CRC TRR 247.

[1] J. Rossmeisl, Z. W. Qu, H. Zhu, G. J. Kroes, and J. K. Nørskov, *J. Electroanal. Chem.* 607, 83 (2007).

[2] S. Rafiezadeh, A. Chaitram, R. Pentcheva, *ChemCatChem* (2025), DOI: 10.1002/cctc.202501290.

O 23.8 Mon 18:00 P2

Probing the active state of Cu(111) for plasma-catalytic CO_2 hydrogenation

— •Luka Babić and Roland Bliem — ARCNL, Materials & Surface Science for EUVL, Science Park 106, 1098 XG Amsterdam, The Netherlands

Plasma catalysis combines the concept of heterogeneous catalysis with the activation of reactants by a plasma discharge. The activation of strong molecular bonds is expected to change the kinetics of challenging reactions such as the hydrogenation of CO_2 to methanol. This reaction proceeds in a mixed H_2/CO_2 plasma, which consists of a multitude of species, including radicals, atoms, and ions with energy stored in various states and degrees of freedom. The state of surfaces interacting with this complex mixture is poorly understood, even for well-defined single-crystalline model catalysts.

Here, we use in situ X-ray photoelectron spectroscopy (XPS) and residual gas analysis to disentangle reaction pathways and the evolution of a Cu(111) model catalyst surface during exposure to radicals generated in plasma. Optical emission spectroscopy (OES) is used to characterize plasma and to assess the species hitting the surface during the exposure. XPS reveals the formation of adsorbed oxygen, followed by Cu(I) and finally Cu(II) oxides. Carbon is fully absent during the reaction with neutral activated CO_2 species. Upon reduction by plasma-activated hydrogen, hydroxides are formed. Depending on the operating conditions, we thus expect the active surface of a Cu plasma catalyst to be either Cu hydroxide or Cu metal.

O 23.9 Mon 18:00 P2

Size selected Pt clusters on a CeO_2(111) support: mobility, reactivity and dimensionality

— •Fabian Heisinger, Johanna Reich, Mina Soltanmohammadi, Rasmus Bischoff, Friedrich Esch, and Barbara A.J. Lechner — TU Munich, Germany

Ceria is a renowned material for its exceptional oxygen storage capacity with applications in catalysis. Central to this functionality are oxygen vacancies and their mobility. In interaction with metal catalyst particles, this reducible oxide is highly versatile, as we demonstrate for size-selected Pt clusters on a single-crystalline ceria film. We study oxidation reactions as a function of cluster size, dimensionality, support reduction, and gas environment. With conventional and fast STM, we directly observe the dynamics of surface vacancies and supported clusters to determine cluster shape changes related to defect density and sintering. We combine this cluster height and coverage monitoring with LEED and XPS to characterize the CeO_2 films in crystallinity, thickness, oxidation state, and Pt coverage. We demonstrate that the Pt cluster dimensionality during sintering can be steered by controlling the oxygen vacancy coverage on the support[1]. Through STM, we track the mobility of O vacancies in an effort to correlate their dynamics with cluster properties, and the cluster dynamics to unravel the influence of their shape on stability and catalytic activity. These dimensionality-tuned, size-selected clusters provide an ideal platform to study the structural dynamics of small metal clusters during an ongoing oxidation reaction.

[1] Reich, Johanna, et al. ACS catalysis 15 (2025): 18369-18382.

O 23.10 Mon 18:00 P2

Metal clusters on rutile TiO_2(110) as model catalysts: Stability and reactivity under near-ambient pressure conditions

— •Jonathan Paul, Marina Isabel de la Higuera Domingo, Lorenz Falling, Florian Kraushofer, Matthias Krinninger, and Barbara A. J. Lechner — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, 85748 Garching, Germany

Clusters frequently exhibit strongly size-dependent catalytic properties and have discrete electronic states, often leading to a particularly high activity in heterogeneous catalysis. However, at the elevated temperatures typically employed in industrial applications, clusters tend to sinter into larger particles, which can lead to a decrease in catalytic activity. Reducible oxide supports, such as titania (TiO_2), are effective materials for stabilizing clusters and can further modify their catalytic behavior through encapsulation effects induced by the strong metal-support interaction (SMSI).

Here, we employ near-ambient-pressure scanning tunneling microscopy (NAP-STM) to investigate how reducing, oxidizing and reaction atmospheres influence the stability, structural dynamics and geometry of Pt and Ni clusters supported on rutile TiO_2(110).[1] Structural insights obtained from microscopy are complemented by a highly sensitive sniffer setup for activity measurements, investigation of reaction mechanisms and determination of turnover frequencies.[2]

[1] F. Kraushofer, et al. J. Am. Chem. Soc. 2025, 39846-39859.

[2] J. Reich, et al. Top. Catal. 2024, 880-891.

O 24: Solid-liquid interfaces: Reactions and electrochemistry – Poster

Time: Monday 18:00–20:00 Location: P2

O 24.1 Mon 18:00 P2

Real-Time Electrochemical AFM Observation of Lithium Plating and Dissolution on HOPG: Surface Morphology and Mechanistic Insights — •Luca Kaufer[1,2], Daniel Ebeling[1], André Schirmeisen[1], and Jürgen Janek[2] — [1]Institute of Applied Physics, Justus-Liebig-University, Gießen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University, Gießen, Germany

This investigation demonstrates the utilisation of atomic force microscopy (AFM) to examine the interactions between liquid electrolytes and Highly Ordered Pyrolytic Graphite (HOPG) electrodes. In particular, the focus is on the deposition of lithium on HOPG surfaces, a crucial process in lithium batteries. Atomic force microscopy measurements facilitate precise analysis of the surface structure, topography, and mechanical properties. In addition, they permit observation of dynamic changes during lithium deposition. This, in turn, provides a deeper insight into the mechanisms of electrode surface reactions and the quality of the electrode surface. Such measurements are of great importance to improve the efficiency and lifetime of batteries by helping to understand and control processes such as dendritic growth or non-uniform deposition.[1,2] We will demonstrate the use of Asylum Research's Fast Force Mapping mode in relation to the mechanical changes in HOPG during lithium deposition. [1] J. Phys. Chem. C 2011, 115, 25484*25489. [2] ACS Appl. Mater.Interfaces 2015, 7, 25441*25447

O 24.2 Mon 18:00 P2

Influence of electrolyte and electrode parameters on the current voltage characteristics during high voltage and plasma electrolysis — •Benjamin Schilling, Lukas Forschner, Justus Leist, Timo Jacob, and Albert K. Engstfled — Ulm University, Ulm, Germany

Electrolysis at gas evolving electrodes at high voltages, up to several hundreds of volts, leads to vivid bubble formation at the electrode, which ultimately leads to the ignition of a plasma in a gas sheath forming around the significantly smaller driving electrode. [1] Depending on the applied voltage, the approach can be used to tailor the electrodes structural properties or to modify the electrolyte, to form nanoparticles or generate H2O2. Systematic studies to elucidate the fundamental physical properties are still scarce [2], which are, however, highly relevant to understand the aforementioned changes on the electrode and electrolyte. In this work we focus on the influence of the electrolyte concentration and composition, voltage scan rate, working electrode geometry and material, electrode distance and electrolyte convection. The electrode structural properties are studied by SEM imaging, the dynamics of the gas film around the electrode are monitored using a high-speed camera and the temperature is proved locally by multiple temperature probes. By correlating these results, we discuss the parameters influencing the temporal changes of the system's properties and their consequences for the application of high-voltage electrolysis. [1] Yerokhin et al., *SURF COAT TECH* **122** (1999) 73-93. [2] Forschner et al., *J. Phys. D: Appl. Phys* **58** (2025) 215204.

O 24.3 Mon 18:00 P2

Predicting Potential-Dependent Binding Energies at the Electrified Metal/Water Interface — •Ann Kathrin Tran, Elias Diesen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Density-functional theory studies of electrified metal/water interfaces present many challenges and uncertainties. Even the methodology for computing the thermodynamics of adsorption is not yet well-established, albeit crucial to e.g. heterogeneous electrocatalysis. Here, we discuss common approaches and approximations in a systematic study of electrochemical binding energies. We choose Au(111) as our model system and focus on the adsorption of key intermediates during O_2 electro-reduction. Firstly, we benchmark predictions from three increasingly advanced models of the double layer: an applied saw-tooth potential in vacuum, an implicit solvent model, and explicitly modelled H_2O via *ab initio* molecular dynamics (AIMD). This comparison disentangles the purely electrostatic energy contribution from stabilization due to explicit H-bonding with the solvent. The latter contribution can be sizeable, yet is only captured by atomistic H_2O in expensive AIMD. We next address the issue of predicting grand-canonical energetics, that is, energies under realistic constant-potential conditions. In this context, we present workfunction information within constant-charge AIMD data, the emerging workfunction-charge relation, as well as different transformation techniques toward constant-potential results. This analysis reveals notable caveats for each approach and highlights the need for further systematic benchmark studies.

O 24.4 Mon 18:00 P2

molecular dynamics simulations of belite-water interactions using HDNNPs — •Usman Tafida[1,2], Maite Böhm[1,2], Henry Wang[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Advances in the development of machine learning potentials (MLPs), such as High-Dimensional Neural Network Potentials (HDNNPs), have enabled *ab initio*-level accuracy for molecular dynamics (MD) simulations of high dimensional systems at greatly reduced computational cost. In this work, HDNNPs are trained on DFT-D3 energies and forces data of beta-belite (Ca_2SiO_4) clusters in water, which serve as model systems for complex oxide-water interfaces. Here, we present the dataset construction scheme, training and validation of the potential. Moreover, MD simulations have been performed to study the structural and dynamical properties of interfacial water at these clusters.

O 24.5 Mon 18:00 P2

High-Dimensional Neural Network Potentials for Molecular Dynamics Simulations of Mineral-Water Interfaces — •Maite Böhm[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In recent years, High-Dimensional Neural Network Potentials (HDNNP) have emerged as a popular tool for atomistic simulations of complex systems such as mineral-water interfaces. In this work, we present the construction of an HDNNP based on density functional theory energies and forces for tricalcium aluminate (C_3A)-water interfaces. We discuss the development of a dataset that includes the relevant solid-liquid interface interactions by active learning and propose approaches for an accelerated extension of the dataset. The trained potential is applied in Molecular Dynamics simulations of the (100) surface of C_3A in contact with water, which are further investigated with respect to the structure and dynamics of water on the surface.

O 24.6 Mon 18:00 P2

Developing High-Dimensional Neural Network Potentials for Studying Tricalcium Silicate-Water Interfaces — •Henry Wang[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

The emergence of machine learning potentials (MLP) trained on energies and forces from electronic structure calculations has revolutionized the simulation of solid-liquid interfaces by molecular dynamics (MD). For instance, High-Dimensional Neural Network Potentials (HDNNP) have shown excellent accuracy for describing the interaction of water with several solid minerals. In this study, we investigate interfaces of liquid water with alite (Ca_3SiO_5), a calcium silicate forming several polymorphs, which is characterized by a particularly high reactivity with water. Insights into the behavior of water at calcium silicate surfaces at an atomistic level are crucial to reach a better understanding of general hydration reactions of this class of materials. An approach for realizing high-accuracy, large-scale MD simulations is presented.

O 24.7 Mon 18:00 P2

Exploration of the Pt(111)-water interface by high-dimensional neural network potentials — •Daniel Trzewik[1,2], Moritz R. Schäfer[1,2], Alexander L. Knoll[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In-depth knowledge of solid-liquid interfaces is essential for understanding numerous catalytic and electrochemical processes. However, accurately describing these interfaces with first-principles methods is computationally demanding, limiting the system sizes and complexities that can be explored. Modern machine learning potentials offer a powerful alternative, delivering near-first-principles accuracy at a fraction of the cost. In this work, we use high-dimensional neural network potentials (HDNNPs) to examine the Pt(111)-water interface in detail. Trained on DFT reference data, these models enable molecular dynamics simulations which reveal the structural and dynamical behavior of water molecules at the interface.

O 25: Solid-liquid interfaces: Structure, spectroscopy – Poster

Time: Monday 18:00–20:00 Location: P2

O 25.1 Mon 18:00 P2

Role of Interfacial Water for CO_2 Reduction Reactions in Ionic Liquid/Acetonitrile Electrolytes — •Björn Ratschmeier[1], Arik Geringswald[1], Alisa Kamaric[1], Angel Cuesta[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]Advanced Centre for Energy and Sustainability (ACES), School of Natural and Computing Sciences, University of Aberdeen, UK

Room-temperature ionic liquids (RTILs) such as 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide ($[BMIM][NTf_2]$) are promising electrolytes for CO_2 reduction reaction (CO_2RR), where the availability of water at the electrode/electrolyte interface is known to play a decisive role in the reaction mechanism. We find that the addition of acetonitrile (ACN) to $[BMIM][NTf_2]$ with 1.5 M H_2O markedly increases the CO yield, while the onset potential for CO formation remains essentially unchanged. *In situ* IRAS of bulk intermediates formed during CO_2RR are indicative for a reaction pathway [1] via a [BMIM]-COOH intermediate that requires the presence of interfacial H_2O as shown in previous work. In contrast, *in situ* ATR-SEIRAS reveals ACN-induced modifications of the electrode/electrolyte interface. OH vibrational bands increase significantly at cathodic potentials, indicating enhanced water accumulation at the interface, thus, causing larger availability of water for CO_2RR. Ref.: [1] Ratschmeier et al. ACS Catalysis 14, 1773 (2024).

O 25.2 Mon 18:00 P2

Capacitance of Nanoconfined Salt Solutions: Interplay between Concentration and Temperature — •Caterina Sartori, Haoyuan Quan, Louis Lehmann, and Roland Netz — FU Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin, Germany

The capacitance of confined aqueous salt solutions is important for a variety of applications, including thermal energy conversion, but remains poorly understood. Performing Molecular Dynamics simulations and treating bulk electrolytes as a reservoir, we determine the temperature and bulk-concentration dependent density, slit concentration and capacitance of confined salt solutions. On a microscopic level, the capacitance is determined by the inverse dielectric profile, which we also present. Our results constitute a crucial step towards understanding the electrostatic behavior of confined electrolytes.

O 26: Plasmonics and nanooptics: Fabrication, characterization and applications – Poster

Time: Monday 18:00–20:00 Location: P2

O 26.1 Mon 18:00 P2

Extending multiphysics crystallization models for phase-change materials with parameters derived from machine learning — •Luis Schüler[1,2], José Moreira[2], Andrei Lupuleasa[2], Wenjing Lei[2], Keerthika Kalavalapudi[2], Matthias Wuttig[2], Thomas Taubner[2], and Dmitry Chigrin[1,2] — [1]AMO GmbH, Aachen — [2]I. Institute of Physics (IA), RWTH Aachen

Optical metasurfaces based on dielectric or metallic scatterers such as nanoantennas provide advanced control over light-matter interactions. Dynamic tuning can be realized with phase-change materials (PCMs), which can be reversibly switched between amorphous and crystalline states with a strong difference in refractive index. Especially metallic nanostructures can significantly influence the crystallization dynamics of PCMs, resulting in deviations from the expected spectral behavior of the metasurface. Therefore, Multiphysics simulations that couple electrodynamics, heat transport, and crystallization kinetics are essential for understanding these effects and optimizing device geometry. However, it is experimentally challenging to obtain key crystallization parameters, such as viscosity or free energy density, over the relevant temperature range. Here, we use machine-learned interatomic potentials trained molecular dynamics data to compute the required material parameters. Furthermore, we use machine learning to predict the viscosity of chalcogenide-based PCMs using data from related glasses. This approach broadens the range of phase-change materials that can be reliably simulated and provides a pathway toward the systematic design of dynamically tunable metasurfaces.

O 26.2 Mon 18:00 P2

Toward Plasmonic Pump-Probe Spectroscopy of a Hot-Electron-Driven Reduction Reaction — •Marcel Schalling, Lukas Schmidt, Ferdinand Bauer, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth

Plasmon-induced hot electrons offer a promising way to drive surface-catalytic chemical reactions with enhanced efficiency and selectivity. We want to follow the dynamics of the hot carriers by pump-probe spectroscopy.

In our approach, an initial laser pulse excites surface plasmons in the gold taper, generating hot electrons. These subsequently reduce adsorbed metal complexes on the taper's surface. This reduction is expected to locally modify the refractive index, which we probe by a second laser pulse. We show our first steps towards this goal. We start from the opto-electrochemical model system of methylene blue, and gradually add plasmonics and hot-electron generation towards the full implementation of the plasmonic pump-probe concept.

O 26.3 Mon 18:00 P2

Dissipation engineered plasmonic ratchet — •Anna Sidorenko[1], Jan Mathis Giesen[2], Sebastian Eggert[2], and Stefan Linden[1] — [1]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, 53115 Bonn, Germany — [2]Physics Department and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

This joint theoretical and experimental study presents a new design of a plasmonic ratchet, where directional transport is implemented purely by dissipation. Using Floquet theory, we identify resonant driving regimes depending on driving frequency and dissipation rates. An experimental observation of the ratchet effect in arrays of evanescently coupled plasmonic waveguides is provided by utilizing leakage radiation microscopy. Remarkably, we find that on resonance the transmitted signal shows lower losses for stronger local dissipation.

O 26.4 Mon 18:00 P2

Is the linkng number a topological invariant? — •Maja Manten[1], Alexander Neuhaus[1], Pascal Dreher[1], Phillip Gessler[1], Bettina Frank[2], Tim Davis[1,2,3], Harald Giessen[2], Michael Horn-von Hoegen[1], Karin Everschor-Sitte[1], and Frank Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany. — [2]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany. — [3]School of

Physics, University of Melbourne, Parkville, Victoria 3010 Australia

Optical near fields, like they occur in surface plasmon polaritons, exhibit a wide range of topological textures, including skyrmions, merons, and optical vortices carrying orbital angular momentum. Near fields that carry a fractional orbital angular momentum rather than integer orbital angular momentum, however, pose a challenge: they form a complex phase-vortex landscape and break the simple picture of a single vortex carrying the topological charge. When the fields become distorted, the situation becomes more complicated as more and more vortices appear. The sequence of vortices and antivortices can extend to infinity and evade global topological classification in real space. Here we show that a global topological invariant, the linking number, can be found in Fourier space. We show how the linking number of a plasmonic field can be determined from a time resolved polarimetric photoemission microscopy experiment and demonstrate the robustness of the linking number against deformation of the excitation structure.

O 26.5 Mon 18:00 P2

Reconfiguring resonator shapes optically to tailor the resonator modes of phonon polaritons in hBN using In$_3$SbTe$_2$ — •Arvid Schick, Lina Jäckering, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

The van der Waals material hexagonal boron nitride (hBN) hosts hyperbolic Phonon Polaritons (HPPs) with high volume confinement and low losses, suitable for nanophotonic devices [1]. Restricting the HPPs to resonators enables ultra-confined resonances [2]. Conventionally, resonator fabrication requires cumbersome lithography processes. Instead, resonators can be fabricated via optical programming of the phase-change material In$_3$SbTe$_2$ (IST), as IST can reversibly be switched between a metallic and a dielectric phase in the infrared [3]. Optical programming of reconfigurable, circular resonators for HPPs in hBN has been demonstrated and allowed for tailoring the field confinement [4]. We investigate square, rectangular and triangular resonators. We reconfigure resonator shape and aspect ratio to tailor the resonator modes that we investigate with scattering-type scanning near-field optical microscopy (s-SNOM). By decreasing the resonator size, we find confinement of up to $\lambda/69$ and a Q-factor of 49. Our results pave the way for rapid and reconfigurable prototyping of confined polariton resonators of arbitrary shape for various 2D materials. [1] Dai et al. *Science* **343**, 1125-1129 (2014); [2] Sheinfux et al. *Nat. Mat.* **23**, 499-505 (2024); [3] Conrads et al. *Opt. Mater. Express* **15**, 2664-2687 (2025); [4] Jaeckering et al. *Nano Lett.* **25**, 15809, (2025)

O 27: Plasmonics and nanooptics: Light-matter interaction, spectroscopy – Poster

Time: Monday 18:00–20:00 Location: P2

O 27.1 Mon 18:00 P2

Charge reservoir as a design concept for plasmonic antennas — •Rostislav Řepa, Michal Horák, Tomáš Šikola, and Vlastimil Křápek — Brno University of Technology, Brno, Czechia

Plasmonic antennas exploit localized surface plasmons to shape, confine, and enhance electromagnetic fields with subwavelength resolution. The field enhancement is contributed to by various effects, such as the inherent surface localization of plasmons or the plasmonic lightning-rod effect [1]. Inspired by nanofocusing observed for propagating plasmons [2], we test the hypothesis that plasmonic antennas with a large crosssection represent a large charge reservoir, enabling large induced charge and field enhancement. Our study reveals that a large charge reservoir is accompanied by large radiative losses, which are the dominant factor, resulting in a low field enhancement.

[1] Křápek et al., arXiv:2407.09454.

[2] Babadjanyan et al., J. Appl. Phys. **87**, 3785-3788 (2000).

O 27.2 Mon 18:00 P2

Distinct Multiphoton Orders in Photoelectron Spectra of Individual Silver Nanoparticles — Waqas Pervez[1], •Frithjof Harmsen[1], Kevin Oldenburg[2], Moha Naeimi[1], Sylvia Speller[1], and Ingo Barke[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Life, Light & Matter, University of Rostock, Germany

We investigate how the multiphoton photoemission process of individual metal clusters deposited on a non-metallic substrate is affected by the particle shape and its local environment. Here we present photoelectron spectra acquired by time-of-flight spectroscopy using a photoemission electron microscope (PEEM). Size-selected particles produced in a magnetron cluster source are deposited in-situ onto silicon substrates. The cluster source can produce single particles as well as agglomerates with characteristic plasmon modes [1], as revealed by transmission electron microscopy (TEM). Photoelectron spectra are obtained using illumination by a femtosecond laser at wavelengths around 800 nm, where at least 3 photons are required to overcome the work function. In addition, we observe well-separated above-threshold processes (ATP / ATI) of 4th order and up to 7th order for agglomerates. No noticeable resonances are observed across the spectral range, in contrast to illumination around 400 nm [2], i.e., at the plasmon energy. Mechanisms are discussed in view of symmetry properties and dipole selection rules.

[1] K. Oldenburg et al., Phys. Rev. Research 7, 023267 (2025)

[2] K. Oldenburg et al., J. Phys. Chem. C 123, 1379 (2019)

O 27.3 Mon 18:00 P2

Plasma-assisted defect modification in hBN studied with cathodoluminescence spectroscopy — •Bharti Garg, Masoud Taleb, and Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Germany

In this work, we study exfoliated hexagonal boron nitride (hBN) flakes treated with argon plasma for different durations and compare their optical response using cathodoluminescence (CL) spectroscopy. Emission spectra collected before and after plasma exposure allow us to isolate the effects of the treatment. hBN is known for defect-dependent optical emission, and plasma processing is a commonly used method to introduce or modify the density and the atomic structure of defects. We observe that longer plasma exposure leads to stronger defect-related emission and broader CL features, indicating an increase in defect density. The emission though occurs at the same wavelength before and after the plasma treatment, allowing us to conclude that the atomic structure of the defects remains similar even after the plasma interaction with the surface of hBN. These results clarify the influence of plasma treatment on defect formation in hBN and highlight the role of exposure time in tuning its optical properties.

O 27.4 Mon 18:00 P2

Tunable Stokes-shifted photoluminescence and defect emission from hBN excited with a supercontinuum laser — •Prabhdeep Singh, Bharti Garg, Maximilian Black, Masoud Taleb, and Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

We investigate the photoluminescence (PL) of hexagonal boron nitride (hBN) flakes placed on holey carbon grids under tunable supercontinuum excitation from 460 to 650 nm. The spectra consistently show a fixed defect emission around 537 nm together with a stokes-shifted peak that moves linearly with the excitation wavelength. The excitation emission energy differences cluster around 0.17 eV and 0.20 eV, matching the in-plane E_1u and E_2g phonon modes of hBN. Cathodoluminescence measurements on the same flakes exhibit only the defect line, along with phonon sidebands. On a gold substrate, we additionally observe a weak third moving peak at the sum of the two phonon energies, arising from surface enhanced Raman spectroscopy scattering (SERS). Spatial PL maps, intensity variations, and measurements with different optical density filters further allow us to evaluate the local emission characteristics and estimate the down-conversion efficiency. The results provide a consistent picture of phonon-mediated optical processes in hBN. Using tunable supercontinuum excitation, we reveal phonon-assisted stokes emission in hBN and a SERS phonon-combination peak on gold an excitation scheme not previously explored for Raman-type processes in this material.

O 27.5 Mon 18:00 P2

Energy and momentum distribution of surface plasmon-induced hot carriers — •Ellen Brennfleck[1], Christopher Weiss[1], Jannis Lessmeister[1], Laurenz Rettig[1], Tobias Eul[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Institute of Physics, University of Augsburg, Germany

Are the spectroscopic properties of plasmon- and photon-induced carriers fundamentally different? This question is crucial for advancing plasmonic energy conversion. Initial studies have suggested characteristic energy and momentum distributions for the photoemission of both bulk plasmon resonances and surface plasmons. For surface plasmons, however, the separation of plasmon and photon-induced emission patterns by their inherent spatial and temporal dynamics remains challenging [1].

To further characterize the electron emission pattern of surface plasmons, we combine a femtosecond laser system with a spatial light modulator to generate a vector vortex beam to excite surface plasmon polaritons at an annular structure. Our photoemission electron microscope enables us to compare the spectroscopic properties of photoemitted electrons and those generated by plasmonic emission at the center of the structure, providing valuable insights into the distinct emission mechanisms.

[1] Hartelt et al., ACS Nano 15, 12 (2021), 19559–19569

O 27.6 Mon 18:00 P2

Hot electron generation in tapered plasmonic waveguides — •Ferdinand Bauer, Valentin Dichtl, Marcell Schalling, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth, Germany

The efficient generation of hot electrons is important for applications such as photochemical catalysis. Hot electron-hole pairs are created by Landau damping of surface plasmon polariton (SPP) and decay through electron-electron scattering.

A symmetric taper in a waveguide enhances the generation of hot electrons. At one end the waveguide is excited by a laser pulse. The emission at the other end is then used as a metric for the transmission and thus the creation of hot electrons.

Numerical simulations (COMSOL) are used to find a high energy density at the hot spot. Within the simulations, Beer's law holds for a broad range of taper lengths and can be used to make geometry optimisation more efficient.

We demonstrate how to maximize energy density in the waveguide hot spot by using numerical simulations and experimental data, thereby optimising the production of hot electrons.

O 27.7 Mon 18:00 P2

Optical Response of Noble Metals based on Metal Boltzmann-Bloch Equations — •Robert Lemke, Andreas Knorr, and Jonas Grumm — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The optical response of plasmonic noble metals can be attributed to the interplay of electronic intra- and interband processes. These processes are addressed by coupled metal Boltzmann-Bloch equations derived from microscopic many-body theory. The specific properties of noble metals are caused by an anisotropic band structure in the vicinities of the X and L high symmetry points.

In order to analyse the line broadening of intra- and interband excitations we consider linearised electron-phonon and electron-electron scattering. Our approach allows to connect spectroscopic signatures directly to microscopic processes, not possible with phenomenological Drude-Lorentz models.

O 28: Oxide and insulator surfaces: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 28.1 Mon 18:00 P2

Probing Reactions at the Plasma-Catalyst Interface — •Maarten van Dorp and Roland Bliem — ARCNL, Amsterdam, The Netherlands

Efficient conversion of CO2 into value-added chemicals is a major step towards tackling climate change. However, chemical activation of CO2 by conventional catalysis requires exceedingly high reaction temperatures, straining energy efficiency and consequently industrial viability. Plasma-assisted catalytic conversion (PLAC) circumvents this by activating CO2 dissociation through the repeated impact of *hot* electrons from a non-thermal plasma, lowering the reaction barrier while selectively heating chemically activated CO2 species. However, to rationally design new PLAC catalysts, and therefore unlock the full potential of PLAC, crucial information about the short-lived intermediates is still unknown.

Here, a NiAl(110) substrate with an epitaxially grown alumina layer (Al10O13) was selected as well-defined support for carrying Cu-nanoparticles as a model system for the hydrogenation of CO2 with PLACIn this model system, a complete characterization of transient intermediates * both within the ECR microwave plasma and on the catalyst surface * requires a combination of complementary spectroscopic techniques, such as XPS, in-situ IRAS, LEED, and OES. . We establish the model system for plasma applications by synthesizing different alumina thicknesses, characterizing them with LEED, and testing their stability during exposure to plasma-activated species using in situ XPS.

O 28.2 Mon 18:00 P2

Influence of sample temperature on electron-beam-induced modifications in ultrathin CaF_2 films on Si(111) — •Luis Witte, Chris Schröder und Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

The development of modern transistor technologies based on 2D materials requires gate dielectrics with low defect densities and high chemical stability. CaF_2 layers on Si(111) are well suited for this purpose due to their low lattice mismatch and large band gap. However, a crucial aspect is their stability under electron irradiation, e.g. during LEED analysis of the layers, which can lead to structural and chemical changes.

In this study, ultrathin CaF_2 layers were deposited on Si(111) using molecular beam epitaxy. First, a growth temperature study was carried out at substrate temperatures between 400 °C and 700 °C. In a second step, the influence of the sample temperature during LEED measurements on the structural stability of the layers was studied. The electron beam of the LEED served both as a source of excitation for structural changes and as a probe for detecting these modifications. The measurements were conducted at sample temperatures from -150 °C to 600 °C in order to systematically investigate temperature-related effects. The results show that modifications induced by the electron beam exhibit a pronounced temperature dependence. In addition, ex-situ XPS measurements were performed to analyse chemical changes.

O 28.3 Mon 18:00 P2

Growth of MgO on Ag(100) for promoting charge transfer of organic molecules — •Christian Haberland, Felix Otto, Maximilian Schaal, Jonas Brandhoff, Leon Bojunga, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Integer charge transfer between metal substrates and adsorbed organic molecules is a central mechanism governing interfacial electronic structure and thus the functionality of molecular devices. To control this process, ultrathin insulating films offer a powerful strategy by decoupling molecular orbitals from metallic states while still enabling quantized charge exchange. In this work, we report the successful preparation of MgO monolayer films on Ag(100) using controlled deposition of Mg and annealing procedures in an oxygen atmosphere. The resulting MgO/Ag(100) system provides a reliable platform for studying charge-transfer phenomena at oxide-supported interfaces. Comprehensive characterization was performed using photoelectron spectroscopy (UPS, XPS, XPD), revealing the electronic structure and stoichiometry, while scanning tunneling microscopy confirmed atomic-scale order and film continuity. The established growth of MgO serves as a robust model system for investigating integer charge transfer in metal/organic hybrid interfaces.

O 28.4 Mon 18:00 P2

Epitaxy of ultrathin α-Fe_2O_3(0001) and Fe_3O_4(111) on α-Al_2O_3(0001) — •Hanna Laguta, Tobias Pollenske, Chris

Schröder, Luis Witte, Felix Johannsmann, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Iron oxides have a lot of technological applications and occur in magnetic, catalytic or electronic devices. Fe_3O_4 (magetite) and α-Fe_2O_3 (hematite) belong to the most stable iron oxides which can be found in nature.

Hematite is antiferromagnetic and has a lot of potential to be used for magnetic data storage. Thus it is of interest to study ultrathin hematite films. In this work, on the one hand α-Fe_2O_3 was grown directly onto the α-Al_2O_3(0001)-substrate using MBE. On the other hand Fe_3O_4 was deposited first to be oxidised to hematite in a second step. The magnetite films underwent exposures of oxygen between $6 \cdot 10^{-3}$ mbar·s and $180 \cdot 10^{-3}$ mbar·s, one sample was oxidised step-by-step.

The samples were respectively investigated using Soft and Hard X-ray Photoelectron Spectroscopy to determine the stoichiometries of near-surface and subsurface regions. Low Energy Electron Diffraction is used to determine the surface structure of the ultrathin oxide films and to distinguish hematite (α-Fe_2O_3) from maghemite (γ-Fe_2O_3) films. Additional measurements using SQUID provide insight into the magnetic properties of the samples.

O 28.5 Mon 18:00 P2

STM and LEED studies on the stabilization of two-dimensional scandium oxides on Pt(111) by Ba and Ti incorporation

— •Selina Schmechel, Muriel Wegner, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The formation of two-dimensional oxides on metal support crucially depends on a charge transfer between the film and the substrate. For the particular case of M_2O_3 transition metal oxide honeycomb (HC) structures, it was found that potentially di- and quadrivalent metal cations form HC structures by charge exchange with the support [1]. This is not possible for trivalent metals and, therefore, they do not form 2D oxides.

Here we study the growth of submonolayer scandium oxide films. We confirm the 3D growth for the binary Sc_2O_3 compound with the bulk lattice parameter of 3.2Å. However, when incorporating Ti an immediate transition into a 2D layer is observed. For different compositions, these mixed Sc-Ti-O films develop long-range ordered 2D wagonwheel structures. By incorporating Ba into Sc_2O_3 we succeed in the formation of a HC structure. In this case, all HC pores are filled with Ba ions, which donate their valence electrons to the substrate. This HC posses a lattice parameter of 6.1Å as determined from LEED. This points to an increased Sc-Sc distance as compared to bulk conditions. This host atom-assisted HC stabilization will be applied to the preparation of lanthanide HC oxides in the future.

[1] J. Goniakowski et al., J. Phys. Chem. C **123**, 9272 (2019)

O 28.6 Mon 18:00 P2

Oxidation behaviour of nickel on magnesium oxide (001): An in situ study of structural development.

— •Tobias Pollenske, Laurenz Hüffmeier, Hannah Hilmer, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Precise control of nickel oxidation on magnesium oxide (MgO)(001) surfaces under ultra-high vacuum (UHV) conditions is of fundamental importance for understanding metal/oxide interfaces and developing novel materials with tailored magnetic, electronic or catalytic properties. In this study, an approximately 15 nm thick Ni layer was deposited on MgO(001) using molecular beam epitaxy (MBE) and oxidised in situ at 250°C, 300°C and 400°C under 1×10^{-5} mbar O_2. The structural changes during oxidation were monitored by X-ray diffraction (XRD) near the MgO(002) Bragg reflection. In addition, GIXRD, XRR and soft XPS measurements were performed between the oxidation steps. The results show that structured NiO formation only occurs at 400°C, while lower temperatures only lead to surface-limited oxidation. The soft XPS data confirm that the Ni surface oxidises almost immediately once a sufficient temperature is reached, with longer exposure to oxygen having little additional effect. Furthermore, the diffraction data show that annealing above 250°C improves the crystalline order of the Ni film. These combined in situ measurements provide a detailed picture of the oxidation kinetics and temperature-dependent structure development at the Ni/MgO(001) interface.

O 28.7 Mon 18:00 P2

Initial stages of gold nanoparticle growth on sapphire

— •Hannah Hilmer[1], Chris Schröder[1], Tobias Pollenske[1], Timo Kuschel[2,4], Arno Jeromin[3], and Joachim Wollschläger[1] — [1]Institute of Physics, Univ. Osnabrück, 49076 Osnabrück, Germany — [2]Faculty of Physics, Univ. Bielefeld, 33615 Bielefeld, Germany — [3]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Sychrotron DESY, 22607 Hamburg, Germany — [4]Institute of Physics, Johannes Gutenberg Univ. Mainz, 55128 Mainz, Germany

Gold nanoparticles are of great interest for applications in catalysis, sensor technology, and electronics due to their shape- and size-dependent optical, electrical, and chemical properties. Their morphological and electronic properties depend heavily on the growth conditions. Al_2O_3(0001) is particularly well suited as a substrate due to its chemical stability and well-defined surface structure.

For this purpose, gold was deposited in ultra-high vacuum using thermal molecular beam evaporation at different deposition durations and varying substrate temperatures. In addition, thermal post annealing was carried out at different temperatures.

The growth processes of Au on Al_2O_3(0001) substrates were characterized using XRR, XPS and LEED. The results show that gold grows on sapphire in the initial stage according to Volmer-Weber growth as discontinuous islands. SEM and EDX analyses show clearly defined gold particles whose size and distribution depend strongly on the substrate temperature, the evaporation time per interval, and annealing temperature.

O 28.8 Mon 18:00 P2

Local Characterization of Structural and Electronic Properties of the ZnO(0001) Surface

— •Yuyang Zhang and Martin Wenderoth — IV Physical Institute, University of Göttingen

Zinc oxide (ZnO) serves as a key model system for understanding Proton-Coupled Electron Transfer (PCET) at interfaces.[1] To unravel electron dynamics on hydrated and doped surfaces, a profound understanding of the pristine surface is the indispensable baseline. Here, high-quality single-crystalline ZnO (0001) surface were prepared under ultra-high vacuum (UHV) conditions. The desired reconstruction was achieved by optimizing cycles of Ar+ sputtering and annealing. The structural properties were characterized by Low-Energy Electron Diffraction (LEED), confirming the long-range order and the intrinsic hexagonal surface symmetry. Similar to [2], Scanning Tunneling Microscopy (STM) revealed an ordered morphology dominated by atomically flat terraces with a high concentration of defects characteristic of polar face. Complementary atomic force microscopy (AFM) measurements provided additional information on the mesoscale morphology. Tunneling current measurements were utilized to probe the local electronic properties, providing insight into the surface band structure. This work was financially supported by the DFG through the CRC1633. [1] Hammes-Schiffer et al, ACS Nano 2017, 11, 10295-10302 [2] Diebold et al, Surf. Sci. 2002, 519, 201-217

O 29: Oxides and insulators: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 29.1 Mon 18:00 P2

Impact of atomic oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the angular and velocity distributions of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. Adsorption processes are evaluated and their influence on the surface structure and resulting changes regarding AO reflection is revealed. A strong dependence on the angle of incidence and the initial velocity is found. A high ratio of specular reflection can be obtained for grazing angles of incidence and hyperthermal initial velocities.

O 29.2 Mon 18:00 P2

First Principles investigation of the electronic properties and OER activity of (sub)stoichiometric $\mathbf{WO_{3-x}}$ (x =0.0, 0.1) — •Jeel Swami and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Tungsten trioxide (WO_3) exhibits a rich sequence of temperature and defect-driven structural phase transitions. Using density functional theory (DFT) calculations with the SCAN0 (with and without a Hubbard U term) and HSE06 functionals, we explore the influence of oxygen defects on the electronic properties of WO_{3-x}. For substoichiometric Magnéli phase $WO_{2.9}$ our results show partial localization of charge at the interface exhibiting weak magnetisation and n-type conductivity. We further investigate the application of WO_3 as anode material for the oxygen evolution reaction. At the (001) facet we consider various surface terminations. Gibbs free energy plot reveal that *OOH formation is the potential determining step for WO_3(001) facet.

We acknowledge computation time at the MagnitUDE and AmplitUDE HPC systems at the University of Duisburg-Essen.

O 29.3 Mon 18:00 P2

Interaction of atomic Oxygen with Silica Surfaces — •Ahmad Kassem Arrak, Stephen Hocker, Hansjoerg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

In order to increase the lifetime of VLEO (very low earth orbit) satellites, the drag forces on the satellite and the degradation of the surface material must be reduced. Both arise mainly from atomic oxygen (AO) impinging on the satellite surfaces at hyperthermal velocities. We investigate the influence of AO impact on silica surfaces using molecular dynamics simulations (LAMMPS). A focus is on adsorption, reflection and chemical reactions. Three interaction potentials were used, one from Vashishta, a Tersoff potential and a PACE machine learning potential. We prepared three (001) surface structures of alpha silica differing by their surface layers. The oxygen impact simulations revealed that the interaction processes occurring at the surface depend strongly on the chemical composition of the surface layers. At the oxygen-rich surface the formation and desorption of O2 can be observed while reflection or adsorption of AO is favored at other surfaces.

O 30: Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 30.1 Mon 18:00 P2

Structural analyses for S and Te on transition metal chain-like phases on the Ir(100) substrate — •Eric Engel, Alexander Wegerich, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The magnetic properties of one-dimensional transition metal oxide chains Ir(100)-(3×1)-MO_2 (M = Mn, Fe) [1,2] may in the case of Mn be tuned by changing the number of oxygen atoms in the chain structure [3]. Here, we present our attempts to replace O by S and Te and the quantitative LEED-IV analyses of the resulting structures.

Dosing H_2S to the MnO_2 or FeO_2 chains leads to the formation of a dominant $c(2 \times 2)$ superstructure. The structural analyses reveal with Pendry R-factors $R_P < 0.11$, that reduced transition metal chains remain as ordered (3×1) structures in the surface layer. The true unit cell of the system is hence a $c(6 \times 2)$ but with only little deviations in the S adsorbate layer from a $c(2 \times 2)$.

For Te, MO_2 chains were reduced in H_2 first, followed by Te deposition. In the case of 1/6 ML Te on the Ir(100)-(3×1)-$FeIr_2$ a (3×2)-Te superstructure emerges, where the Te atoms take positions on pure Ir hollow sites between the Fe-chains ($R_P = 0.123$). For 1/2 ML Te a dominant $c(2 \times 2)$ superstructure appears, again with only slight influences of the metal chains in the Ir(100) surface adsorbate positions.

[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)
[2] M. Schmitt et al., Phys. Rev. B **100**, 054431 (2019)
[3] J. Qi et al., Phys. Rev. B **107**, 060409 (2023)

O 30.2 Mon 18:00 P2

Structure of Standing Tetracyanoethylene Molecules on Cu(111) and Cu(100) — •Lorenz Brill[1], Jonas Brandhoff[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich Schiller University Jena, Germany — [2]Graz Universtiy of Technology, Austria

Tetracyanoethylene (TCNE) has been predicted to go through a standing-lying transition on Cu(111) depending on the deposition conditions. However, only disordered growth with a mix of standing and lying molecules has been observed in the past. Here, we present the first evidence of well ordered structures of standing TCNE molecules grown on Cu(111) and Cu(100), observed by low energy electron diffraction and scanning tunneling microscopy. We compare the obtained structures to predictions calculated in thermodynamic equilibrium.

O 30.3 Mon 18:00 P2

Quantitative sputter depth profiling: LEIS measurements and SDTrimSP simulations on silicon oxide — •Julian Pichler, Camil Bocaniciu, Alper Tunga Celebi, and Markus Valtiner — Technische Universität Wien, Wiedner Hauptstr. 8-10, Vienna, 1040, Austria

Precise surface characterization is crucial in semiconductor devices, to guarantee highest quality and optimal device fabrication.

This involves identifying defects, accurate handling of layers and surface contaminations, as well as determining elemental concentrations. This study focuses on a combined interpretation of Low Energy Ion Scattering Spectroscopy (LEIS) measurements on silicon oxide by quantification with references and Monte Carlo simulations with the SDTrimSP code [1]. We calculate surface erosion rates from simulations to deduce layer thicknesses in target materials, under consideration of atomic intermixing effects induced by sputtering.

For silicon oxide on pure silicon we find good quantitative agreement in sputtering depth profiles between LEIS measurements and SDTrimSP simulations for oxide layer thicknesses around 2 nm. We provide an estimation of layer thicknesses within a few Ångstrom and demonstrate intermixing at the interface induced by sputtering.

References [1] Mutzke et al., SDTrimSP Version 6.00, IPP report (2019)

O 30.4 Mon 18:00 P2

Should Doping be illegal at inorganic/organic Interfaces — •Aleksey Sokolov, Christoph Wachter, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, 8010, Austria

Organic/inorganic-semiconductor interfaces are central to the performance of devices such as organic light-emitting diodes and photovoltaic cells. The geometric arrangements of the molecules at the interface, known as polymorphism, heavily influence the properties of the interface, such as ionization energy, electron affinity, and charge mobility. Which arrangement molecules assume under given deposition conditions is governed by a variety of factors, such as the molecular size and shape, the intermolecular interactions as well as the molecule-substrate interactions, particularly the adsorption-induced charge-transfer. The amount of charge transfer, however, is critically determined by the substrate's doping concentration. Although there are now successful methods in predicting stable polymorphs, the role of the substrate doping for the interface polymorphism is not sufficiently understood. In this work, we use density functional theory in combination with the machine learning-driven structure search method SAMPLE to investigate how doping-induced charge transfer influences the thermodynamically stable phases of the example of F4TCNQ on ZnO. The results give insight into the interplay between doping, charge transfer, and interface structure, which can be used to generalize the effects in similar systems.

O 31: Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 31.1 Mon 18:00 P2

Investigating the native oxide layer of CoCrFeNi(100) by co-adsorption of O_2 and H_2: an XPS study — •Peter Richter, Kavya Harsha Kumar, Susanne Wolff, and Thomas Seyller — Technische Universität Chemnitz, Chemnitz, Deutschland

High-entropy alloys (HEAs) are a relatively new class of materials with potential applications under ambient conditions. Hence, understanding the formation and the properties of their native oxides is essential. In this study, we use X-ray photoelectron spectroscopy to investigate the native oxide layer present on CoCrFeNi(100) as well as on the clean surface subjected to controlled exposures of O_2 and H_2.

To evaluate the stability of the native oxide layer, samples were annealed in ultra-high vacuum at temperatures in the range of 350 to 1100 °C. Oxide reduction increased significantly at 700 °C and was complete at 1100 °C. The exposure of clean CoCrFeNi(100) surfaces to 1 to 1000 L of O_2 leads to controlled oxidation, with Cr contributing most to oxide formation, followed by Co and Fe. The subsequent introduction of H_2 at sample temperatures of up to 500 °C leads to systematic changes in the surface chemistry.

Experimentally, the information of the bonding configuration is best observed in the 2p core levels of Co, Cr, Fe and Ni. However, when using the Al K_α line, several Auger peaks overlap with the Co2p and Fe2p core levels. In addition, multiplet splitting and satellite features further complicate the evaluation of the XPS data. To improve this, we performed reference measurements and developed fitting models for the Auger lines using pure metal foils.

O 31.2 Mon 18:00 P2

Molecular bottom up: Site-selective adsorption of cyclooctyne on partially passivated Si(001) — Jannick A. Peters[1], •Sophie Göbel[1], Dominik Scharf[2], Ulrich Koert[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany

Organic molecular structures on the technologically most important Si(001) surface are of great potential for future applications in terms of "more than Moore". The synthesis of organic structures on semiconductor surfaces requires several aspects to be considered, such as precise choice of adsorbates and their functional groups, as well as a well-prepared surface where the reaction sites can be controlled. For a lateral ordering of the organic layer, pre-patterned substrates are seen as promising starting point; e.g., alternating passivated and non-passivated surface areas are generated by means of STM in hydrogen desorption lithography. A self-organized approach might be based on ethylene on Si(001) which is known to show a well-ordered adsorbate structure on Si(001) in the submonolayer regime due to nearest-neighbor interactions. The reaction of cyclooctyne and its derivatives on the Si(001) surface pre-passivated with ethylene was studied by means of XPS and STM. Whereas C_2H_4 shows strongly reduced reactivity at the remaining, unreacted silicon dimers, cyclooctyne with its direct reaction channel on clean Si(001) shows high reactivity also at these strongly hindered sites. Furthermore, the reaction of bifunctional cyclooctynes was observed to be more selective than on clean Si(001).

O 31.3 Mon 18:00 P2

Quantitative imaging of surface potential of PTCDA molecules on Ag(111) and Pb(111) — •Sandhya Anchamkudy[1], Janine Lorenz[1,2], Amin Karimi[1], Christian Wagner[1,2], Ruslan Temirov[1,3], Henry Thake[4], Reinhard Maurer[4], Stefan Tautz[1,2], and Felix Lüpke[1,3] — [1]Peter Grünberg Institut (PGI 3), Forschungszentrum Jülich, Germany — [2]Institut für Experimentalphysik IV A, RWTH Aachen, Germany — [3]Institute of Physics II, Universität zu Köln, Germany — [4]Department of Chemistry, University of Warwick, United Kingdom

Scanning Quantum Dot Microscopy (SQDM) enables quantitative imaging of surface dipoles with unprecedented energy and spatial resolution. In the past, SQDM has been applied to molecular adsorbates, adatoms, defects, and atomic assemblies on silver [Phys. Rev. Lett. 115, 026101 (2015), Nat. Mater. 18, 853 (2019)] - and provided valuable benchmarks for theory where metal-organic hybrid systems are particularly challenging. Here, we investigate the adsorption geometry dependent effects of isolated perylene tetracarboxylic dianhydride (PTCDA) molecules on Ag(111). We identified two preferred orientations of PTCDA molecules: along the <1-10> and <11-2> directions of the Ag(111) surface. In SQDM measurements, the two orientations yield distinct dipole moments of -0.51 D and -0.65 D, respectively. In addition, we carried out SQDM of a single PTCDA molecule on superconducting Pb(111) and found that the dipole is seven times larger compared to PTCDA on Ag(111). This difference can be attributed to a significantly higher charge transfer and adsorption height on Pb(111).

O 31.4 Mon 18:00 P2

Redox Molecules on Gold Surfaces: Insights into Triboelectric Behavior through Simulations — •Zohreh Izadi[1,2], Michael Moseler[1,2,3], Michael Walter[1,2,3], and Leonhard Mayrhofer[3] — [1]Cluster of Excellence livMatS @Freiburg Center for Interactive Materials and Bioinspired Technologies(FIT), University of Freiburg, Freiburg, Germany — [2]Institute of Physics, University of Freiburg, Freiburg, Germany — [3]Fraunhofer IWM, MikroTribologie Centrum μTC, Freiburg, Germany

Triboelectricity, the electrostatic charge generated during the contact and separation of materials, remains poorly understood at the microscopic level. Redox-active molecules on metal surfaces provide a controlled platform to probe these charge-transfer processes. We studied donor and acceptor molecules adsorbed on Au(111) and evaluated their adsorption geometries and binding energies, as well as the electronic signatures associated with interfacial charge transfer. We also considered different environments and found that humidity was a key factor facilitating charge transfer between the molecules and the surface. Our results are in very good agreement with the experimental findings from our joint study, offering insight into how redox-driven charge transfer at metal-molecule interfaces contributes to triboelectric behavior.

Reference: N. Ranjan, Z. Izadi et al., Contact Electrification via Redox-Active Molecules, Angewandte Chemie International Edition, 2025, e10031. DOI: 10.1002/anie.202510031.

O 31.5 Mon 18:00 P2

TPD Studies of Metal-Substrate Interactions in LOHCs and Polyfluorinated Compounds — Kassandra Zoltner, •Evelyn Versok, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Metal-substrate interactions critically govern catalytic reaction pathways and degradation mechanisms. Here, we investigate two chemically contrasting classes of adsorbates - hydrogen-rich liquid organic hydrogen carriers (LOHCs) and fluorocarbons - to clarify their stability and reactivity on metal surfaces. LOHCs such as decalin and tetralin are attractive hydrogen-storage materials but are prone to side reactions and catalyst-induced decomposition. In contrast, fluorocarbons including all-cis-hexafluorocyclohexane and perfluoromethylcyclohexane exhibit exceptional thermal and chemical stability, which is technologically valuable yet contributes to unwanted environmental persistence. Understanding molecule-metal interactions is therefore important for both hydrogen-storage chemistry and fluorocarbon degradation strategies. We employ temperature-programmed desorption (TPD) to determine adsorption energies, reaction kinetics, and product distributions. Systematic analysis of the selected LOHCs and fluorinated compounds on Au(111), complemented by comparison with partially dehydrogenated and defluorinated analogues, reveals detailed metal-induced transformation pathways. These insights advance the mechanistic understanding of hydrocarbon and fluorocarbon degradation on metal surfaces and support catalyst development.

O 31.6 Mon 18:00 P2

Orientation-dependent Adsorption and Manipulation of a Boron-doped Polycyclic Aromatic Hydrocarbon — •Elishka Vaz[1], Matthias Schnitzlein[2], Frank Würthner[2], Matthias Bode[1], and Jing Qi[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie, Organische Chemie II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The incorporation of boron atoms into polycyclic aromatic hydrocarbons (PAHs) alters their electronic properties since the boron centres act as π-acceptors [1]. In this contribution, we present a novel boron-centered PAH with terminal bromine-substituents. Upon adsorption on the Cu(111) surface, the B-PAHs adopt twelve distinct azimuthal orientations: six aligned with the crystallographic directions of the (111) surface, and six rotated by 30°. Differential-conductance spectroscopy and apparent-height analyses reveal a pronounced influence of the substrate on both the topographic appearance and electronic structure. Atomic-resolution imaging enables assignment of adsorption sites via interpolation of the surface atomic rows. Moreover, lateral tip-induced manipulation demonstrates controlled stacking along the molecular short axis. Finally, we identify a double-chain arrangement, likely composed of intact molecules, which exhibits a notable spectral shift in the differential-conductance signature relative to isolated adsorbates.

[1] M. Schnitzlein *et al.*, ChemistryEurope **3**, e202500135 (2025)

O 32: Topical Talk Witte

Time: Tuesday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 32.1 Tue 9:30 TRE/PHYS

Excitons in molecular solids: from unitary films to donor-acceptor co-crystals — •Gregor Witte — Renthof 7, 35032 Marburg

Their strong light-matter interaction makes organic semiconductors (OSCs) promising candidates for optoelectronic devices. However, the microscopic picture of photophysical excitations and their properties is still incomplete. Reasons for this are the different nature of excitons in inorganic and organic SCs and the frequently used simplified description of excitons in OSCs within the framework of H- and J-aggregates, which disregards high-energy states and the delocalization of wave functions. Optical transmission-absorption measurements on single crystals or films with large crystalline domains enable the spectroscopy of higher energy excitons and, by means of polarization- and direction-resolved measurements, also a correlation with the molecular packing motif. Among OSCs, acenes represent an ideal platform for exciton studies, as they allow both polymorph-selective crystallization and versatile modification of the molecular electronic structure through chemical substitutions. Furthermore, also highly ordered acene-perfluoroacene cocrystals can be produced, which enable detailed characterizations of heteromolecular charge transfer excitons in molecular donor-acceptor systems with well-defined internal interfaces. In this talk I will present some of our recent exciton studies on various acenes, which combine polarization-resolved optical spectroscopy with modern ab initio calculations based on density functional theory and many-body perturbation theory.

O 33: Graphene: Growth, structure and substrate interaction (joint session O/HL)

Time: Tuesday 10:30–12:30 Location: HSZ/0201

Invited Talk O 33.1 Tue 10:30 HSZ/0201

During-synthesis functionalization of graphene layers — •Cristina Africh — CNR-IOM, Trieste, Italy

Introducing heteroatoms into graphene is a powerful way to modulate its catalytic, electronic, and magnetic properties. During the last decade, we developed a clean and scalable functionalization strategy that exploits the sponge-like properties of nickel substrates as well as the catalytic role played by transition metal (TM) single atoms at graphene edges during Chemical Vapor Deposition synthesis [1]. Following this route, it is possible to grow N-doped, B-doped and TM-doped graphene as well as co-doped layers [2,3,4]. The potential of the functionalized networks for sensing and, as a perspective, for catalysis, was evaluated by monitoring their response upon gas exposure [5,6].

[1] C. Africh, M. Peressi and G. Comelli, Surf. Sci. 753, 122652 (2025). [2] S. Fiori et al., Carbon 171, 704-710 (2021). [3] S. Patil et al., Surf. Interfaces 51, 104700 (2024). [4] V. Chesnyak et al., Sci. Adv. 10, eado8956 (2024). [5] D. Perilli, S. Fiori et al., J. Phys. Chem. Lett. 11 8887-8892 (2020). [6] D. Perilli, V. Chesnyak et al., Angew. Chem. Int. Ed. 64, e202421757 (2025).

O 33.2 Tue 11:00 HSZ/0201

Heterotriangulene Kagome Graphene Films: Growth and Effect of Kinetic Reaction Parameters — •Wyatt Behn[1], Simon Briesenick[1], Chang Wan Kang[2], Manuel González-Lastre[3], Pablo Pou[3], Rubén Pérez[3], Dmytro Perepichka[2], and Peter Grutter[1] — [1]Dept. of Physics, McGill — [2]Dept. of Chemistry, McGill — [3]Universidad Autónoma de Madrid

Nanoporous graphenes featuring Kagome lattices formed by heterotriangulene units continue to attract interest for their correlated electronic properties. Their symmetry gives rise to flat bands and Dirac cones [1,2]. Covalent organic frameworks (COFs) like these are often synthesized by surface-assisted Ullmann coupling, and are susceptible to defects such as voids, irregular-sided linkages, and limited grain sizes of around 100 nm [3,4]. We perform a series of polymerizations over a range of sample temperatures (180-250 C) for tribromo- and triiodotrioxaazatriangulene precursors on the Au(111) surface. Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) we interrogate how deposition conditions and choice of halogen affect the final polymer film quality, which we quantify using minimum spanning tree and persistent homology approaches. We also investigate the prevalence of halogenated edge terminations and of undesired organometallic intermediates. Experimental results are complemented by simulated STM and nc-AFM analyses. [1] C. Steiner, et al. Nat. Commun. 8, 14765 (2017). [2] G. Galeotti, et al. Nat. Mater. 19 (2020). [3] M. Lackinger, Chem. Commun. 53 7872 (2017). [4] T. Qin, et al. Commun. Chem. 7 154 (2024).

O 33.3 Tue 11:15 HSZ/0201

Defect-Driven Formation of Distinct 2D-Ag Phases at the Graphene/SiC Interface — •Sawani Datta[1], Boyang Zheng[2], Arpit Jain[2], Vibha Reddy[1], Kathrin Küster[1], Joshua A. Robinson[2], Vincent H. Crespi[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalation of two-dimensional (2D) materials at the graphene/SiC interface is important for improving environmental stability of the intercalant and tuning graphene's electronic properties. However, the underlying mechanisms remain complex and are still not fully understood. In this study, we show that by modifying the intercalation process, specifically through defect engineering, it is possible to selectively stabilize two distinct phases of intercalated silver (Ag). The previously established phase (Ag$_1$) aligns with nearly (1×1) registry of SiC [1, 2], while the second phase (Ag$_2$) develops a denser $(3\sqrt{3}\times3\sqrt{3})R30^\circ$ superstructure on a (5×5) SiC unit cell, producing a 6.25×6.25 Moiré pattern with respect to graphene, as seen in the low energy diffraction (LEED) pattern [2]. Angle-resolved photoemission spectroscopy (ARPES) reveals a striking kaleidoscopic modulation of the Ag$_2$ and graphene bands, absent in Ag$_1$, along with notable differences in charge transfer between the two phases. These results demonstrate that defect-controlled, phase-selective intercalation offers a promising pathway to design and explore exotic 2D electronic states at graphene/SiC interfaces. [1] PRB 101, 201407(R) (2020). [2] arXiv:2511.07151v1 (2025).

O 33.4 Tue 11:30 HSZ/0201

Strain-Induced 2D Pb phases confined between graphene and SiC — •Sergii Sologub[1,2], Markus Gruschwitz[1], Zamin Mamiev[1], Chitran Ghosal[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The intercalation of metals beneath graphene offers a powerful route to stabilizing and protecting novel 2D phases. We performed a detailed intercalation study of Pb beneath the ZLG on SiC(0001) using low-energy electron diffraction (at the temperatures from 70 to 600° C) as well as scanning electron and tunneling microscopy [1]. Our analysis reveals the formation of different 2D Pb monolayer phases, such as stripes and hexagons, which emerge due to the interplay between substrate pinning and strain within the Pb layer, depending on local coverage. The interface reconstruction of Pb was shown can be tuned by varying the details of the intercalation protocol. Based on our experiments combined with recent simulations [2], an intercalation model, accounting for the different periodicities observed in the interface layer, was proposed. These findings provide new insights into the strain-driven stabilization of intercalated metal layers and highlight the potential of graphene as a versatile platform for engineering low-dimensional materials.

[1] Adv. Mater. Interfaces 12, no. 21: e00617 (2025); [2] Appl. Surf. Sci. 681, 161572 (2025).

O 33.5 Tue 11:45 HSZ/0201

Strain engineering in graphene on Ru(0001) — Paula García-Mochales[1] and •Antonio J. Martínez-Galera[1,2,3] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

The ability to induce and characterize strain in the atomic lattice of 2D materials, localized within only a few nanometers around specific positions, is a major challenge for the development of straintronics. In this work, the interaction between Si nanoparticles and the surface of graphene/Ru(0001) is employed to induce local strain in the latter. The strain field has been mapped at the nanoscale by scanning tunneling microscopy (STM), using the moiré pattern intrinsic to graphene/Ru(0001) surfaces as a magnifying lens. The induced strain is found to be confined within only a few nanometers around each nanoparticle. To achieve more accurate control, strain engineering at the nanometer scale was successfully performed by manipulating nanoparticles through the STM tip. This approach to controlled strain could provide a key tool for exploring new physics arising by strain in 2D materials.

Reference:

P. García-Mochales and A. J. Martínez-Galera, Nano Lett. 25, 16097-16103 (2025).

O 33.6 Tue 12:00 HSZ/0201

Subsurface carbon controls graphene growth on Ir(111) — •Smruti Ranjan Mohanty, Lothar Brendel, Marko Kriegel, Niels Ganser, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

The CVD growth of 2D materials is governed by a balance between adsorption, surface diffusion, and nucleation. For transition metal substrates, dissolution into the bulk acts as an additional parameter. By employing in-operando low-energy electron microscopy (LEEM) to monitor graphene growth on Ir(111), the effect of the growth temperature and the precursor pressure on the nucleation behavior is studied. The island nucleation density exhibits two distinct regimes, described as separate cases within Venables nucleation theory [1]. For a critical nucleus size $i^* = 5$, low dosing pressures yield a low nucleation density that is governed by incomplete condensation with a scaling exponent of 2.5. At higher-dosing pressures, adsorptions at island edges dominate over the adatoms loss into the substrate, resulting in a higher nucleation density and a strongly reduced scaling exponent. Kinetic Monte Carlo simulations that incorporate bulk dissolution reveal both nucleation regimes and find a universal, temperature-independent scaling law. The results indicate a universal nucleation behavior for 2D materials with finite, non-negligible solubility in the supporting metal substrate.

[1] J A Venables et al 1984 Rep. Prog. Phys. 47 399

O 33.7 Tue 12:15 HSZ/0201

Thermodynamics of heteroatom-doped graphene: Brute forcing the partition function — •Lukas Hörmann[1,2], Benedict Saunders[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, United Kingdom — [2]University of Vienna, Austria

The introduction of dopants into graphene can be used to tune material properties for specific applications, such as electronics, sensors, or catalysis. Achieving such tunability requires precise control over the composition and concentration of dopants within the lattice. This demands a fundamental understanding of the thermodynamics that govern the phase space of heteroatom superstructures in the two-dimensional graphene framework. We present a comprehensive approach to determining dopant structures that enables the near-exhaustive enumeration of all relevant heteroatom superstructures. The approach combines Density Functional Theory and machine learning to build a transferable energy model for dopant formation. Our method's efficient data handling and fast inference enable the evaluation of more than 150 million possible structures, allowing us to effectively brute force the partition function and derive all thermodynamic properties from it. We show the capabilities of our approach for free-standing graphene doped with nitrogen atoms, establishing a thermodynamic model to investigate how temperature affects the configuration space of doped graphene. Our analysis yields physical insights into defect interactions. We observe a characteristic peak in the heat capacity, indicating an order-to-disorder transition, and present a mechanistic understanding of how this peak arises.

O 34: Catalysis and surface reactions I

Time: Tuesday 10:30–12:30 Location: HSZ/0204

O 34.1 Tue 10:30 HSZ/0204

From Global Optimization to Transition State Search: Automatic Workflow for Surface Reaction Kinetics — •Hyunwook Jung[1], Emanuel Colombi Manzi[1], Johannes T. Margraf[1,2], Hendrik H. Heenen[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Reaction-barrier calculations present the major bottleneck in the systematic exploration of surface reaction networks via atomistic simulations. Each involved transition-state search introduces a high-dimensional configuration space, comprised of many initial and final state combinations, that must be explored to identify the minimum-energy pathway with the lowest activation barrier. Typically, this task is delegated to human chemical intuition as user-input to e.g. a nudged elastic band (NEB) calculation, since its automation remains a significant challenge. Here, we introduce a fully automated workflow for transition-state optimization that does not require any human intervention. Initial and final geometries are generated through global optimization and subsequent alignment, followed by an atom-mapping and index permutation to arrive at the nonequivalent transition pathways. This process still leads to a large combinatorial number of possible interpolations from which we select a tractable subset using heuristic reaction-distance metrics. We demonstrate the workflow across a range of reactions and surface combinations from the OC20NEB database and discuss its overall performance.

O 34.2 Tue 10:45 HSZ/0204

Machine-learning Driven Approach of Surface Adsorption Energy Prediction — •Karlo Sovic and Johannes Margraf — University Bayreuth, Bayreuth, Germany

Heterogeneous catalysis is a cornerstone technology across industrial chemistry, materials science, and environmental engineering, effectively promoting and redirecting key chemical reactions in various applications. In these processes, control of surface adsorption energies is paramount for designing efficient catalysts. However, in the case of large adsorbates, the high computational cost of accurate DFT calculations limits comprehensive exploration of the corresponding potential energy surface. Machine-learning interatomic potentials offer a promising solution to this challenge. Leveraging recently reported pre-trained models, the complex interactions crucial for accurate surface chemistry can be captured with effectively via fine-tuning.

Here, a data-efficient workflow for describing the glycerol hydrodeoxygenation mechanisms leading to propanediols on M(111) and M(211) surfaces (M=Pt, Cu, Ni) is reported. With our approach, the fine-tuned model yields high-fidelity adsorption energies with near-DFT accuracy at low computational cost. Furthermore, analysis of thermodynamic properties was carried out to accurately determine the overall Gibbs free energetics of investigated reaction pathways. Based on these comprehensive insights, we propose a versatile workflow for the accelerated screening of catalytic systems, enabling the rapid construction of adsorption energy databases and exploring relevant reaction mechanisms.

O 34.3 Tue 11:00 HSZ/0204

Modeling Solvothermal Reactions at Surfaces with Machine Learning Interatomic Potentials — •Maciej Baradyn[1], Nils Gönnheimer[1,2], and Johannes T. Margraf[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]Fritz-Haber Institute, Berlin, Germany

Dynamical processes such as adsorption, desorption and diffusion are vital elementary reactions involved in heterogeneous catalytic reactions. In solvothermal reactions, the presence of solvent molecules has significant effects on the dynamics of the adsorbates, which must displace hydration layers to diffuse or adsorb on the surface and undergo resolvation during desorption. The presence of solvent molecules also affects the interactions between surfaces and adsorbates, and can contribute to the (de-)stabilization of the adsorbed species.

In this contribution, we explore the robustness of machine learning potentials based on the MACE-MP-0 foundation model for describing dynamical processes under these conditions. This is demonstrated on a representative system of a glycerol molecule interacting with the Cu(111) surface in explicit water. Enhanced sampling methods are used to compute free energy profiles of the studied processes, and to reflect the experimental reaction conditions under which they occur in industrial applications.

O 34.4 Tue 11:15 HSZ/0204

Converting MoS$_2$ to MoO$_2$ by Thermal Treatment Under Dilute O$_2$ — •Armin Sahinovic[1], Jixi Zhang[2], Osamah Kharsah[1], Marika Schleberger[1], Rossitza Pentcheva[1], and Rodney Smith[2] — [1]Department of Physics and Center for Nanointegration, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Chemistry, University of Waterloo, ON N2L 3G1 Waterloo, Canada

The reaction of MoS$_2$ with O$_2$ at elevated temperatures introduces the risk of structural and functional degradation that decrease the lifespan of MoS$_2$-based devices [1]. In experiment, variable-temperature Raman measurements indicate that depending on the O$_2$ concentration in the environment the MoS$_2$ is converted into either MoO$_3$ or MoO$_2$. To elucidate the specific mechanism of this reaction, density functional theory (DFT) calculations were performed including the van der Walls dispersion correction. We show that the S-vacancy formation energy as well as O substitution energy are lowered with increasing O content. DFT calculations show that at high O contents in MoS$_{2-x}$O$_x$ the P2$_1$/c phase is energetically preferred over the 2H-MoS$_2$ structure. A *P-T* phase diagram of the Gibbs free energy obtained from DFT shows that the partial O pressure tunes whether MoO$_3$ or MoO$_2$ is the dominant product of the reaction. We explored the band structure of multiple vacancies in MoS$_2$ and find additional in-gap states compared to the monovacancy. Our results offer insight into the conditions that control the degradation of MoS$_2$-based devices.

[1] J. Gao, et al., ACS Nano, 10 (2), 2628 (2016)

O 34.5 Tue 11:30 HSZ/0204

2D TiS2 Nanoparticles in reductive and oxidative Atmospheres as Model (Photo-)Catalysts — •Niko Kruse[1], Justin Klimek[1], Aaron von Seggern[1], Martin Hedevang[2], Sergi Camposs Jara[2], Jeppe Vang Lauritsen[2], and Lars Morhusen[1] — [1]Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]iNano Center, Aarhus University, Aarhus, Denmark

Sustainable materials for the thermal and photochemical utilization of (waste) carbon dioxide (CCU) become more and more demanded.[1] Titanium-based 2D materials such as TiS2 can directly harvest sunlight and have demonstrated high CO2 conversion activity.[2] To illuminate atomistic structure-property relationships of such catalytic systems, we present a model system consisting of 2D TiS2 nanoparticles on Au(111) and TiO2 (110) surfaces, rendering it suitable for atomic-level microscopy and spectroscopy. A direct synthesis route was developed by Ti metal evaporation in the presence of benign organic S precursors.[3] The resulting materials were characterized by combined STM, XPS, and NEXAFS experiments, along with DFT calculations.[4] We demonstrate the substrate-dependent structure and compositional detail of the nanoparticles and highlight the chemical potential of S as the relevant shape descriptor. In addition, the surface chemistry of 2D TiS2 nanoparticles in reactive atmospheres will be presented, highlighting the strong stability even in oxidative & reductive conditions. [1] R. Guil-López, N. M. et al., Materials 2019, 12. 3902. [2] A. Aljabour, et al, ACS Catal. 2020, 10, 66. [3] F. Besenbacher et al., J. Catal. 2021, 403, 4. [4] N. Kruse et al., Small 2025, 21, e06023.

O 34.6 Tue 11:45 HSZ/0204

In situ X-ray Imaging of PtPd Core-Shell Nanoparticles under Methane Oxidation Conditions — •Lydia J. Bachmann[1,2], Thomas F. Keller[1,2], Ivan A. Vartanyants[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY — [2]University of Hamburg

Due to the high global warming potential of methane, the release of any methane into the atmosphere needs to be avoided. Therefore, catalysts are used for the emission control. Common catalyst nanoparticles (NPs) for methane oxidation consist of Pd or Pt. Combining them allows to build more stable NPs. Since the surface chemical composition is crucial for the activity, segregation and mixing processes need to be taken into account. In this study we successfully tuned the initial chemical composition of one core-shell and one partially alloyed NP. We confirmed these elemental distribution by Bragg coherent diffraction imaging (BCDI). During in situ BCDI measurements under methane oxidation at temperatures between 320°C and 560°C, Pt segregated to the {111} oriented facets of the initial core-shell NP. Conversely, the initially partially alloyed NP did not exhibit such facet-dependent segregation, but rather observed the formation of a Pd core, Pt shell structure at 680°C. Since the initial Pt core, Pd shell NP showed Pd-Pt mixing at 620°C, we hypothesize that this NP would form such an inverted core-shell structure under higher temperatures as well. These results demonstrate opportunities for systematically investigating promising core-shell NPs and their catalytic activity, offering valuable insights for the design of advanced catalysts.

O 34.7 Tue 12:00 HSZ/0204

The mechanism and Rate-Determining Step of Catalytic Ammonia Oxidation on Pd(332) at High Temperatures — •Jan Fingerhut[1], Jessalyn DeVine[2], Rongrong Yin[3], Mark Bernard[2], Alice Bremer[4], Dmitriy Borodin[2], Kai Golibrzuch[2], Theofanis Kitsopoulos[5], Daniel Auerbach[2], Hua Guo[3], and Alec Wodtke[2] — [1]Leiden Institute of Chemistry, Leiden, the Netherlands — [2]Max-Planck-Institute for Multidisciplinary Science, Göttingen, Germany — [3]University of New Mexico, Albuquerque, USA — [4]Georg-August-Universität, Göttingen, Germany — [5]University of Southern Mississippi

Despite its immense practical importance in industrial production of nitric acid, the mechanisms of catalytic ammonia oxidation on platinum group metals remain controversial. In this work, we employ velocity-resolved kinetics to study ammonia oxidation on a model Pd(332) catalyst between 600 and 700 K. We obtain the temporal evolution of gas-phase reactants (NH_3), products (NO, H_2O) and - with the help of femtosecond laser-induced desorption - of a reaction intermediate, N*. The reaction exhibits the prompt appearance of H_2O and the delayed formation of NO; the rate-determining step is the reaction N* + O* → N*O occurring at step sites. This means that N* is the longest-lived reaction intermediate, an insight that helps explain formation of byproducts like N_2 and N_2O. We present a mechanism that explains all experimental observations, based on transition-state theory calculations and using input from density functional theory. We also show that N*O desorption is accelerated by coadsorbed oxygen.

O 34.8 Tue 12:15 HSZ/0204

Promoting Role of Isolated Surface Hydroxyls on Selective Dehydrogenation of 2-Propanol over Co3O4 Catalyst — •Jan Smyczek[1], Patrick Hubert[1], Hauke Scheele[2], Carsten Schröder[1], Sharif Najafishirtari[2], Paul Kohlmorgen[1], Malte Behrens[2], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 1, 24118 Kiel, Germany — [2]Institute of Inorganic Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 2, 24118 Kiel, Germany

This study investigates the catalytic decomposition of 2-propanol to acetone over Co_3O_4 catalysts, examining both powdered materials under ambient pressure and model $Co_3O_4(111)$ surfaces in ultrahigh vacuum. Water pretreatment at elevated temperatures substantially enhanced acetone formation rates. Scanning tunneling microscopy and infrared spectroscopy revealed that high-temperature water pretreatment creates isolated hydroxyl groups (O_sH) involving lattice oxygen atoms, whereas low-temperature deposition forms an extended, partly dissociated OH/H_2O network layer. The role of isolated O_sH groups can most likely be attributed to their function as hydrogen acceptors for H atoms leaving from either 2-propanol or the propoxy intermediate. Critically, dissociation occurs only with isolated O_sH species, not within the extended OH/H_2O network, which nearly completely suppresses both abstraction steps. The isolated O_sH groups function as efficient hydrogen acceptors, proving substantially more effective than adsorbate-free lattice oxygen.

O 35: Organic molecules on inorganic substrates: Adsorption and growth II

Time: Tuesday 10:30–12:15 Location: HSZ/0401

O 35.1 Tue 10:30 HSZ/0401

Phophangulenes on Au(111): comparing the influence of the environment on single molecule rotation — •Wyatt Highland[1], Sajjan Mohammad[1], Paul Philip Schmidt[1], Roberto Robles[2], Milan Kivala[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [3]Institute of Organic Chemistry, Heidelberg University, Heidelberg, Germany — [4]University of Applied Sciences of the Grisons, Switzerland

Bowl-shaped phosphangulenes represent a promising class of rotor molecules for molecular energy-storage applications on surfaces, owing to their fixed rotational axis defined by the central phosphorus atom, which simultaneously serves as the anchoring group on gold substrates. For low coverge, the phosphangulenes stay isolated on Au(111). We examined their adsorption configurations and subsequently, the possibility for rotational motion using both the STM tip and thermal activation as external triggers. At higher coverage, phosphangulenes form compact self-assemblies that suppress their rotational motion. To overcome this, we employ porous, hydrogen-bonded trimesic-acid networks to isolate individual phosphangulenes at the surface. Comparing their rotational dynamics inside and outside the pores allowed to directly reveal the influence of the immediate surroundings on the rotational motion.

O 35.2 Tue 10:45 HSZ/0401

Self-assembly and electronic properties of functionalized norbornadiene photoswitches on Au(111) and graphene/Ir(111) — •Shreya Garg[1], Roberto Robles[2], Pedro Ferreira[3], Kasper Moth-Poulsen[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department of Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián 20018, Spain, SanSebastián, Spain — [3]Universitat Politecnica de Catalunya, Barcelona, CT, Spain — [4]University of Applied Sciences of the Grisons, Switzerland

The norbornadiene/quadricyclane (NBD/QC) system represents a notable class of photoswitches, in which the low-energy NBD isomer can be transformed into its metastable QC isomer upon exposure to external energy. Here, we investigate the self-assembly and electronic properties of a benzoic acid-functionalized NBD on Au(111) using STM, STS, and DFT. Two distinct adsorption conformations are identified; nevertheless, the overall structure of the self-assembled layers remains governed by hydrogen bonding between the carboxyl groups. To further elucidate molecule-substrate coupling effects, we examined NBD derivatives on graphene/Ir(111), which offers a reduced density of states near the molecular levels, thereby providing partial electronic decoupling. This approach revealed differences in electronic properties compared to Au(111), emphasizing the critical influence of the substrate and contributing to the optimization of their switching performance in future electronic systems.

O 35.3 Tue 11:00 HSZ/0401

Validation of the Rotational Degrees of Freedom in Azobenzene Subphthalocyanine — •Dominik Volavka[1], Wyatt Highland[1], Bartosz Szczefanowicz[1], Rebecci Samuele[1], Roberto Robles[2], Nicolas Lorente[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]University of Applied Sciences of the Grisons, Switzerland

Azobenzene mounted on Subphthalocyanine (Azo-SubPC) via a single covalent oxygen bond is predicted to exhibit interesting rotational and switching properties due to the single bonding character of the boron-oxygen-carbon. Recent attempts at observing these rotational actions through scanning tunneling microscopy were hindered because of the self-assembling nature of Azo-SubPC when deposited on Au(111) and Ag(111). In each case, one-dimensional arrangements of Azo-SubPC formed, wherein molecules were neighbored by additional Azo-SubPC molecules on both sides. The resulting configuration of the molecules thusly led to a high steric hindrance and ultimate restriction of Azo-SubPC's anticipated rotational degree of freedom. Alternative preparation methods of Azo-SubPC are herein proposed and evaluated in the attempt of depositing and identifying isolated Azo-SubPC molecules with preserved rotational freedom. Isolated Azo-SubPC molecules can give insight into the underlying principles dictating the mechanisms of rotation in rotor molecules.

O 35.4 Tue 11:15 HSZ/0401

TPD/R Investigations of Metal-Substrate Interactions of Polyfluorinated Molecules on Au(111) — •Stefan R. Kachel, Evelyn Versok, Leonard Neuhaus, Kassandra Zoltner, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Interfaces between organic molecules and metal surfaces are crucial in heterogeneous catalysis, organic electronics, and related nanotechnological and sensing applications. Molecules with large dipole moments are particularly relevant, as dipole enhancement through tailored fluorination can strongly influence adsorption geometries, adsorbate-substrate interactions, and thus the electronic properties of molecule-metal interfaces. Among nonionic, saturated compounds, all-cis-hexafluorocyclohexane (HFCH) exhibits the highest known polarity (μ = 6.2 D). Here, we use temperature-programmed desorption and reaction (TPD/R) to investigate the desorption kinetics and energetics of HFCH and two reference compounds, perfluoromethylcyclohexane and cyclohexane, on Au(111). The polar HFCH shows markedly stronger interactions with the substrate than the two reference compounds, and all systems display desorption behavior that deviates substantially from structurally related aromatic species. The pronounced polarity and stacked packing motif of HFCH render it a promising model system for studies in supramolecular chemistry and organic materials research, including potential applications in organic ion-conducting materials.

O 35.5 Tue 11:30 HSZ/0401

TPD Studies on LOHC-relevant Cycloalkanes and Aromatics on Au(111) — •Kassandra Zoltner, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie and mar.quest, Philipps-Universität Marburg, Germany

Liquid organic hydrogen carriers (LOHCs), such as the decalin/tetralin pair, are promising compounds for hydrogen storage, yet their (de)-hydrogenation cycles are limited by catalyst-induced side reactions. In this context, molecule–surface interactions fundamentally determine adsorption strength and reactivity, thereby controlling catalytic selectivity and activity. This work presents surface analytical studies using temperature-programmed desorption (TPD) to investigate the desorption kinetics and energetics of decalin, perhydroazulene, and (partially) dehydrogenated analogues on Au(111). The study focuses on how the degree of hydrogenation, structural motifs including ring connectivity, and configurational isomerism as well as electronic properties influence substrate and intermolecular interaction strengths. The results reveal distinct differences in desorption characteristics: aromatic molecules (naphthalene, azulene, tetralin) exhibit stronger adsorption to the metal substrate and repulsive intermolecular interactions, arising from their π-electron system, whereas saturated hydrocarbons (decalin, perhydroazulene) show weaker substrate binding and intermolecular attraction. The findings provide molecular-level insights into LOHC adsorption properties on metal surfaces and contribute to the development of improved hydrogen storage–catalysis systems.

O 35.6 Tue 11:45 HSZ/0401

MAD-SURF: a general Machine-Learning Potential for molecular adsorption on metal surfaces — •Manuel González Lastre[1], Joakim S. Jestilä[2], Rubén Pérez[1], and Adam S. Foster[2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain — [2]Department of Applied Physics, Aalto University, 00076, Espoo, Finland.

Predicting how organic molecules adsorb, assemble and interact on metal surfaces is central to surface chemistry, molecular electronics and scanning probe microscopy. Yet, the application of first-principles simulations to interfaces is hampered by the computational cost for evaluating the electronic structure for the large number of atoms typically involved. Here we present MAD-SURF, a general Machine-Learning Interatomic Potential tailored for molecular adsorption on metal surfaces. Trained on a broad dataset spanning diverse molecules, adsorption motifs, surfaces, molecular dynamics and non-covalent aggregates, MAD-SURF achieves near quantum-mechanical accuracy while enabling simulations that are orders of magnitude faster than Density Functional Theory. The model reliably reproduces energies, forces and adsorption geometries across different surfaces. We demonstrate its versatility by capturing experimentally observed systems, ranging from organic monolayers and polycyclic aggregates to flexible biomolecules and long-range metal surface reconstructions. By combining accuracy, speed, and generalizability, MAD-SURF offers a practical framework for accelerating atomistic simulations in surface science.

O 35.7 Tue 12:00 HSZ/0401

Using Machine Learning to predict molecular conformations from STM images — •Tim J. Seifert[1], Dhaneesh Kumar[2], Stephan Rauschenbach[3], Klaus Kern[2], Markus Etzkorn[1,4], Kelvin Anggara[2], and Uta Schlickum[1,4] — [1]Institute of Applied Physics, TU Braunschweig, Braunschweig — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Department of Chemistry, Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom — [4]Laboratory for Emerging Nanometrology LENA, Braunschweig

Single-molecule imaging of biologically essential building blocks such as saccharides and peptides by scanning tunneling microscopy (STM) holds immense promise, enabling key insights into their structure and biological functions. However, automatic structural analysis remains bottlenecked by the lack of available experimental training data. We overcome this fundamental limitation through a novel workflow that rapidly generates vast datasets of high-fidelity synthetic STM images from geometric molecular models. We train a custom Machine Learning architecture on this synthetic data to predict atomic coordinates directly from STM images, enabling fully automated reconstruction of molecular conformations. Validated on two distinct organic systems - glycans and polypeptides - the method achieves atomic positional accuracies below 4 Å and 2 Å, respectively, with unsupervised conformer classification of polypeptides exceeding 97% accuracy. The trained models transfer robustly to experimental STM data, delivering visually convincing structural predictions.

O 36: Focus Session: Mineral-water interfaces II

The Focus Session discusses recent advances in the understanding of mineral-water interfaces. These interfaces are ubiquitous in nature, host of many geological and biological processes, intimately linked to the global carbon cycle, and therefore highly relevant for Earth*s climate. For example, silicate weathering removes carbon dioxide from the atmosphere on geological timescales, acting as a stabilizing feedback mechanism since weathering rates increase with temperature. In the oceans, carbonates dissolve and precipitate in response to changing atmospheric carbon dioxide concentrations, thus far mitigating part of the anthropogenic impact of CO_2 emissions. In addition, numerous industrial and technological processes involve mineral-water interfaces, including seawater desalination, scaling and incrustation prevention, as well as various biochemical applications. However, and despite their importance, many fundamental aspects of mineral-water interfaces remain poorly understood, including water binding and diffusion, structure formation, ice nucleation, growth, or desorption.

This DPG Focus Session will address these aspects at the molecular level, elucidating fundamental processes involving both single water molecules and bulk water in contact with mineral surfaces. The session brings together scientists investigating mineral-water systems under ultrahigh vacuum conditions as well as at mineral-water interfaces in bulk aqueous environments. We aim for a balanced Session with contribution from both renowned experts and young investigators active in the field.

Organized by Philipp Rahe (U Osnabrück), Angelika Kühnle (U Bielefeld), Jan Balajka (TU Vienna), Wolf Gero Schmidt (U Paderborn).

Time: Tuesday 10:30–12:30 Location: HSZ/0403

Invited Talk O 36.1 Tue 10:30 HSZ/0403

Acidity in nanoconfinement from ab initio and NNPs simulations — Anthony Baldo[2], Muhammad Saleh[1], Kevin Leung[2], and •Marialore Sulpizi[1] — [1]Department of Physics and Astronomy, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Geochemistry Department, Sandia National Laboratories, Albuquerque, New Mexico, USA

Chemical and physical properties in nanoconfined systems may substantially differ from bulk, a phenomenon that can be exploited for the development of new industrial processes for energy generation and storage. Here we consider the specific behavior of acids within silica nanopores, a topic of relevance to the geochemistry and the nanofluids communities.

Starting from ab initio molecular dynamics simulations we develop neural network potentials (NNPs) capable of describing the solid/liquid interfaces and the nanoconfined liquids* behavior over a wide range of temperatures. These NNPs can capture the change in acidity constants when e,g acetic acid is confined in nanoscale slit or when it approaches the interface. Our approach can be further extended to more complex geometries and solution compositions.

O 36.2 Tue 11:00 HSZ/0403

Ab initio exploration of water clusters on CaF_2 — •Isaac Azahel Ruiz Alvarado[1], Wolf Gero Schmidt[1], Paul Laubrock[2], Jonas Heggemann[2], and Philipp Rahe[2] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, Paderborn, Germany — [2]Institut für Physik, Universität Osnabrück, Osnabrück, Germany

The electronic and structural properties of the $CaF_2(111)$ surface-water interface are investigated from first-principles calculations. The energetic landscape for single molecular adsorption is calculated using standard DFT with London dispersion forces corrections. Single water molecules are found to preferentially adsorb on surface Ca atoms while large diffusion energy barriers are determined that restrict lateral movement of the water molecules. Additionally, the adsorption energies for the intact water molecule are compared to dissociative adsorption.

Multiple water molecules are included in the calculations to simulate the ice-like clusters observed experimentally by high-resolution AFM data acquired with CO-terminated tips. In order to understand the formation of these clusters, hexagonal rings similar to the ice I_h motif are modeled on top of the CaF_2 surface slab. The ice-surface incommensurability coupled with large diffusion barriers and preferred adsorption sites is suspected to limit the formation of a closed water monolayer. Complete water overlayers and additional structures are also calculated using molecular dynamics aided by machine learning force fields trained from ab initio calculations.

O 36.3 Tue 11:15 HSZ/0403

Surface Structure of Polar Silver Iodide (0001) in Various Liquids: No Indication for a Surface Reconstruction — •Kim Noelle Dreier, Annamaria Latus, Ralf Bechstein, and Angelika Kühnle — Physical Chemistry I, Department of Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

Silver iodide (AgI) has long been known as a material that induces precipitation in clouds. The superior ice nucleation ability is commonly explained by the close lattice match between β-AgI(0001) and the basal plane of ice. However, this surface is polar, indicating that a stabilization mechanism should be present. Here, we investigate the Ag-terminated β-AgI(0001) and the I-terminated β-AgI(000-1) surfaces in water and compare the results with images recorded in n-dodecane, 0.1 M NaCl and 0.1 M KI aqueous solutions. Strikingly, high-resolution images consistently reveal a bulk-truncated structure. These findings align with observations at a larger scale, which neither indicate any surface reconstruction. Although the observed structures reveal a variety of features and depend on the surface termination, some general conclusions can be drawn. Firstly, in solvents with poor AgI solubility, only minor changes are observed. Secondly, the images taken in KI solution exhibit patterns that are characteristic of mineral dissolution and growth. Thus, even in a situation where AgI can and does dissolve, no indication for a surface reconstruction can be found. These results shed new light onto the surface structure of β-AgI(0001), challenging the expectation that a surface reconstruction is present under ambient conditions.

Invited Talk O 36.4 Tue 11:30 HSZ/0403

Living Interfaces: Dissolution and Precipitation Processes at Mineral-Brine Interfaces Revealed by AFM — •Igor Siretanu, Vincenzo Alagia, Saravana Kumar, Shilpa Mohanakumar, Max Nederstigt, Chinmay Shukla, Michel Duits, and Frieder Mugele — Physics of Complex Fluids Group and MESA+ Institute, Faculty of Science and Technology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Mineral-brine interfaces are dynamic systems where dissolution and precipitation govern reactivity and morphology. Using in-situ Atomic Force Microscopy (AFM), we examine olivine ([Mg,Fe]2SiO4) and calcite. Olivine, a candidate for carbon mineralization, shows etch-pit-mediated surface retraction with morphology strongly dependent on solution chemistry. In H2SO4, pits are larger and deeper than in HCl, while oxalic acid induces anisotropic complexation, forming rectangular pits and stepped terraces aligned with crystallographic directions. These changes accelerate step retreat and Mg release, offering mechanistic insight into dissolution kinetics relevant for CO2 sequestration. At calcite-water interfaces near equilibrium, AFM force spectroscopy reveals two regimes: (A) DLVO-type forces with low surface potentials (<5 mV) and (B) long-range viscoelastic repulsion from a soft interfacial layer formed by coupled dissolution-precipitation. This dynamic interphase explains inconsistencies in reported surface forces and highlights how solution composition, crystallography, and transient phases control mineral reactivity, with implications for geochemistry, biomineralization, and carbon capture.

O 36.5 Tue 12:00 HSZ/0403

Water Organization and Speciation at the Calcite (10.4)-Water Interface at High pH — •Tobias Dickbreder[1], Frank Heberling[2], and Ellen H. G. Backus[1] — [1]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria. — [2]Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Calcite dissolution and precipitation are central for various environmental processes including the geological carbonate-silicate cycle, buffering of sea- and freshwater pH values and biomineralization. Since these processes take place at the calcite-water interface, the structure and properties of the interface between water and the most stable calcite (10.4) surface have been well studied. Despite this effort the protonation state of surface-bound water and interfacial carbonate groups remains poorly understood, because dissolution and carbonate buffering complicate studying calcite de-/protonation experimentally.

Here, we apply vibrational sum frequency generation (SFG) spectroscopy to directly assess the water species present at the calcite-water interface. As reported previously, the SFG spectrum at neutral pH is almost featureless due to the opposite orientation of the first two water layers [1]. At very high pH, however, we observe the emergence of spectral features suggesting surface charging and the presence of interfacial hydroxyl groups. Our study, thus, confirms the presence of hydroxyl groups at the calcite-water interface, facilitating the development of more-accurate models of the calcite-water interface.

[1] Söngen et al., J. Phys. Chem. Lett. 12 (2021), 7605 - 7611.

O 36.6 Tue 12:15 HSZ/0403

The mechanism of selenite incorporation into the calcite surface revealed by atomic-scale imaging — •Marie Luigs, Ralf Bechstein, and Angelika Kühnle — University of Bielefeld, Bielefeld, Germany

Selenium is an essential trace element for human health. However, the margin between its required and toxic intake is very narrow, making its distribution in soils and waters an important subject of research. Moreover, the interaction between the nuclear waste component 79Se and minerals in the Earth's crust is relevant for the selection of nuclear waste disposal sites. Selenium in the form of selenite can be incorporated into the mineral calcite by substituting for carbonate ions. However, the mechanism of selenite incorporation into calcite remains unknown. Here we demonstrate that selenite incorporation occurs at step edges during calcite crystal growth. Atomic-scale atomic force microscopy (AFM) images of the calcite surface exposed to a selenite-rich calcium carbonate growth solution shows that calcite layers grown in the presence of selenite displayed a significantly higher defect density than layers that were exposed to selenite only after their formation. These observations indicate that significant selenite incorporation into calcite, reflected by an increased defect density, does not occur via ion exchange on terraces but via step edge growth. Our results give further insights into the conditions required for selenite incorporation into calcite and present the first atomic-scale AFM images of a selenite-rich calcite surface.

O 37: Electronic structure theory I

Time: Tuesday 10:30–12:30 Location: TRE/PHYS

Invited Talk O 37.1 Tue 10:30 TRE/PHYS

Calculations of excited electronic states by converging on saddle points on the electronic energy surface — •Hannes Jonsson — University of Iceland, Reykjavik, Iceland

Calculations of excited electronic states are important in various contexts, e.g. photocatalysis and molecular motors. They are challenging as commonly used optimization methods are based on minimization and thereby converge on the ground state. A time-dependent formulation of density functional theory (TD-DFT), especially within the linear response and adiabatic approximations, is therefore often used to estimate excited states, but can fail especially when significant charge transfer occurs and when states are close in energy. Alternatively, by converging on a saddle point on the electronic energy surface, the orbitals can be optimised for an excited state to provide a solution of the underlying Kohn-Sham equations with higher energy than the ground state. This turns out to a give more robust estimate of the excitation energy than TD-DFT with computational effort similar to that of a ground state calculation. Several applications of this approach with commonly used density functionals will be presented, as well as calculations using a self-interaction corrected functional giving improved results. In particular, excited states involving twisting of a C=C bond, e.g. in molecular motors, and Rydberg states have been analysed. As a solid state application, the various states involved in the optical preparation of a pure spin state in nitrogen/vacancy defect in diamond will be presented. The results show close agreement with more computationally demanding calculations as well as experiments.

O 37.2 Tue 11:00 TRE/PHYS

Probing quantum coherence with free electrons — •Hebrew Crispin and Nahid Talebi — Christian-Albrechts-Universität, Kiel, Germany

Advances in ultrafast electron microscopy have enabled the study of coherent interactions between free electrons and quantum systems with high spatial resolution. Recent works have examined the coupling of free electrons to two-level systems, including the use of coherently shaped electron wavefunctions to probe coherence in individual or collective quantum emitters. Coherence can also be accessed through sequential time-resolved cathodoluminescence spectroscopy, which has demonstrated the ability to measure ultrafast radiative decay and dephasing in single emitters with femtosecond resolution. In addition, there is increasing interest in time-resolved electron energy-loss spectroscopy (EELS) techniques capable of tracking system dynamics.

Here, we present a general theoretical framework for coherent interactions between free electrons and quantum emitters prepared in arbitrary initial superposition states. We employ a fully quantum, time-dependent description of both the propagating electron wavepacket and the emitter. Quantum coherence manifests as transient oscillations in both the emitter populations and in the zero-loss peak of the spectral energy-loss probability density, even for an unmodulated electron wavepacket. Our work reveals novel coherent dynamics in the interactions between free electrons and quantum systems.

O 37.3 Tue 11:15 TRE/PHYS

Phonons in polar materials: a DFPT extension in the FLAPW method *FLEUR* — •Friedrich Hanrath[1,2], Thomas Bornhake[1,2], Gustav Bihlmayer[1], Gregor Michalicek[1], Daniel Wortmann[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, D-52074 Aachen, Germany

Phonons play a pivotal role in determining many essential properties of solids. Using Density Functional Perturbation Theory (DFPT), a state-of-the-art approach for computing fundamental physical response properties from first principles, phonon calculations have previously been realized [1] within the full-potential linearized augmented plane-wave (FLAPW) method *FLEUR* [2]. In polar materials, zone-center vibrations are altered by their interaction with long-range electric fields, giving rise to the characteristic LO-TO splitting in the long-wavelength limit. In this talk, we present the extension of the DFPT framework in *FLEUR* to a macroscopic electric-field perturbation, enabling the calculation of high-frequency dielectric tensors and Born effective charges, quantities required to describe LO-TO splitting, and compare our results with experiments.
This work was supported by the CoE-MaX (EuroHPC Joint Undertaking, Grant 101093374) and DFG through CRC 1238 (Project C01).

[1] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).

[2] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de

Invited Talk O 37.4 Tue 11:30 TRE/PHYS

Many-Body Theory meets Electrochemistry: Electronic Structure of Cathode Materials — •Silke Biermann — Centre de Physique Théorique, UMR7644, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France

Progress in dynamical mean field-based electronic structure methods over the last years has provided us with precious tools allowing for a microscopic understanding of electronic mechanisms at work in correlated materials, including functional materials. In this talk, we will focus on layered transition metal compounds studied for battery applications. Analysing the electronic structure, energetics and intercalation voltage, we find that Hund's exchange coupling plays a crucial role for the electrochemistry of these compounds. We identify the battery charging process as a transition from a high-spin Mott insulator to a low-spin correlated metal. We argue that a deeper understanding of the microscopic mechanisms at work in such materials might contribute to paving the way to better battery materials in the future.

O 37.5 Tue 12:00 TRE/PHYS

Massively parallel and GPU-accelerated evaluation of three-center integrals for numerical atomic orbitals (NAOs) — •Moritz Leucke, Antonio F. Delesma, and Dorothea Golze — Julius-Maximilians-Universität Würzburg, Germany

Four-center electron repulsion integrals appear in many electronic structure methods, such as many-body perturbation methods like the Random-Phase-Approximation or GW and others. To reduce their computational cost, the resolution-of-the-identity (RI) approximation is commonly employed. RI refactors the four-center integrals into three- and two-center integrals, among which the three-center integrals remain a computational bottleneck, particularly when using NAOs.

We present a global RI scheme combined with a local metric (attenuated Coulomb) within an all-electron NAO framework, treating molecules and solids on equal footing. Central to the approach is a novel GPU-accelerated algorithm for computing 3-center integrals that relies on domain decomposition to improve load balancing and strong scaling.

We demonstrate that our RI implementation achieves linear scaling with system size and maintains meV-level accuracy for GW energies. Performance benchmarks show scalability across thousands of CPU cores and substantial speedups with GPU support.

[1] Delesma et al., NIC Symposium Proceedings, 52(2025), 113-123.

O 37.6 Tue 12:15 TRE/PHYS

Efficient all-electron implementation of the Bethe-Salpeter method using crystal symmetries — Jörn Stöhler, Stefan

Blügel, and •Christoph Friedrich — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

We describe an implementation of the Bethe-Salpeter equation (BSE) method in the full-potential linearized augmented-plane-wave (FLAPW) method. As in most implementations, the BSE is solved by the diagonalization of a two-particle Hamiltonian matrix, whose dimension is proportional to the number of **k** points. Due to the large number of **k** points required to converge the spectra, the resulting matrix becomes large even for small unit cells. We describe a method that exploits the crystal symmetries to accelerate the construction and diagonalization of the two-particle Hamiltonian. In particular, we employ group theoretical tools to bring the Hamiltonian into block-diagonal form. It is shown that, in many cases, only one of the blocks needs to be taken into account, which leads to a considerable speedup of the diagonalization step. In the case of Si, for example, the dimension of the Hamiltonian is reduced by a factor of five, giving rise to a speedup factor of 125 in its diagonalization. The optical absorption spectrum calculated with a 60×60×60 **k** mesh is very close to the experimental spectrum. The code allows for the inclusion of spin-orbit coupling and is parallelized with the possibility of storing the Hamiltonian in distributed memory over many nodes. We also show results for LiF and the MoS_2 monolayer.

O 38: Ultrafast electron dynamics at surface and interfaces II

Time: Tuesday 10:30–12:30 Location: TRE/MATH

O 38.1 Tue 10:30 TRE/MATH

Ultrafast momentum microscopy of exciton dynamics at ZnO surfaces — •Hashima Marukara, Paul Werner, Jan Philipp Bange, G S Matthijs Jansen, Wiebke Bennecke, Junde Liu, and Stefan Mathias — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

ZnO is a prototypical wide-band-gap material with long-lived excitons, making it a central platform for modern optoelectronic and catalytic technologies, especially for investigating exciton-related phenomena [1]. Excitons*bound electron*hole pairs that can exist in various forms near the surface, significantly shape the material*s optical and electronic response and play an essential role in interfacial energy-conversion processes [2]. However, studies that directly characterize these excitons, particularly if they are defect-mediated, localized or mobile, or predominantly Frenkel- or Wannier-type, remain limited.

Here we address these questions using time-resolved momentum microscopy to map the fingerprints of excitons in energy, momentum and time [3]. We present first experimental momentum-space maps of the ZnO(10-10) surface exciton states and track their real-time evolution following photoexcitation. We observe clear signatures of surface exciton formation, including their emergence in the unoccupied band structure and their subsequent relaxation dynamics on ultrafast timescales.

[1] Gierster *et al.*, Nat Commun 12, 978 (2021) [2] Deinert *et al.*, Phys. Rev. Lett. 113 057602 (2014) [3] Bennecke *et al.*, Nature Phys. (2025), https://doi.org/10.1038/s41567-025-03075-5

O 38.2 Tue 10:45 TRE/MATH

Investigating the light-induced metallization of ZnO through time-resolved photoemission spectroscopy — Gian Marco Pierantozzi[1], Federico Motti[1], Matteo Gatti[2], •Monika Schied[1], Alice Crosato[3], Thomas Sartori[3], Riccardo Cucini[1], Giorgio Rossi[1,4], Fausto Sirotti[2], and Giancarlo Panaccione[1] — [1]CNR – Istituto Officina dei Materiali (IOM), Trieste, Italy — [2]École polytechnique, Paris, France — [3]Università Ca' Foscari Venezia, Italy — [4]Università degli Studi di Milano, Italy

With a direct bandgap of ∼3.4 eV and a high exciton binding energy (∼60 meV), ZnO is ideal for optoelectronics and excitonic studies. Under optical excitation, the system shows ultrafast metallization with several relaxation timescales [1,2]. The relevance of defects in stabilizing the photoinduced metallic state is known, but many aspects of the processes remain unclear. Here we investigate the ultrafast dynamics of the optically populated conduction band and the Zn 3d core level with time- and angle-resolved photoemission spectroscopy after resonantly pumping, in order to disentangle the excitations of defect levels. Our experiments cover the whole metallization process in ZnO. We observe a fast rise in the conduction band population within 100 fs, a slower temperature-dependent rise, probably due to carrier transport and redistribution, a decay on the ns timescale and a long-lasting metastable state. All these dynamics occur also pumping below resonance, albeit to a lower extent, highlighting the role of the defect levels.

[1] L. Gierster et al. Nat. Comm. 12:978 (2021);

[2] L. Gierster et al., Far. Disc. 237, 58 (2022)

O 38.3 Tue 11:00 TRE/MATH

Ultrafast electron dynamics in charge-transfer insulators $LaFeO_3$(001) and $BiFeO_3$(001) — •Friederike Wührl, Antonia Rieche, Anne Oelschläger, Kathrin Dörr, and Wolf Widdra — MLU Halle-Wittenberg

The electron dynamics in strongly correlated systems, where electron-electron correlation leads to band gap opening, are highly unexplored. One example is the prototypical charge transfer insulator NiO, which shows a remarkable short lifetime of <10 fs at the conduction band minimum, relaxing in a many-body in-gap state, which couples to the antiferromagnetic spin system [1]. Here we are extending our time-resolved studies to the unoccupied states of epitaxial antiferromagnetic $LaFeO_3$(001) and ferroelectric $BiFeO_3$(001) thin films grown on $SrRuO_3$/$DyScO_3$(001) substrates. We use two-photon photoemission in a UV-UV pump-probe experiment, exciting electrons across the band gap, which opens between strongly hybridized oxygen 2p/Fe 3d and Fe minority states for both perovskites. We find in both sytems a broad state at $\sim 1.3\,\mathrm{eV}$ above E_F with a short lifetime of 20 fs, whereas the conduction band minimum shows a multiexponential decay with timescales in the femtosecond to picosecond range. The different decay channels show an energy dependent increase of lifetimes towards the Fermi level. Comparing $BiFeO_3$ and $LaFeO_3$, the decay channels differ solely in their amplitudes, with a higher probability for the fast decay channel in $LaFeO_3$.

[1] Gillmeister *et al.* Nat. Commun. **11**, 4095 (2020).

O 38.4 Tue 11:15 TRE/MATH

Ultrafast Formation and Annihilation of Strongly Bound Anisotropic Excitons in CrSBr — •Lawson T. Lloyd[1], Tommaso Pincelli[1,2], Mohamed A. Wahada[1], Alessandro De Vita[1,2], Ferdinand Menzel[3], Kseniia Mosina[4], Túlio H. L. G. Castro[1], Alexander Neef[1,2], Andreas V. Stier[3], Nathan P. Wilson[3], Zdeněk Sofer[4], Jonathan J. Finley[3], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany — [3]Technische Universität München, Garching, Germany — [4]University of Chemistry and Technology Prague, Prague, Czech Republic

Excitons dominate the optical response and determine the functionality of atomically thin semiconductors. In the van der Waals magnetic semiconductor CrSBr, strongly bound, anisotropic excitons couple to the underlying spin order, which could be leveraged in next-generation opto-spintronics. However, mechanisms of exciton formation, dissociation, and interaction with free carriers remain largely unexplored. Employing time- and angle-resolved photoemission spectroscopy, we probe the nature of the exciton in CrSBr by directly imaging the nonequilibrium electronic states, extracting fundamental properties of the excitonic wavefunction and revealing the driving mechanisms of exciton relaxation on ultrafast timescales. Notably, we observe an excitation-density-dependent interconversion between bound excitons and quasi-free carriers, indicating that many-body effects govern the excited state dynamics during the initial stages of relaxation.

O 38.5 Tue 11:30 TRE/MATH

Large relative delays for photoemission final states less than 1 eV apart — •Tillmann Schabbehard, Andreas Gebauer, Walter Enns, Luis Maschmann, and Walter Pfeiffer — Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

The reconstruction of attosecond beating by interference of two-photon transitions (RABBITT) allows probing photoemission dynamics in atoms, molecules and solids. However, the interpretation of retrieved relative delays between different emission channels in particular for emission from solids is controversial. Here we employ spin-orbit delays in GaSe by RABBITT, i.e., relative delays for emission from the different initial states of the spin-orbit doublet, to investigate the relative photoelectron kinetics in emission channels, which differ less than 1 eV in their final state energy (E_{final}). Despite the small spin-orbit splitting for both Ga3d and Se3d the extraction of relative delays for the two spin-orbit doublets yields 180±53 as and 94±45 as. These unexpectedly large delays can neither be attributed to intraatomic delay mechanisms nor to kinetic propagation effects in the final state continuum. This challenges common concepts about photoelectron emission dynamics, which predict much smaller delays for E_{final} differences below 1 eV. Notably, the Se3d spin-orbit delay in GaSe agrees well with those observed in Bi_2Se_3 and WSe_2 indicating a general high variability of emission dynamics as function of the E_{final}. Predictions based on the one step model, which take into account transport via propagating and evanescent states match observations much better, while modelling based on propagation effects in the final state alone fail.

O 38.6 Tue 11:45 TRE/MATH

Lightwave-driven flat bands in a van der Waals crystal — •Changhua Bao[1], Vincent Eggers[1], Manuel Meierhofer[1], Jakob Helml[1], Lasse Münster[1], Suguru Ito[2], Leon Machtl[1], Sarah Zajusch[2], Giacomo Inzani[1], Ludwig Wittmann[1], Marlene Liebich[1], Robert Wallauer[2], Ulrich Höfer[1,2], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Philipps-University of Marburg, Marburg, Germany

Flat bands lead to an extremely high density of states and suppressed kinetic energy, thereby increasing electronic correlations and leading to intriguing light-matter interaction. Here, we reveal the band structure of the van der Waals crystal $NbOCl_2$ using photoelectron momentum microscopy. We directly map out an electronic band that is flat throughout the entire Brillouin zone and well isolated from both the conduction and remote valence bands. By utilizing subcycle photoemission spectroscopy [1,2], the dynamics of the flat band under atomically strong mid-infrared light fields are explored. Intriguingly, the carrier field of light induces long-lived collective modes, which are resolved with subcycle precision. These collective modes not only accelerate the electrons but also renormalize the energy of the flat band. We investigate the microscopic mechanisms of these dynamics, highlighting novel possibilities of flat bands in strong-field physics.

[1] Reimann *et al.,* Nature **562**, 396 (2018); [2] Ito *et al.,* Nature **616**, 696 (2023)

O 38.7 Tue 12:00 TRE/MATH

Spin-orbit entangled exciton formation in a 2D correlated semiconductor — •Tania Mukherjee[1,2], Lawson T. Lloyd[1], Alessandro De Vita[1,2], Martin Wolf[1], Laurenz Rettig[1], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany

Excitons govern the magneto-optical properties in spin-ordered 2D materials. $NiPS_3$, a layered antiferromagnetic semiconductor, has recently gained significant attention because of its unconventional excitonic behaviour. Previous literature suggests that excitons are composed of bound electron and holes pairs in a highly spin and orbitally entangled Zhang-Rice-singlet state, resulting in strong coupling with the underlying magnetic ordering.However, the microscopic mechanism that governs the exciton formation remains elusive and unexplored. Using time- and angle-resolved photoemission spectroscopy, we map the electronic structure and the excited state dynamics of $NiPS_3$ across the magnetic phase transition and, for the first time, observe directly the long-lived exciton footprint below the Néel temperature. This paves the way for exploring similarly complex excitonic behavior in other layered correlated materials.

O 38.8 Tue 12:15 TRE/MATH

Understanding resonantly enhanced light-induced superconductivity in K3C60 — •Michael A. Sentef[1,2], Juan I. Aranzadi[1], Paul Fadler[1], and Joseph Tindall[3] — [1]Institute for Theoretical Physics, University of Bremen — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [3]Center for Computational Quantum Physics, The Flatiron Institute, New York

Light-induced superconducting-like responses have been observed in K3C60 when driving with mid-infrared laser pulses [1], with a pronounced 10 THz resonance reported more recently [2]. Here we address the microscopic origin of this resonance. Using numerical calculations on finite clusters for a realistic multi-orbital model of K3C60 we simulate the effect of a periodic drive on the strongly correlated system. We find a sharp enhancement of pairing correlations when the drive frequency is tuned close to 10 THz, in agreement with experiment. The microscopic origin of this enhancement and its potential implications for a light-induced hidden phase [3] will be discussed. Our results thus provide a microscopic explanation for the resonantly enhanced light-induced superconducting-like state in K3C60 and strengthen its interpretation as being closely connected to superconducting pairing rather than to purely optical or nonthermal population effects.

[1] Mitrano et al., Nature 530, 461-464 (2016). [2] Rowe et al., Nature Physics 19, 1821-1826 (2023). [3] Budden et al., Nature Physics 17, 611-618 (2021).

O 39: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces I

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Tuesday 10:30–12:30 Location: WILL/A317

O 39.1 Tue 10:30 WILL/A317

Influence of Tip Apex Modification on Force Microscopy at the Solid-Liquid Interface — •Lucas Andreas Scheibel and Andrea Auer — Institute of Physical Chemistry, Innsbruck, Austria

Recent advances in electrochemical atomic force microscopy (EC-AFM) at the electrified solid-liquid interface using stiff, self-sensing quartz cantilevers (qPlus sensors [1]) have enabled high-resolution imaging of both electrode surfaces and interfacial solvent structures.[2,3] This interfacial region plays a decisive role in determining the performance of electrocatalysts, fuel cells, and electrochemical processes. In this work, we introduce chemically modified Si tips functionalized with charge-neutral hydrophobic or hydrophilic groups to identify how charge buildup at the tip apex influences the ability to resolve solvent structures and distinguish water from ion layering at the Au(111)-electrolyte interfaces across a range of pH values. These strategies provide new insight into atomic-scale contrast mechanisms of liquid AFM and highlight the role of tip-apex chemistry[2] in resolving the interfacial organization of solvent molecules at well-defined electrified solid-liquid interface.

[1] F. J. Giessibl, Rev. Sci. Instrum. 90, 011101 (2019)

[2] A. Auer, F. J. Giessibl, J. Kunze-Liebhäuser, ACS Nano, 19, 9, 8401-8410 (2025)

[3] A. Auer, X. Ding, A. S. Bandarenka, J. Kunze-Liebhäuser, J. Phys. Chem. C, 125, 9, 5020-5028 (2021)

O 39.2 Tue 10:45 WILL/A317

High-Resolution Hydration Layer Mapping: Does a Hydration Structure above Gold Imply a Clean Surface? — •Antonia Köhler[1], Ralf Bechstein[1], Michael Reichling[2], and Angelika Kühnle[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Institut für Physik, Osnabrück, Germany

Solid-liquid interfaces are pivotal in a broad range of fields, including electrochemistry, catalysis and geochemistry. In electrochemistry, the molecular structure of the electrode-water interface is decisive for understanding and improving electrochemical reactions. In this context, the Au(111) surface constitutes a prototypical model system as gold is believed to be a relatively inert and well-characterized sample material. So far, however, little is known about the hydration structure at the Au(111)-water interface at the molecular level. Here, we present atomic force microscopy data on a gold sample carefully cleaned according to standard electrochemistry preparation recipes. Our three-dimensional atomic force microscopy data reveal a vertically ordered hydration structure with layer-to-layer distances of 0.36 nm as expected for water. Strikingly, despite our extensive cleaning efforts (validated by cyclic voltammetry measurements), our two-dimensional data reveal stripe-like structures at the Au(111)-water interface. The dimensions of these structures differ from the well-known herringbone reconstruction of the gold surface, which is why we interpret them as surface contamination. Our work, hence, demonstrates that the presence of a hydration structure is no evidence for a clean gold surface.

Invited Talk O 39.3 Tue 11:00 WILL/A317

Electric double layer of platinum electrodes — •Marc Koper — Leiden University

Platinum is the most studied electrode material in electrocatalysis, but its electric double layer properties are still incompletely understood. Only Pt(111) has a true double layer window, which charges purely electrostatically. However, the properties of the electric double layer of Pt(111) do not follow the classic Gouy-Chapman-Stern theory. Lower coordination sites and facets on platinum are always covered by either hydrogen or hydroxyl adsorbates, which have an important influence on its double layer properties, as will be illustrated by recent results of double-layer measurements on stepped Pt single-crystal electrodes combined with ab initio molecular dynamics simulations and mean-field modeling. In addition, we show that at low electrolyte concentrations, which are often necessary for double-layer measurements, Pt(111) displays strong constant-phase element behavior, which complicates the accurate measurement of its double layer capacitance. The possible origin of this nonideality will be discussed. Finally, the effect of adsorbates on the electric double layer of platinum will be discussed on the basis on hydrogen-covered Pt(111).

O 39.4 Tue 11:30 WILL/A317

Nonequilibrium density-potential functional theoretical approach of electrochemical plasmonics — •Lulu Zhang[1,2], Michael Eikerling[1,2], and Jun Huang[1,2] — [1]Forschungszentrum Juelich GmbH, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany

Electrochemical plasmonics enables in-situ optical probing and modulation of electrochemical interfaces. Experiments have revealed that localized surface plasmon resonance (LSPR) in metal nanoparticle-solution systems is sensitive to surface charge, morphology, electrolyte composition and chemisorption. However, resolving nanoscale interfacial structures from the measured LSPR is rarely practiced; all existing theoretical methods fall in short of simulating the electrochemical plasmonics of nanoparticles under realistic conditions, namely, at a constant electrode potential for a particle with a diameter above 10 nm immersed in an electrolyte solution with a moderate concentration below 100 mM. We are developing a nonequilibrium density-potential functional theoretical (DPFT) approach to enable LSPR simulations under realistic conditions, considering coupled electron-ion-solvent interactions under a terahertz electromagnetic perturbation and on the mesoscale. It ensures constant-potential simulations, scalability to realistic systems, consistency for electronic effects under equilibrium and nonequilibrium, and systematic analysis under working conditions. The fundamental insights into coupled light-electron interactions at electrochemical interfaces are provided, including the extinction spectra, enhanced electric fields and perturbed electron densities.

O 39.5 Tue 11:45 WILL/A317

Insights into the Structure and Dynamics of Co_3O_4–Water Interfaces Using a High-Dimensional Neural Network Potential — •Amir Omranpour[1,2] and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Co_3O_4 is an important catalyst for the oxygen evolution reaction and for the oxidation of organic molecules in the liquid phase. Therefore, understanding the Co_3O_4–water interface is essential for understanding the mechanistic aspects of those catalytic processes. The interactions at such complex interfaces, including hydrogen-bond fluctuations, hydroxylation, proton transfer, and solvent structuring, are inherently reactive atomistic processes that cannot be fully described by continuum or implicit-solvent models. On the other hand, *ab initio* molecular dynamics with explicit solvent remain restricted to only a few picoseconds and a few hundred atoms. In this work, we overcome these limitations by training a high-dimensional neural network potential (HDNNP) on density functional theory data, which enables us to greatly extend the accessible time and length scales. Using this HDNNP, we carry out simulations that uncover the structure, dynamics, and reactivity of Co_3O_4–water interfaces in detail. Our simulations show that different surface terminations give rise to significantly different hydration structures. They also reveal how each termination templates the interfacial water network, affects hydroxylation, and determines the degree of structural ordering at the interface.

Invited Talk O 39.6 Tue 12:00 WILL/A317

First-principles modelling of electrochemical interfaces — •Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm

Electrochemical processes occur at the interface between an electron conductor, the electrode, and an ion conductor, the electrolyte. From an atomistic point of view, the liquid nature of electrolytes requires appropriate statistical averages which can be numerically rather demanding. Still it has become possible to model these interfaces using using first-principles quantum chemical methods [1,2]. In this talk I will present which insights can be gained from such studies, but I will also identify limititations of this approach and discuss how they can be overcome, contrasting the cases of solvated cations and anions [3, 4] as one example.

[1] A. Groß and S. Sakong, Chem. Rev. **122**, 10746 (2022).
[2] A. Groß, Curr. Opin. Electrochem. **40**, 101345 (2023).
[3] F. Gossenberger, F. Juarez, A. Groß, Front. Chem. **8**, 634 (2020).
[4] F. Dominguez-Flores, A. Groß, W. Schmickler, J. Phys. Chem. C **129**, 9179 (2025).

O 40: Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

O 40.1 Tue 14:00 P2

Nonequilibrium phonon dynamics after laser-excitation — Tobias Held, Christopher Seibel, Markus Uehlein, •Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Electron-phonon coupling is a fundamental process governing the energy relaxation dynamics of solids excited by ultrafast laser pulses. While this coupling is often described in terms of an effective electron temperature, recent works have highlighted the important roles of both nonequilibrium electronic distributions and detailed phononic properties.

In this study, we investigate how nonequilibrium electron occupations, phonon stiffness, and wavenumber-resolved coupling collectively shape the energy exchange between electrons and the lattice in metals. We find that deviations from thermal electronic distributions can substantially modify the coupling parameter, challenging the conventional assumption that electron temperature alone determines the coupling strength. We further identify a roughly quadratic scaling of the coupling parameter with phonon stiffness, with high-wavenumber phonon modes consistently dominating the interaction. Finally, we demonstrate that this preferential coupling leads to the emergence of hot phonons near the Brillouin-zone boundary, which in turn induces a collapse of the overall energy transfer rate and significantly delays electron-phonon equilibration.

O 40.2 Tue 14:00 P2

Comparing temperature change during light-matter interaction of thermal and athermal electron systems — •Fabio A. Müller, Tobias Held, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When an ultrashort laser pulse irradiates a metal, the electronic system initially absorbs energy and is driven far from equilibrium. This transient nonequilibrium distribution modifies the light-matter interaction, in part through changes in Pauli blocking, while electron-electron scattering concurrently drives the system toward a hot Fermi-Dirac distribution. Consequently, ultrashort laser pulses of the same fluence but different duration lead to different absorption, even in the linear regime.

Here, we investigate how the capability of an electron ensemble to absorb photons depends on its instantaneous energy distribution. Specifically, we compare the absorption arising from nonequilibrium electron distributions with that of Fermi-Dirac distributions carrying the same energy density. Our results show that, for realistic materials, the relative absorption is highly sensitive to the photon energy, a behavior that can be traced back to distinct features in the electronic density of states.

O 40.3 Tue 14:00 P2

Role of non-thermal electrons on energy dissipation and phase transition in laser excited metals — •Lukas Jonda, Tobias Held, Markus Uehlein, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics andResearch Center OPTIMAS, RPTU Kaiserslautern-Landau

The influence of non-equilibrium electrons on energy dissipation and phase transitions is not well understood. It is known that during femtosecond laser irradiation of a surface, electrons are excited to a state of non-equilibrium in space and energy. These highly excited electrons then transport energy ballistically into the bulk. On a picosecond timescale, electrons transfer energy to the lattice via electron-phonon collisions. If the transferred energy is large enough to reach the melting point, the crystal lattice can undergo a phase transition.

We developed a hybrid model that combines a kinetic Monte Carlo simulation and a two-temperature model. The latter describes diffusive transport as well as electron-phonon equilibration, and the former describes primary electron excitation by the laser pulse, transport of non-equilibrium electrons, and secondary electron generation.

We present results for gold, where the influence of non-equilibrium electrons on energy transport is expected to be significant, due to the long mean free path of its electrons. Finally, we are interested in the influence of non-equilibrium electrons on the melting process.

O 40.4 Tue 14:00 P2

Capturing thermalization through electron-electron scattering with machine learning — •David L. Kaiser, Tobias Held, Christopher Seibel, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Ultrafast excitation of metals by optical laser pulses induces nonequilibrium energy distributions in the electron system. This nonequilibrium gives rise to complex electron-electron scattering processes, which typically restore a Fermi-Dirac distribution on a femtosecond timescale. Accurately modelling the thermalization requires evaluating the full electron-electron collision integral, which is however computationally costly.

In this study, we explore the possibility to use machine learning to emulate the dynamics generated by the full collision integral. Our goal is to significantly accelerate these calculations, enabling efficient simulations of bulk and multilayer systems. This approach opens the door to uncovering new relaxation pathways and predicting the response of complex material systems to ultrafast excitation.

O 40.5 Tue 14:00 P2

Studies of laser ablation of band-gap materials — •Markus Bonifer[1,2], Sebastian T. Weber[1], Nils Cremer[2,3], Gabriel Schaumann[2,3], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Focused Energy GmbH, Im Tiefen See 45, 64293, Darmstadt, Hessen, Germany — [3]Institute of nuclear physics (IKP), Technische Universität Darmstadt, Darmstadt, Germany

We aim to explore laser ablation as a possible approach for creating clean, well-defined microholes in polymers used for laser fusion targets where symmetry and control of surface roughness are important. Because polymers differ widely in their properties, general insights into laser material interaction are sought through modeling of density-dependent excitation in band-gap materials.

The theoretical models used are based on the density-dependent two-temperature model (nTTM) and extended multiple rate equations (EMRE). These calculations are intended to guide experimental studies carried out in collaboration with Focused Energy to identify suitable processing conditions and improve overall feature quality.

O 40.6 Tue 14:00 P2

Thermalization of optically excited electrons in metals: electron-electron scattering dynamics — •Stephanie Roden, Christopher Seibel, Tobias Held, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When a metal is irradiated with a short-pulsed optical laser, the electron distribution is disturbed into a state far from equilibrium. On a femtosecond timescale, the non-thermal electrons thermalize by collisions with each other, which drives the electrons towards a hot Fermi distribution.

In this work, we present a derivation of the full electron-electron Boltzmann collision integral within the random-$\boldsymbol{k}$ approximation. Building on this approach, we trace the temporal evolution of the electron energy distribution in metals after ultrafast excitation. Furthermore, we examine to which extent the resulting dynamics can be captured by the numerically simpler relaxation time approach, applying a constant and an energy-dependent relaxation time derived from Fermi-liquid theory.

We find a better agreement with the latter, while specific features caused by the balance of scattering and reoccupation can only be captured with a full collision integral.

O 40.7 Tue 14:00 P2

Time-resolved PEEM and μARPES using a 100 kHz ToF momentum microscope — •Isabella Alexandra Hofmeister[1,2], Michael Herb[1,2], Maria Federl[1], Franz Seitz[1], and Isabella Gierz[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy - RUN, Regensburg, Germany

Momentum microscopy provides energy-resolved imaging in real and reciprocal space with < 100 meV resolution, combining PEEM

($\Delta x < 40\,\mathrm{nm}$ lateral resolution) and μARPES ($\Delta k < 0.02\,\text{Å}^{-1}$) capabilities. We implemented an ultrafast setup with a time-of-flight momentum microscope and a 100 kHz laser system delivering 6 eV probe pulses and pump pulses tunable from the mid-infrared to visible range. Procedures for converting time-of-flight to kinetic energy and for establishing spatial and temporal pump-probe overlap are discussed. Proof-of-principle time-resolved PEEM and μARPES experiments on the topological insulator Bi$_2$Se$_3$ demonstrate femtosecond-resolved carrier dynamics with high spatial and momentum precision.

O 40.8 Tue 14:00 P2

First steps with a qPlus-based MIR AFM — •Furkan Özyigit, Lukas Böhm, Leonie Weiss, Jay Weymouth, Rupert Huber, and Franz Giessibl — University of Regensburg, 93053 Regensburg

We report initial progress in an ultrafast non-contact atomic force microscope/scanning tunneling microscope (NC-AFM/STM) platform based on qPlus sensors, integrated with a CEP-stabilized mid-infrared (MIR) pump-probe system and tunable optical parametric amplifier (OPA) for versatile excitation. In first experiments, we successfully induced transient tunneling currents on Cu(111) using MIR pulses, demonstrating precise control of ultrafast electronic excitation at the atomic scale via laser-coupled tunneling. While the tunneling cur- rent reflects the ultrafast electronic excitation dynamics, the qPlus sensor permits complementary force detection to monitor subsequent structural or electrostatic interaction changes, such as those resulting from induced charge redistribution or lattice relaxation. This enables simultaneous probing of electronic and mechanical dynamics with femtosecond time and sub-nanometer spatial resolution. Beyond investigations of transient electrostatic forces, this versatile system facilitates a broad class of ultrafast nanoscale experiments, including scattering-type scanning near-field optical microscopy (s-SNOM) for imaging carrier and phase dynamics, time-resolved tip-enhanced spectroscopy for molecular states, and pump-probe tunneling spectroscopy.

O 40.9 Tue 14:00 P2

Image potential states of oxide quasicrytals — •Barbara Drobinski[1], Friederike Wührl[1], Richard Kraska[1], Konrad Gillmeister[1], Stefan Förster[1], Cheng-Tien Chiang[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of Atomic and Molecular Sciences , Academia Sinica, Taipeh, Taiwan

Quasicrystals are aperiodically ordered materials that lack translational symmetry. Their aperiodic potentials give rise to an infinitely dense set of Fourier components, which can induce gaps and mini-gaps in the electronic band structure. Here, we investigate this phenomenon for nearly free-electron-like image-potential surface states, where electrons propagate in front of the surface while experiencing the aperiodic potential. Using momentum-resolved two-photon photoemission, we determine both the electronic dispersion and relaxation dynamics of oxide quasicrystals (OQCs) based on Ba-Ti-O/Pt(111) [1] and Eu-Ti-O/Pt(111). The latter is obtained via Eu decoration of a Ti$_2$O$_3$ honeycomb precursor [2]. In both systems, we observe n=1 and n=2 image potential states, located 340 meV (360 meV) and 150 meV (190 meV) below the vacuum level for Ba-Ti-O (Eu-Ti-O), respectively. The states exhibit parabolic dispersions without apparent gap openings. We discuss the momentum-dependent electron lifetimes in the context of possible mini-gaps in the underlying aperiodic potential.
[1] S. Förster *et al.*, Nature **502**, 215 (2013)
[2] M. Haller *et al.*, http://arxiv.org/abs/2510.11426

O 40.10 Tue 14:00 P2

Ultrafast Electron Diffraction Study of Lattice Dynamics in Elemental Chromium — •Justus Richter[1,2], Victoria Taylor[1], Hyein Jung[1,2], Ralph Ernstofer[1,2], and Yoav William Windsor[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institut für Physik und Astronomie, Technische Universität Berlin

Femtosecond electron diffraction (FED) allows to quantitively study ultrafast atomic motion. Here we use FED to study photoinduced atomic motion in Cr. We saw that measurements taken above- and below T_N exhibit qualitatively different responses from the lattice, hinting to the effect of the spin-induced periodic lattice distortion within the antiferromagnetic Cr phase, though further investigation is required. A two temperature model (TTM) was used to model the energy flow between the electronic and lattice subsystems by which we extract an estimate for the electron-phonon coupling constant $G_{ep} = (4.8 \pm 0.6) \times 10^{17}$ Jm^{-3}K^{-1}, which fits into the wide range of values reported in literature. Finally, we measured Cr side-by-side with Pt and demonstrate qualitative differences in their temporal responses, including a significantly faster thermalization of the Cr lattice and differences in the shape of their temporal response.

O 40.11 Tue 14:00 P2

Ultrafast electron dynamics in the valence-fluctuating intermetallic EuIr$_2$Si$_2$ — •Abeer Arora[1], Túlio de Castro[1], Amine Wahada[1], Lawson Lloyd[1], Tommaso Pincelli[2], Kristin Kliemt[3], Cornelius Krellner[3], Denis V. Vyalikh[4,5], Yoav Will Windsor[2], Martin Wolf[1], Ralph Ernstorfer[1,2], and Laurenz Rettig[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institut für Physik und Astronomie, TU Berlin, Germany — [3]Physikalisches Institut, Göthe-Universität Frankfurt, Germany — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

EuIr$_2$Si$_2$ is a valence-fluctuating intermetallic compound that, despite its non-magnetic bulk, develops 2D ferromagnetic order below 48 K in the topmost Eu layer due to a stable Eu^{2+} configuration. Its heavy Ir ions generate strong Rashba spin-orbit coupling, which interacts with magnetic exchange and influences the surface electronic states. Probing the non-equilibrium dynamics of the 2D electrons in the Si-Ir-Si surface layer offers a direct way to study the coupling of the spin-orbit and surface magnetic interaction. Using femtosecond XUV time- and angle-resolved photoemission spectroscopy, we investigate how the surface states evolve following photoexcitation with a 1.55 eV pulsed laser. Our preliminary results show an ultrafast quenching of the surface-state splitting, which we discuss in terms of demagnetization of the Eu 4f moments and modified spin-orbit coupling.

O 40.12 Tue 14:00 P2

Ultrafast STEM locked to GHz sample excitation — •Andreas Wendeln[1], Alexander Schröder[1], Sakal Singla[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Ultrafast transmission electron microscopy (UTEM) has been an established method for investigating nanoscale dynamics for several years, combining the nanometer spatial resolution of TEM with the femtosecond temporal resolution of a pump-probe approach. In recent years, there have been numerous advances in the development of new femtosecond electron sources, such as laser-driven Schottky [1] or cold-field emitters [2]. A combination of these sources with advanced electron optical elements, such as a probe aberration corrector, is expected to deliver even smaller electron spot sizes and to increase the available pulsed current but was not yet demonstrated. Here, we present a measurement scheme for ultrafast STEM with a focus on magnetic imaging, utilizing an aberration corrector and a laser-driven cold-field emitter. In initial measurements using a continuous photoelectron beam, the measurement method is characterized regarding experimental parameters, such as probe currents, focal spot sizes, and stability. Subsequently, we report the locking of femtosecond electron pulse train at repetition rates between 100 kHz up to 80 MHz to GHz radiofrequency currents which we aim to employ for DPC and ptychography imaging schemes of current-driven magnetic dynamics. [1] Feist et al., Ultramicroscopy, 2017. [2] Schröder et al., Ultramicroscopy, 2025.

O 40.13 Tue 14:00 P2

Probing Ultrafast Structural Dynamics in Multilayer Graphene Using ULEEM — •Simon Briesenick[1,2,4], Johannes Otto[1,2,4], Leon Brauns[1,2], Philip Schädlich[3], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [4]authors contributed equally

Multilayers of graphene (MLG) exhibit electronic and structural properties that vary strongly with, e.g., layer number and stacking order, making MLG a suitable model platform for studying ultrafast phenomena in two-dimensional materials [1]. We investigate the behavior of MLG after excitation with ultrashort light pulses using our newly developed ultrafast low-energy electron microscope (ULEEM) [2]. The instrument allows for the investigation of surface structural dynamics with sub-picosecond and nanometer spatial resolution, utilizing low-energy ($\leq$ 100 eV) ultrashort probe electron pulses. We present first data on the light-induced Debye-Waller effect in MLG, demonstrating the potential of ULEEM studies for resolving ultrafast structural behavior in MLG.

[1] K. V. Emtsev, et al. Phys Rev B. 77, 155303 (2008) [2] J. Otto et al. (in preparation)

O 40.14 Tue 14:00 P2

Hot-electron dynamics in moiré structures studied with resonant scanning tunneling spectroscopy — •Martin Lülff, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

To study hot-electron dynamics in Gr-metal heterostructures, image-potential states (IPSs) serve as ideal model system. While their energies are known to be highly sensitive to the respective Gr-metal distance variation within the moiré unit cell [1, 2], recent two-photon photoemission experiments suggest moiré-site dependent lifetimes [3].

Here, utilizing the high spatial resolution of resonant scanning tunneling microscopy (STM) and spectroscopy (STS) we study the moiré-site dependent IPSs' lifetimes for highly corrugated Gr/Fe/Ir(111) and Gr/Ir(111), respectively. Comparing these resonant STS data with those recorded on bare Fe/Ir(111) and Ir(111), respectively, enables the influence of the varying Gr-metal distance on the lifetimes to be distinguished from that of the underlying metal substrate. We analyse the IPSs' lifetimes for a Stark shift in their energies by applying various electric field strengths in current-dependent STS series, and discuss the results in terms of their resulting energetic positions with respect to the underlying unoccupied electronic band structure. Our work contributes to an in-depth understanding of electron transfer processes at Gr-metal interfaces.

[1] M. Bazarnik and A. Schlenhoff, ACS Nano **19**, 25812 (2025)
[2] N. Armbrust *et al.*, New J. Phys. **17**, 103043 (2015)
[3] N. Armbrust *et al.*, Phys. Rev. Lett. **108**, 056801 (2012)

O 40.15 Tue 14:00 P2

Photo-induced electron pressure drives THz phonon in Platinum-Copper superlattice — •Jan-Etienne Pudell[1], Maximilian Mattern[2,3], Marc Herzog[2], Alexander von Reppert[2], Daniel Schick[3], Chandan Singh[4], Peter M. Oppeneer[4], Michel Hehn[5], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Roman Shayduk[1], Wonhyuk Jo[1], Johannes Möller[1], Jörg Hallmann[1], James Wrigley[1], Matias Bargheer[2,6], and Anders Madsen[1] — [1]European XFEL — [2]University Potsdam — [3]MBI, Berlin — [4]Uppsala University — [5]IJL, Université Lorraine — [6]HZB Berlin

Using ultrafast X-ray diffraction (UXRD) at the MID end-station at the European XFEL, we investigate the ultrafast lattice dynamics of metal-metal superlattice (SL) with few atomic layers of Pt and Cu upon femtosecond photoexcitation. Our results reveal that the absorbed optical energy is rapidly localizes within the Pt layers, driving the excitation of a coherent artificial THz phonon mode defined by the superlattice period. The signal's amplitude and phase modulation of the SL Bragg peaks induced by the lattice excitation i.e. the artificial THz phonon, are predominantly driven by electron pressure within the first picosecond. This response is faster than the Debye-Waller effect, which is limited by the electron-phonon coupling time.

O 40.16 Tue 14:00 P2

Experimental realization of an interferometric XUV-trARPES experiment with phase-stabilized IR pulses — •Antonius Naujok[1], Gregor Zinke[1,2], Franz Spartz[1], Sebastian Hedwig[1], Tobias Eul[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Re search Center OPTIMAS, RPTU University Kaiserslautern- Landau, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, 86159 Augsburg

Layered 2D van der Waals materials, such as TMDCs, have been extensively studied for their optical properties and coherent responses. However, exploring coherent excitations and dephasing processes in such materials using time-resolved ARPES is challenging because the key points of the materials' band structure cannot be accessed using phase-stabilized pulses in the visible regime, as has been done in most experiments thus far [1]. To overcome this limitation, we introduce a modified version of coherent multidimensional spectroscopy. This new method is based on time-resolved ARPES and utilizes a pair of phase-stabilized femtosecond infrared (fs-IR) pulses in combination with femtosecond XUV pulses for photoionization. We demonstrate the feasibility of our approach by focusing on the A-exciton excitation and the subsequent carrier dynamics in WSe_2. Through temporal Fourier-analysis of the entire ARPES spectrum, we're able to resolve distinct frequency components within characteristic features of the WSe_2 electronic band structure. [1] M. Aeschlimann et al., Phys. Rev. B. 105, 205415 (2022)

O 40.17 Tue 14:00 P2

Implementation of white light continuum probing for pump-probe spectroscopy — •Joris Wicker, Tim Titze, Maximilian Staabs, Jacob Kutzner, Stefan Mathias, and Daniel Steil — University of Göttingen, 1. Institute of Physics, Göttingen, Germany

We integrated a white-light continuum (WLC) probe together with a prism spectrometer in a conventional two-color femtosecond pump-probe setup. Further, we developed a custom measurement program using Microsoft's .NET Framework and Python, enabling instrument control, automated measurement sequences, and preliminary data analysis. To test the modified setup and software, we investigated the transient evolution of the reflectivity in metallic thin film systems and perovskite oxides using 1030 nm pumping. Spectrally and temporally resolved reflectivity variations were observed, confirming the proper functionality of the system. Furthermore, the stability of the WLC source was characterized. Possible future improvements include integrating a Wollaston prism to enable spectrally and time-resolved magneto-optical Kerr effect (MOKE) measurements.

O 40.18 Tue 14:00 P2

Investigation of the light-dressed bandstructure of graphene — •Lina Segerer[1], Marco Merboldt[1], Mattis Langendorf[1], Paul Werner[1], Jan Philipp Bange[1], Junde Liu[1], Wiebke Bennecke[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Philipps-Universität Marburg, Germany

Time-periodic driving of solids with strong laser fields enables optical control of material properties. Photon-driven systems not only exhibit replicas of their equilibrium band structure, known as Floquet-Bloch states, but can undergo non-trivial topological phase transitions when excited with circularly polarized light. Recent advances in angle-resolved photoemission spectroscopy (ARPES) have shown that Floquet-Bloch states can be generated in graphene using linear polarized laser pulses [1,2]. However, the oblique incidence angle of the pump pulse so far has limited the realization of a purely circularly polarized light field. In this study, we overcome this challenge by integrating an extra beam path in our ultrafast momentum microscopy (MM) setup enabling backside normal-incidence excitation with linearly and strictly circularly polarized IR pump pulses. We observe light-induced Floquet-Bloch states and investigate the polarization dependence of Floquet-Volkov interference as well as modifications in the light-dressed band structure of epitaxial graphene.

[1] M. Merboldt *et al.*, Nat. Phys. **21**, 1093 (2025).
[2] D. Choi *et al.*, Nat. Phys. **21**, 1100 (2025).

O 40.19 Tue 14:00 P2

Table-top 3D ultrafast momentum microscopy with a time-preserving EUV-monochromator — •Lennart Weinhagen[1], Wiebke Bennecke[1], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Bent van Wingerden[1], Thi Lan Dinh[2], Fabio Frasetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russel Luke[2], Stefan Mathias[1], and G.S. Matthijs Jansen[1] — [1]1st Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, Padova, Italy

Photoemission momentum microscopy with tunable probe-photon energy gives unique access to electronic and molecular structures, enabling Fermi-surface imaging, photoemission electron diffraction (PED) and 3D orbital tomography (3D-POT). However, such measurements have largely relied on synchrotron radiation, thus limiting their use in femtosecond-resolved experiments. Here, we present a table-top EUV source with a time-preserving monochromator driven by a 1030 nm femtosecond laser, using an off-plane grating at grazing incidence to reduce spatial chirp. Integrated into our time-resolved momentum microscope [1], it delivers femtosecond, photon-energy-tunable EUV probe pulses. Demonstrated on PTCDA/Ag(110), the setup enabled full 3D reconstruction of the frontier orbitals highlighting the potential of laboratory-scale, energy-selective momentum microscopy [2].

[1] Schmitt *et al.*, Nature 608, 499-503 (2022).
[2] Bennecke *et al.*, arXiv:2502.18269 (2025).

O 40.20 Tue 14:00 P2

Multimode momentum microscopy of cleaved 1T-TaS_2 crys-

tals — ●Bent van Wingerden[1], Olena Tkach[2], Hashima Marukara[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Marcel Reutzel[3], Junde Liu[1], Gerd Schönhense[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Johannes Gutenberg-Universität Mainz, Germany — [3]Philipps-Universität Marburg, Germany

Ultrafast momentum microscopy has evolved as one of the most powerful tools to study non-equilibrium electronic structure dynamics of 2D quantum materials [1]. However, the large electric field strength generated by the immersion lens limits its versatility in terms of sample systems. One critical issue is related to vacuum-cleaved van-der-Waals-crystals that often show microscopic protrusions, which are prone to field-induced electron emission and flashovers, both of which can destroy the sample itself as well as the microscope's electronics. In our work, we test the momentum imaging capabilities of a newly designed multimode momentum microscope [2,3] in combination with an EUV table-top HHG source. Using vacuum-cleaved bulk crystals of $1T$-TaS$_2$, we show that operating in modes of reduced electric field strength at the sample position suppresses field emission, while still preserving the field-of-view and imaging quality. We carry out detailed comparisons of different operating modes with the new lens system.
[1] Reutzel, Jansen, Mathias, *Adv. in Phys. X* 9, 2378722 (2024).
[2] Tkach & Schönhense, *Ultramicroscopy* 276, 114167 (2025).
[3] Tkach et al., arXiv:2401.10084 (2024).

O 40.21 Tue 14:00 P2

Towards time-resolved momentum microscopy of plasmon excited quantum materials — ●Mattis Langendorf[1], Lina Segerer[1], Paul Werner[1], Marco Merboldt[1], Jonas Pöhls[1], Tobias Meyer[1], Daniel Steil[1], Junde Liu[1], Jan Philipp Bange[1], Wiebke Bennecke[1], G. S. Matthijs Jansen[1], R. Thomas Weitz[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Philipps-Universität Marburg, Germany

For the realization of Floquet*Bloch engineering as well as for the study of formation and propagation of excitons in two-dimensional quantum materials using time- and angle-resolved photoemission spectroscopy (ARPES), a highly localized excitation on a micron scale seems ideal [1]. However, achieving such spatial confinement poses a significant experimental challenge. Surface plasmon polaritons (SPPs) offer a promising solution, as these collective charge-carrier oscillations enable strong electromagnetic field localization and can therefore provide the required tightly focused excitation conditions [2]. In combination with femtosecond momentum microscopy that enables spatiotemporal access to electron and exciton dynamics [3], we investigate the concept of exploiting SPPs as a driving field to excite quantum materials.
[1] Merboldt *et al.*, Nat. Phys. **21**, 1093*1099 (2025).
[2] Dreher *et al.*, Nanophotonics **11**, 3687-3694 (2022).
[3] Reutzel, Jansen, Mathias, Adv. in Phys. X **9**, 2378722 (2024).

O 41: Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

O 41.1 Tue 14:00 P2

Manipulation of topological surface states by switchable molecules. — Lukas Staiger[1], Jannis Lessmeister[1], ●Ralf Hemm[1], Juliusz Wolny[1], Volker Schünemann[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Three-dimensional topological insulators host spin-momentum-locked surface states protected by time-reversal symmetry, giving them potential for spintronic devices. Controlling these states remains challenging but is crucial for opening gaps, shifting the Dirac point and tailoring spin textures for applications. In our work, we utilize a monolayer of the spin-crossover complex Fe(phen)$_2$(SCN)$_2$ on the topological insulator Bi$_2$Se$_3$ to break the time-reversal symmetry of the substrate. Employing angle-resolved photoemission spectroscopy, we trace the evolution of the electronic structure as a function of molecular coverage and temperature. Despite a conspicuous energy shift and modified dispersion, there is no clear evidence for a band gap opening after deposition of a molecular monolayer. Concurrently, additional spectral weight from molecular orbitals emerges, and thermally and optically driven spin-crossover transitions in the Fe(phen)$_2$(SCN)$_2$ layer induce changes in the Dirac-point energy and spectral weight. Our findings demonstrate that a spin-crossover overlayer can quantitatively alter the dispersion of topological surface states, while allowing them to exist due to strong interactions between molecules and surfaces.

O 41.2 Tue 14:00 P2

Deciphering the complex surface of the topological phase in the polar semiconductor BiTeI — ●Adrian Weindl, Christoph Setescak, and Franz J. Giessibl — Faculty of Physics, University of Regensburg, D-93053 Regensburg, Germany

BiTeI is a semiconductor consisting of polar layers that can form Rashba spin-split p-n junctions on its surface due to stacking faults. It has been shown that gentle annealing can transform the surface of BiTeI into a topological insulator with spin-polarized surface modes exhibiting linear dispersion. Previous LEED and RHEED measurements revealed that the surface undergoes a structural change from a non-centrosymmetric triple-layer structure to a quintuple-layer structure. However, the exact surface structure remains elusive. Using scanning tunneling microscopy, atomic force microscopy, and Kelvin probe force spectroscopy we study the surface before and after annealing with atomic resolution. We show that the annealing results in different surface phases that are highly sensitive to the annealing temperature: a chemically homgeneous phase at around 240°C and a inhomogeneous phase with strong charge disorder at 250°C. We determine the termination of each phase and confirm that the surface exhibits the signature of a topological surface state even in the strongly disordered phase.

O 41.3 Tue 14:00 P2

THz-driven nonlinear dynamics studied with high-power THz sources — Atiqa Arshad[1,2], Jan-C Deinert[2], Igor Ilyakov[2], Andreas Gebauer[2], Anjan Kumar N M[1], and ●Stefan Kaiser[1] — [1]TU Dresden,Germany — [2]HZDR, Dresden,Germany

THz pump-photoelectron spectroscopy (ARPES) probe is currently being implemented at the THz facility TELBE at Helmholtz-Zentrum Dresden-Rossendorf. This unique combination of high-field terahertz excitation and tr-ARPES probe will enable groundbreaking experiments on solid surfaces and interfaces. To this aim we have set up a high-repetition rate THz source driven by a 180 W laser source yielding $>$ 50 mW THz output power. We report on the THz generation and characterization scheme as well as on first experiments. A highly promising material class to be studied with these light sources is BiTeI, a dual topological insulator that exhibits two different types of surface states on different interfaces. We present our study on the complex nonlinear dynamics, in particular THz harmonic generation in these compounds.

O 41.4 Tue 14:00 P2

The quasi one-dimensional van der Waals material α-Bi$_4$Br$_4$ — ●Jonathan K. Hofmann[1,2], Serhii Kovalchuk[1,3], Mingqian Zheng[4], Yuqi Zhang[4], Vasily Cherepanov[1], Timofey Balashov[1], Jin-Jian Zhou[4], Zhiwei Wang[4], Yugui Yao[4], Irek Morawski[3], F. Stefan Tautz[1,2], Felix Lüpke[1,5], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Institute of Experimental Physics, University of Wrocław, Poland — [4]Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement, Beijing Institute of Technology, China — [5]II. Physikalisches Institut, Universität zu Köln, Germany

α-Bi$_4$Br$_4$ is a quasi-one-dimensional material: covalently bonded Bi$_4$Br$_4$ chains are arranged in parallel, side-by-side and layer-by-layer, with van der Waals gaps in between. Bulk α-Bi$_4$Br$_4$ is higher-order topological insulator. At step edges on the (001) surface, quantum spin Hall (QSH) edge states are present. Using a scanning tunneling microscope (STM), we observe a significant shift of the chains, relative to each other, which we attribute to shear stress. Scanning tunneling spectroscopy reveals that the edge states are robust against the strain. Density functional theory confirms that a strained monolayer of $\mathrm{Bi_4Br_4}$ is a QSH insulator with $\mathbb{Z}_2 = 1$. Furthermore, we use a four-tip STM to analyze the electrical transport of α-$\mathrm{Bi_4Br_4}$ *in situ*.

O 42: Electronic structure of surfaces: Spectroscopy, surface states – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 42.1 Tue 14:00 P2

Plasmonic lenses for nano-spectroscopy of Van der Waals materials — •Natalie Lehmann[1], David Huber[2], Daiyu Geng[1], Jiabao Yang[1], Stuart Parkin[1], Wolf Widdra[2], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), DE — [2]Martin-Luther-University Halle-Wittenberg, Halle (Saale), DE

Surface plasmon polaritons excited at the edge of Archimedean spirals carved into a gold (111) surface can be focused to a sub-micrometer spot at the spiral center [1, 2]. We aim to use this nano-focused electric field to spectroscopically investigate 2D materials, which are often only a few micrometers in size. Here we present our measurements on gold/graphene samples. Notably, the plasmonic focus remains intact, and the gold surface is effectively cleaned by the graphene; even without sputtering the gold, its characteristic surface state is observed. Furthermore, the measured k-space spectrum shows replicas of the sp orbitals above the Fermi edge, reflecting the dynamics of an excited electron system. We propose that the laser pulse is pumping the system while the plasmon is probing the excited states. These findings demonstrate the feasibility of ultrafast pumped, nano-focused spectroscopy using a single micrometer-sized laser beam.

O 42.2 Tue 14:00 P2

Hydrogen Plasma Cleaning of $\mathrm{Fe_3Sn_2}$ single crystals for surface-sensitive measurements — •Felix Müller[1], Lu Lyu[1], Lilian Prodan[1], Jannis Lessmeister[2], Tobias Eul[1], Martin Aeschlimann[2], István Kézsmárki[1], and Benjamin Stadtmüller[1] — [1]University of Augsburg — [2]RPTU University Kaiserslautern-Landau

Preparing clean and well-defined surfaces is essential for high-resolution photoemission spectroscopy (PES) and other similarly surface-sensitive studies. Typical preparation methods to realize high-quality surfaces include in situ cleaving under ultrahigh vacuum (UHV) conditions. However, this method cannot be universally applied to all crystal structures. Alternative approaches can rely, for instance, on $\mathrm{H_2}$-based plasma cleaning using $\mathrm{H_2}$ sources integrated into a UHV system. Here, we investigate the effectiveness of this method in preparing $\mathrm{Fe_3Sn_2}$ surfaces for spectroscopy and discuss its potential as a general cleaning technique for other topological bulk materials.

We show that the hydrogen plasma efficiently removes common surface contaminants, particularly oxygen and carbon, while preserving the intrinsic surface structure. This enables the observation of sharp spectroscopic features over the whole energy range and significantly enhances the signal quality of subsequent PES measurements. Our results show that plasma can be a simple and reproducible method for achieving contamination-free surfaces of topological bulk materials for surface-sensitive spectroscopy applications.

O 42.3 Tue 14:00 P2

WTe2: a Cool Look at 330 mK — •Rian A.M. Ligthart, Kevin Hauser, Alexander LaFleur, Gleb Neplyakh, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

As silicon-based electronics reach their size limit, two-dimensional (2D) materials, particularly Transition Metal Dichalcogenides (TMDs), emerge as promising alternatives to enhance efficiency at the same length scale. Among them, WTe2 stands out due to its unique properties including topological states, Weyl semimetal character and graphene-like high electron mobility.

We investigate cleaved bulk WTe2 using a Scanning Tunneling Microscope at 330 mK. With scanning tunneling spectroscopy, the electronic properties and their dependence on vector magnetic fields are studied on the surface of bulk WTe*, as well as at step edges and twin domain boundaries. We scrutinize the topological nature of the edge states and observe a reduced density of states around zero bias in bulk WTe2.

O 42.4 Tue 14:00 P2

Chiral-Induced Spin Selectivity in Thia-Bridged Triarylamine Hetero[4]helicenes SAMs: Structural Insights from XPS and NEXAFS — •Yichen Jin[1], Jan Böhnke[1], Lapo Querci[2], Niccolò Giaconi[2], Cornelius Gahl[1], Dominik Stemer[3], Roberta Sessoli[2], Matteo Mannini[2], and Martin Weinelt[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]University of Florence, Via della Lastruccia 3-13, Sesto Fiorentino 50019, Italy — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Helicene enantiomers act as efficient spin filters when assembled on metallic surfaces, making them promising candidates for organic spintronic applications. Previous magnetic conductive AFM studies reported spin polarizations of up to ~60% through the respective chiral enantiomers of Thia-Bridged Triarylamine Hetero[4]helicenes (HelSAc) self-assembled monolayers (SAMs) ascribed to the chirality-induced spin selectivity (CISS) effect. To understand the structural origins underlying this behavior, we investigated HelSAc SAMs on Au(111) using XPS and NEXAFS. Angle-dependent XP spectra of sulphur 2p reveal three chemically distinct components assigned to S*C, S*Au, and atomic sulfur. NEXAFS shows pronounced polarization dependences of the σ^* and π^* resonances, demonstrating the parallel alignment of the HelSAc to the Au surface. Together, these results establish a well-defined chemical and structural picture of HelSAc SAMs, providing the essential foundation for interpreting spin-dependent photoelectron spectroscopy and understanding the CISS effect in this chiral system.

O 42.5 Tue 14:00 P2

Structure and Electronic Properties of (Bi, Pb) Atom Layer Structures studied by ARPES and STM — •Lars Konermann[1], Wen Si[2], Hiroko Abe[1], Masaki Imamura[3], Masahiro Haze[2], Kazutoshi Takahashi[3], Yukio Hasegawa[2], and Akari Takayama[1,4] — [1]Waseda Univ., Shinjuku, Japan — [2]ISSP, Univ. of Tokyo, Kashiwa, Japan — [3]SL Center, Saga Univ., Tosu, Japan — [4]IMRAM, Tohoku Univ., Sendai, Japan

In Single-atom layer (SAL) structures comprised of heavy elements on semiconductor substrates, spin-split electronic states occur due to strong spin-orbit interactions and the breaking of the spatial inversion symmetry, known as the Rashba effect. For (Bi, Pb) on Si or Ge, spin-splitting electronic bands have been demonstrated both theoretically and experimentally. Furthermore, the possibility of a superconducting transition is anticipated suggesting spin-triplet superconductivity. Albeit, experimental confirmation has not yet been obtained.

We investigated the atomic and electronic structures of (Bi, Pb)/Si(111) and Ge(111) structures using cryogenic scanning tunneling microscopy (STM) and spectroscopy (STS), as well as angle-resolved photoemission spectroscopy (ARPES) with synchrotron radiation. A series of experiments was conducted to evaluate the sample: observation of the periodic atomic arrangement, determination of the Pb/Bi composition ratio, detailed band dispersion, and investigation of the electronic states at ultra-low temperatures.

In this presentation, we will present these experimental results and discuss the potential for superconductivity with the Rashba effect.

O 42.6 Tue 14:00 P2

Line-Moiré Phases of an Epitaxial Honeycomb Monolayer AgTe/Ag(111) — •Romana Ganser — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg

Moiré heterostructures offer a versatile platform for engineering electronic band structures by precise control over long-range superlattice potentials that particularly give rise to emergent phenomena [1]. Here, we present angle-resolved photoemission spectroscopy (ARPES) measurements on a highly tunable one-dimensional (1D) epitaxial moiré heterostructure. We show that the electronic structure is strongly altered by the moiré superlattice hosting replica bands and sizable hybridization gaps. From our experimental data, we can trace back to the local, spatially-varying interlayer coupling, shaping the moiré potential. The latter leads to a 1D confinement of the electrons and, interestingly, also gives rise to Dirac nodal lines, which are robustly protected by the superlattice symmetry.

[1] Balents, L. et al. Nat. Phys. 16, 725-733 (2020).

O 42.7 Tue 14:00 P2

Realization of an Acoustic Kagome lattice — •Louis Müller[1,3], Noah Endres[1,3], Begmuhammet Geldiev[1,3], Simon Widmann[2,3], Maximilian Ünzelmann[1,3], and Friedrich Reinert[1,3] — [1]Exp. Physik VII, JMU Würzburg, Germany — [2]Technische Physik, JMU Würzburg, Germany — [3]Würzburg-Dresden Cluster of Excellence ctd.qmat

Hosting Dirac cones, flat bands, and saddle points in their band structure, Kagome materials have recently attracted great attention. We realize an acoustic Kagome lattice using 3D-printed resonators, enabling direct measurement of amplitude and phase to reconstruct wave functions and extract the band structure. Our experiment resolves the flat band, identifies the sublattice character of the van-Hove singularities, and clearly reproduces the Dirac cones in good agreement with tight-binding calculations. This platform provides a highly flexible and intuitive way to investigate lattice-driven effects that are difficult to isolate in electronic Kagome systems. Finally, we compare this data to angle-resolved photoemission spectroscopy measurements on a prototypical Kagome superconductor.

O 42.8 Tue 14:00 P2

Excitation of spin-polarized electrons by Deep-UV Pulses with Orbital Angular Momentum from Au(111) and Cu(111) — •Ruwen Quenter, Paul valerian Möllers, and Helmut Zacharias — Center for Soft Nanoscience (SoN), University of Münster, Busso-Peus-Str. 10, 48149 Münster, Germany

Photoemission can, depending on the substrate and the circularly polarization of the light, result in a longitudinal spin polarisation of the excited electrons. The angular momentum of the light influences the final state determined by the selection rules in a way that corresponds to a specific total angular momentum. Spin-orbit interactions cause an energetical separation of states with different total angular momenta, resulting in a spin imbalance of the excited electrons. This can be measured by e.g. Mott scattering. Orbital angular momentum light has a helical wavefront that carries its orbital angular momentum as a degree of freedom wich may have an influence on the electron orbital angular momentum in the electron excitation process. Spin-resolved photoemission measurements could determine if this influence could result in a changed photoelectron spin polarization. We present preliminary results from measurements on Au(111) and Cu(111).

O 42.9 Tue 14:00 P2

Wavefunction confinement of deeply buried As δ-layers in Si(001) measured with hard and soft X-ray angle-resolved photoemission spectroscopy — •Emily C. McFarlane[1], Enrico G. Della Valle[2], Procopios C. Constantinou[2], Taylor J. Z. Stock[3], Kieran Spruce[3], Christoph Schlueter[4], Sergii Chernov[4], Thiago R. F. Peixoto[4], Moritz Hoesch[4], Gerd Schönhense[5], Hans-Joachim Elmers[5], Vladimir N. Strocov[2], Neil J. Curson[3], Steven R. Schofield[3], and Niels B. M. Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), DE — [2]Paul Scherrer Institute, Villigen PSI, CH — [3]London Centre for Nanotechnology, University College London, London, UK — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, DE — [5]Johannes Gutenberg University, Mainz, DE

Vertically confined regions of high concentration dopants in silicon, so-called “δ-layers”, are potential building blocks of future quantum devices. A momentum-resolved understanding of the wavefunction confinement of the electrons in such systems is required for their future development, which so far has been limited to shallow samples. Here we present both hard and soft X-ray photoelectron spectroscopy studies of shallow (∼3nm) and deeper (∼7nm) buried As δ-layers measured with a momentum microscope and hemisphere at PETRA-III and the SLS. We find that the deeper buried sample has smaller electron confinement than the shallower δ-layer, and different quantum well states are located at different depths of the sample. In contrast, in shallow δ-layers all quantum well states are located near the surface.

O 43: Scanning probe microscopy: light matter interaction at atomic scales – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 43.1 Tue 14:00 P2

Modelling the near-field enhancement for tip-enhanced photoluminescence on non-conductive layers — •Jinhui Guo and Laerte Patera — Department of Physical Chemistry, University of Innsbruck, 6020 Innsbruck, Austria

While scanning tunnelling microscopy (STM)-based tip-enhanced photoluminescence (TEPL) has been demonstrated for molecules adsorbed on 2-3 monolayers (ML) of NaCl/Ag(111) [1], nonradiative quenching due to charge tunnelling through the insulating layer is expected to affect the exciton lifetime. Employing sufficiently thick insulating layers ($>$ 14 ML) strongly suppresses electron tunnelling [2], potentially preserving the photoexcited state. However, such thick insulating layers are incompatible with STM operation, making atomic force microscopy (AFM) an ideal choice. To elucidate the field enhancement in AFM-based TEPL experiments, we performed three-dimensional finite element method (3D-FEM) simulations [3] for various AFM Cu tip geometries and Cu substrates with and without NaCl layers up to 20 ML. Our results indicate that below the tip, a pronounced electric field enhancement in the plane parallel to the sample surface ($E_{/\!/}$) persists even on a 20 ML-thick NaCl layer. This effect arises mainly from the reduced screening of $E_{/\!/}$ within the NaCl layers compared to the metallic Cu substrate. These findings support the exploitation of non-conductive layers for TEPL experiments.

[1] J. Doležal *et al.*, *Nano Lett.* 2024, 24, 1629-1634. [2] W. Steurer *et al.*, *Nat. Commun.* 2015, 6, 8353. [3] COMSOL Multiphysics® v. 6.3. www.comsol.com. COMSOL AB, Stockholm, Sweden.

O 43.2 Tue 14:00 P2

Sub-nanoscale photochemistry without plasmons: Debromination of dibromoterphenyl on Au(111) — Hao Jiang[1,2], Youngwook Park[1], Adnan Hammud[1], Martin Wolf[1], Qiang Sun[2], and •Akitoshi Shiotari[1] — [1]Fritz Haber Institute of the Max Plank Society, Berlin, Germany — [2]Materials Genome Institute, Shanghai University, Shanghai, China

Local control of light-induced reactions is a crucial process for developing molecule-based optodevices and designing photocatalysis. Nanometer- and angstrom-scale photoreaction controls have been demonstrated using scanning tunneling microscopy (STM) combined with laser irradiation [1,2]; however, so far they rely on localized surface plasmon resonance (LSPR) using plasmonic metal tips. Here we report a novel light-assisted reaction that can be induced locally without LSPR. Using laser-coupled low-temperature STM, we observed 4,4”-dibromo-p-terphenyl (DBTP) on Au(111), which is a representative system undergoing Ullmann coupling by heat or far-field illadiation [3,4]. By tuning both the bias voltage at the STM junction and the wavelength of the incident visible laser, the debromination of DBTP is induced at the sub-nanometer scale using non-plasmonic tips. This research opens up the prospect of performing the single-molecule photochemistry for various non-plasmonic systems.

[1] E. Kazuma et al., Prog. Surf. Sci. 93, 163 (2018). [2] Y. Park et al., Nat. Commun. 15, 6709 (2024). [3] H. Jiang et al., ACS Nano 18, 1118 (2024). [4] H. Jiang et al., Nano Lett. 25, 9597 (2025).

O 43.3 Tue 14:00 P2

Photoisomerization of azobenzene derivatives on Au (111) using various photon energies and polarizations — •Haraprasad Mandal[1], Paul Schöngrundner[1], Stefan Hecht[2], and Leonhard Grill[1] — [1]Department of Chemistry, University of Graz, Austria — [2]Department of Chemistry, Humboldt-Universität zu Berlin, Germany

Azobenzene derivatives continue to serve as model systems for studying photoisomerization at surfaces. Among them, tetra-tert-butyl azobenzene (TBA) is particularly suitable due to its chemical stability, large steric groups, and well-defined trans and cis configurations that can easily be identified in scanning tunnelling microscopy (STM) images. In this work, we systematically studied the photon-energy- and polarization-dependent trans-to-cis isomerization of TBA, using a tunable femtosecond laser in combination with STM (working in ultra-high vacuum and at low temperatures). Illumination is done through an optical port, and STM imaging is used to identify the configuration of individual molecules before and after laser exposure. The switching efficiency was then studied for a variety of wavelengths in the range between 350 nm and 800 nm as well as different (s/p) polarization directions of the incoming light. Our results provide direct insight into the parameters that steer TBA photoisomerization on Au(111) and demonstrate the capability of our laser STM platform for controlled photochemical studies of single molecules.

O 43.4 Tue 14:00 P2

Focal phase evolution of single-cycle THz near-field pulses in a scanning tunneling microscope — •Andrea Rossetti, Vivien Sleziona, Alkisti Vaitsi, Luis Enrique Parra Lopez, Martin Wolf, and Melanie Müller — 1Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany

Lightwave scanning tunneling microscopy (LW-STM) employs single-cycle THz pulses as femtosecond bias, enabling imaging at sub-nanometer spatial and sub-picosecond temporal resolution. Control over the polarity and carrier-envelope phase (CEP) of such THz voltage transients is thereby crucial in determining which electronic states contribute to the ultrafast tunneling current. A simple approach for continuous CEP control of the single-cycle THz transients in LW-STM is via the Gouy phase. In this work, using a spintronic THz emitter, we use photoemission sampling from the point-like apex of the STM tip to monitor the local CEP of the tip-enhanced THz pulses along the focal axis of a focused THz beam. We find that the CEP exhibits a non-trivial evolution through the focus that strongly deviates from the expected Gouy phase shift for a monochromatic beam. Using analytical models and numerical calculations, we discuss the influence of the broad bandwidth of the THz pulses as well as their coupling to the STM tip for the local CEP in LW-STM.

O 43.5 Tue 14:00 P2

Development of Cryogenic Photoinduced Force Microscopy: Introduction and Progression — •Shuxia Chen[1], Claudia Felser[1], Lukas Eng[2], and Fabian Menges[1] — [1]Max Planck Institute for Chemical Physics of Solids — [2]Technische Universität Dresden

Photo-induced Force Microscopy (PiFM) provides access to optical properties at atomic length scales through the detection of near-field optical forces. To date, PiFM experiments have been largely restricted to ambient conditions, with only limited demonstrations in extreme environments such as cryogenic temperatures or high magnetic fields. In this work, we aim to expand PiFM operation to low temperatures and large external magnetic fields. This development opens the door to exploring light matter interactions over an expanded parameter space and in exotic quantum materials.

O 43.6 Tue 14:00 P2

Investigation of atomic defects in quasi-freestanding $\mathbf{MoS_2}$ with THz-STM — •Caroline Firschke, Junyoung Sim, Vibhuti N. Rai, Paul Wiechers, Florian Faaber, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Germany

Transition metal dichalcogenides (TMDCs) are an interesting class of materials due to their 2D-like nature and unique band structures. These materials tend to host different types of defects, heavily influencing their optoelectronic properties. THz-driven scanning tunneling microscopy is a unique technique to investigate the nature of these defects on atomic scales with ultrafast time resolution (1).

Here, we grow monolayers of MoS_2 on Au(111) via chemical vapor deposition, which host quasi-freestanding monolayers of MoS_2 with a band gap of around 2.7 eV, the so called "pits" (2). We find structural defects in these pits, which are decoupled from the metal substrate, and show sharp positive ion resonances in the band gap.

These sharp non-linearities of the I-V curve provide favorable conditions for their investigation via THz pulses. We find that these defects show sharp resonances in the light-wave-driven scanning tunneling spectroscopy, which vary depending on the THz field strength, DC bias voltage and tip-sample distance. The THz response of these resonances cannot be modeled with a simple convolution of THz pulses with the static I-V of the junction, suggesting a modulation of the charge state of the defects on ultrafast timescales.

(1) T. L. Cocker et. al. Nature Photon 7, 620-625 (2013)
(2) N. Krane et. al. Nano Letters 2016 16 (8), 5163-5168

O 43.7 Tue 14:00 P2

Photo-switching of azobenzene derivatives on Au(111) — •Matthew J. Timm[1], Robert di Vora[2], Stefan Hecht[3], Birgitta Bernhardt[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Austria — [2]Institute of Experimental Physics, Graz University of Technology, Austria — [3]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The light-induced trans-cis isomerization of azobenzene and its derivatives is of great scientific and technological interest as these molecular photo-switches can be used for nano-scale sensing or information storage. Particularly, 3,3',5,5'-tetra-tert-butylazobenzene (mTBA) adsorbed upon Au(111) has seen much interest, being studied at sub-monolayer coverage (around 0.1 ML) by scanning tunneling microscopy (STM) [1,2] and near monolayer (ML) coverage (0.9 ML) by two-photon photoemission [3]. However, missing is a single-molecule level insight into whether photo-switching at low coverage differs from that at higher but still sub-monolayer coverage - does it matter if only small or large areas of the surface are covered? Here, we combine STM with a self-designed computer-vision algorithm to study photoisomerization induced by pulsed laser radiation ($\lambda = 518$ nm) at a rather high surface coverage of 0.6 ML. This approach can track the isomerization state of thousands of individual mTBA molecules and enables us to detect subtle variations in switching yields among densely packed, similarly oriented molecules. [1] M. Alemani, et al. JACS 128 (2006) 14446. [2] M. J. Comstock, et al. Phys. Rev. Lett. 99 (2007) 038301. [3] S. Hagen, et al. Chem. Phys. Lett. 444 (2007) 85-90.

O 43.8 Tue 14:00 P2

Sub-10-fs compression of NIR pulses for phase-resolved sampling of MIR lightwave transients — •Justus Hess, Ugaitz Elu, Andrea Rossetti, Martin Wolf, and Melanie Müller — Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany

Lightwave scanning tunneling microscopy (LW-STM) employs single-cycle THz pulses as femtosecond bias [1], enabling imaging at sub-nanometer spatial and sub-picosecond temporal resolution. Ultrashort phase-stable mid-infrared (MIR) pulses promise to increase the time resolution in LW-STM. Phase-resolved characterization of the incident and STM tip-enhanced MIR transients requires sampling pulses with a duration of ideally less than 10 fs. For future MIR excitation in our LW-STM, we implement a MIR source and a pulse-compression scheme based on supercontinuum generation in a photonic crystal fiber (PCF) at 2 MHz in our existing LW-STM setup. Near-infrared (NIR) pulses with a duration of ~40 fs at a center wavelength of 1030 nm are spectrally broadened via self-phase modulation in the PCF to a Fourier-limit of 6 fs. Subsequent dispersion control with a transmission-grating compressor yields few-cycle pulses at 30mW average power sufficient for MIR waveform sampling in LW-STM. [1] T. Cocker et al., Nature 539, 263*267 (2016)

O 43.9 Tue 14:00 P2

Excitation of phonons by THz near fields in a quasi-suspended nanoscopic monolayer of MoS2 — •Junyoung Sim, Vibhuti Rai, Caroline Firschke, Christian Lotze, and Katharina J. Franke — Freie Universtiät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Phonons play a central role in describing fundamental physical properties of materials, such as heat capacity and resistivity, and also govern many-body phenomena such as superconductivity and charge-density waves. To resolve ultrafast lattice vibrations at the atomic scale, terahertz scanning tunneling microscopy (THz-STM) has provided important groundworks, where such vibrations are influenced by the presence of atomic-scale defects [1, 2].

In this work, we investigate the phonon dynamics in a monolayer molybdenum disulfide (MoS2) grown on a Au(111) surface. We focus on nanoscopic regions, where the MoS2 layer is suspended and the electronic structure is minimally hybridized with the substrate [3]. We observe an oscillatory behavior in the THz-STM pump-probe spectra on these suspended regions, which we assign to a coherent vibrational mode excited and measured by the tip-enhanced THz near field. To elucidate the excitation mechanism of the phonon modes, we vary the pump/probe field and investigate the influence of defects within the suspended area.

[1] Roelcke et al., Nature Photonics. 18, 595-602 (2024)
[2] Rai et al., arXiv:2506.08219 (2025)
[3] Krane et al., Nano Lett. 2016, 16, 8, 5163-5168 (2016)

O 43.10 Tue 14:00 P2

THz-driven plasmonic STM luminescence — •Alkisti Vaitsi, Luis Enrique Parra López, Vivien Sleziona, Martin Wolf, and Melanie Müller — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We combine THz scanning tunneling microscopy (THz-STM) with visible light detection to investigate ultrafast STM- luminescence (STML) luminescence from atomic-scale plasmonic junctions. The luminescence is driven by single- cycle THz pulses which act as a quasi-static ultrafast bias. This enables femtosecond gating of ultrafast tunneling currents and the excitation of localized surface plasmon (LSP) modes via ultrafast inelastic tunneling. Our measurements, combined with numerical reconstruction of THz-STML spectra from static STML spectra, show that a quantum cutoff is often absent in THz-STML. In addition, THz-STML spectra frequently exhibit a distinct spectral shape that differs from that predicted from quasi-static, single-electron tunneling-induced luminescence. We discuss the role of overbias emission, hot luminescence, and femtosecond plasmon dynamics in THz-gated STML.

O 43.11 Tue 14:00 P2

Design of a light-coupled high-magnetic-field Scanning Tunneling Microscope — •Colin Geuder[1], Marco Mönnich[1], Kurt Lichtenberg[1], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]2Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart.

Light-matter interaction at the nanoscale lies at the heart of many fundamental phenomena ranging from light harvesting to ultrafast lightwave electronics. However, accessing magnetic degrees of freedom through light-matter interaction at the atomic scale presents unique challenges. Scanning tunneling microscopy (STM) is the ideal tool, that can locally probe and excite these different interactions at atomic length scales. Here, we present the design of an STM that combines optical access with a large numerical aperture, magnetic fields up to 5 T, and temperatures below 2 K. We mitigate thermal loads introduced by the high-NA optical access through a combination of fiber coupling and radiation blocks at several stages of the cryostat's shields. This instrument enables studies of magnetic degrees of freedom in nanoscale light-matter interaction, such as magnon-photon coupling or exciton-magnon transport in layered materials.

O 43.12 Tue 14:00 P2

strong-field theory model for ultrafast electron transport in laser-assisted STM — •boyang ma[1], melanie mueller[1], and michael krueger[2] — [1]Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany — [2]Department of Physics, Technion, Israel Institute of Technology, 32000 Haifa, Israel

In ultrafast scanning tunneling microscopy (USTM), the classification of light-driven currents is usually based on the well-known Keldysh parameter. Similar to the description of strong-field photoemission, it is often used to distinguish photon-driven (weak-field) and field-driven (strong-field) tunneling regimes. Here, we discuss the limitations of the Keldysh parameter in classifying light-induced electron transport in nanoscale gaps, and present a theoretical study of laser-induced electron transport in STM [1,2]. In contrast to strong-field effects in spatially extended systems, we show that the Keldysh parameter alone is insufficient to capture the electron transmission dynamics in a confined nanogap. Instead, it must be complemented by an additional parameter, ζ, defined by the laser field strength, frequency, and junction width [2]. Notably, in the THz-STM, ζ alone becomes the decisive parameter, superseding the role of the Keldysh parameter. This reflects the fact that the Keldysh parameter accounts solely for properties of the driving field and neglects geometric confinement of the tunneling junction.

[1] B. Ma and M. Krüger, Phys. Rev. Lett. 133, 236901 (2024)
[2] B. Ma and M. Krüger, Phys. Rev. A 112, 033104 (2025)

O 43.13 Tue 14:00 P2

Addressing Atomic-scale optical Stark-shift Microscopy — Xabier Arrieta[1,2], Sofia Canola[3], Ruben Esteban[1,4], Javier Aizpurua[2,4,5], and •Tomas Neuman[3] — [1]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Donostia- San Sebastián 20018, Spain — [2]Department of Electricity and Electronics, FCT-ZTF, UPV/EHU, Leioa 48940, Spain — [3]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, Prague, 16200, Czech Republic — [4]Donostia International Physics Center, Donostia-San Sebastián 20018, Spain — [5]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza 5, Bilbao 48009, Spain

An applied external electric field can shift the optical transition energies of molecular emitters through the optical DC Stark effect. Conventional Stark-shift spectroscopy applies spatially homogeneous electric fields, allowing to probe variations in molecular dipole moment and polarizability upon photoexcitation. In contrast, molecules in natural environments experience strongly inhomogeneous internal electric fields, where the Stark effect follows different selection rules. We extend the theory of Stark-shift spectroscopy to account for such nanoscale field. Similar field localization naturally arises in light-assisted scanning tunneling microscopy, which could provide spatially resolved access to the electronic response of individual molecules under optical excitation [1,2]. We demonstrate the potential of this technique to develop into atomic-scale Stark-shift microscopy. [1] Roslawska et al., Phys. Rev. X, 12, 011012 (2022). [2] Imada et al., Science, 373(6550), 95-98 (2021).

O 43.14 Tue 14:00 P2

Light emission from dibenzoterrylene (DBT) molecules studied with STML — •Yannis Hilgers, Andreas Reutter, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics, LENA - TU Braunschweig, Braunschweig, Germany

Scanning Tunneling Microscopy induced Luiminescence (STML) has gathered great interest since its development in the late 1980s as it allows studying optical properties with atomic spatial resolution. With this technique, it has become possible to study quantum light sources like individual molecules exhibiting single photon emission, but obtaining high and reproducible photon yields has proven to remain challenging. With our self-built STML-setup, we achieve count rates about an order of magnitude higher than what has been reported in the past, allowing for measurements on more sensitive systems. Here, we present optical properties of dibenzoterrylene (DBT) molecules which have been reported as single photon sources when encapsulated inside a host lattice of Anthracene and Naphthalene. However, since both materials are not stable, we combine DBT molecules with a host lattice consisting of C_{60} multilayers, which is much more robust and even stable in air at room temperature. We found that light emission of individual DBT on C_{60} multilayers is indeed preserved. The emitted light was analyzed by means of photon maps and photon energy spectra.

O 43.15 Tue 14:00 P2

Influence of Polarons on Tunneling and Optical Spectra of Molecules Adsorbed on Dielectric Layers — •Jan Friese — Institute of Physics, Czech Academy of Sciences, Cukrovarnicka 10, Prague, 16200, Czech Republic

Light-assisted scanning tunneling microscopy has enabled the simultaneous probing of transport and optical properties of individual molecules with atomic-scale precision. This technique relies on electronically decoupling the molecules from the metallic substrate by depositing them on dielectric spacer layers. However, these spacers are often formed by ionic crystals, such as NaCl. The phononic response of these ionic layers can significantly impact the observed experimental features due to polaronic effects. Their understanding requires a bottom-up theoretical description accounting for the dynamics of the dielectric layer triggered by electronic transitions in the molecule.

Here we address this challenge and use the polaron-formalism to model the interaction of phonons in the dielectric layer with changes of the charge density in the molecule due to optical or charge transfer excitations. With that, two-time correlation functions and consequently spectral functions can be derived to account for the dynamics involved in substrate reorganization processes following a change of charge density in an adsorbed molecule. The results can be used to calculate features like the reorganization energy, and positions, widths and shapes of peaks in tunneling and optical spectra.

O 43.16 Tue 14:00 P2

Optics of Edge-Modified Graphene Nanoribbons: A Theoretical Perspective — •Jian Cheng Wong[1], Song Jiang[2], Guillaume Schull[2], and Tomáš Neuman[1] — [1]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague, Czech Republic — [2]Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Atomic-scale engineering of graphene nanoribbons (GNRs) provides a versatile means to tune their electronic and optical properties. We present a theoretical study of edge-modified GNRs that describe the process resulting in excitonic emission under scanning tunneling microscopy-induced luminescence (STML). The modified edge structure forms localized states in GNR similar to the end states studied formerly[1]. From the electroluminescence maps, we explore how interactions between two of these localized states change the optical properties depending on the GNR structure. For this, we construct a many-body model which describes the dynamics of tip-induced charging/discharging and relaxation that eventually leads to light emission.

[1] Song et al., Science, 379(6636), 1049-1054 (2023).

O 43.17 Tue 14:00 P2

Utilizing a Tunable Laser for Tip Enhanced Photoluminescence of Single Molecules — •Maximilian Rödel[1], Rodrigo Cezar De Campos Ferreira[1], Jiři Doležal[1], and Martin Švec[1,2] — [1]Institute of Organic Chemistry and Biochemistry (IOCB), Czech Academy of Sciences, Flemingovo náměstí 542/2. CZ16000, Praha 6, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10/112, CZ16200, Praha 6, Czech Republic

The study of organic molecules and their optical properties provides insight into molecular interactions, guiding the design of materials for advanced opto-electronic devices. In this contribution, we present a tip-enhanced photoluminescence (TEPL) scanning tunneling microscope (STM) setup by utilizing a tunable Ti:Sapphire laser not only for resonant excitation of organic molecules like MgPc, but, moreover, for disentangling optical signals.

For this purpose, a parabolic mirror is used for coupling the laser into the nano-cavity, ensuring wavelength-independent imaging and minimizing aberrations, enabling a consistent performance across the entire visible wavelength range. By doing so, high-resolution spectra of single-molecule MgPc at temperatures of <7 K on a Ag111/NaCl surface can be detected and by changing the excitation wavelength the vibronic contribution and the Raman signal can be distinguished.

With this model system, we are able to complement our optical data set and even hope to establish photoluminescence excitation spectroscopy for future measurements.

O 44: Scanning probe techniques: Method development – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 44.1 Tue 14:00 P2

Determining the electrical transmission to the junction of a scanning tunneling microscope — •Guido Hiller, Gaël Reecht, and Manuel Gruber — University of Duisburg-Essen

Stochastic resonance spectroscopy has recently been implemented in STM to probe dynamics at the atomic scale over a wide range of timescales, down to the picosecond range [1]. A key requirement for this method is a modulation voltage at the STM junction with an amplitude independent of the frequency. This, in turn, demands an accurate characterization and compensation of the frequency-dependent transmission of the cabling.

Several studies have focused on quantifying such transmissions. In particular, Paul et al. [2] quantitatively analyzed the radio-frequency induced broadening of a sharp feature in dI/dV spectra. Building on this method, we carried out such analysis in the Fourier space and discuss the associated advantages.

[1] Betz et al., arXiv:2412.12647 (2024) / Hänze et al., Sci. Adv. 7, no. 33 (2021) [2] Paul et al., Rev. Sci. Instrum. 87, no. 7 (2016)

O 44.2 Tue 14:00 P2

Upgrading an LT-STM with a qPlus-AFM system — •René Knispel, Patrick Härtl, and Matthias Bode — Physikalisches Institut, Experimentelle Physik 2, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The invention of the scanning tunneling microscope (STM) by Binnig and Rohrer in 1981 enabled direct imaging of atomic-scale structures in real space [1]. Shortly thereafter, the recognition of tip–sample interactions enabled the development of the atomic force microscope (AFM) [2]. In 1995, Giessibl achieved true atomic resolution with AFM [3] by measuring the force gradient-induced resonance frequency shifts of a silicon cantilever. Quartz-based cantilevers with enhanced stiffness and sensitivity enabled the development of the so-called qPlus-AFM technique, which surpasses STM in spatial resolution and allows STM measurements to be performed concurrently.

To extend the capabilities of our low-temperature STM, we upgraded it with a qPlus-AFM system. The Pan-type scanner was redesigned to enable cantilever excitation and to integrate both differential oscillation signals and the STM tunneling current. A UHV-LT preamplifier for the oscillation signals was also build and mounted inside the liquid-helium shield of the cryostat. The technical implementation and performance of the upgraded microscope will be demonstrated using suitable test samples.

[1] G. Binnig *et al.*, Phys. Rev. Lett. **49**, 57 (1982).
[2] G. Binnig *et al.*, Phys. Rev. Lett. **56**, 930 (1986).
[3] F. J. Giessibl, Science **267**, 68 (1995).

O 44.3 Tue 14:00 P2

Multifrequency Tunnelling Spectroscopy — •Gleb Neplyakh, Philipp E.J. Maier, Carolina A. Marques, Berk Zengin, Kevin Hauser, Rian Ligthart, Alexander LaFleur, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Scanning tunnelling spectroscopy (STS) probes the local density of states by measuring differential conductance as a function of energy. Traditional STS acquires N energy points by sweeping a DC bias with a small modulation superimposed. This requires N sequential measurements, making it impractical for large mapping tasks.

We have developed Parallel Spectroscopy (PS) to overcome this limitation. PS exploits the nonlinearity in the $I(V)$ curve of the materials: a single or multitone AC voltage drive generates a set of higher harmonics that encode the full spectrum. Demodulating N harmonics within one leakage-free integration window enables the energy dependence to be recovered in a single measurement, providing substantial speedups.

We compare conventional STS and single- and multi-frequency PS with respect to signal-to-noise ratio, potential artefacts, and spectral resolution. Using PS in conjunction with compressive sensing could allow us to conduct high-resolution studies of many-body effects in quantum materials.

O 44.4 Tue 14:00 P2

Tip-enhanced Raman Microscopy simulation methods — •Pablo Planelles Prensa, Harshit Sethi, Orlando Silveira Junior, and Adam Foster — Konemiehentie 1, 02150 Espoo / P.O. Box 15600, FI-00076 AALTO

Tip-enhanced Raman Microscopy (TERS) has emerged as a promising technique that overcomes Abbe diffraction limit, which dictates that for green light around 500 nm the spatial resolution is limited to only 250 nm, which is insufficient for studying nanomaterials. In TERS, by using a strongly localized plasmonic field produced at the tip apex, the Raman signal is significantly enhanced, and submolecular resolution can be achieved.

Similar to Scanning Tunneling and Atomic Force Microscopy techniques, TERS relies on a sharp tip. TERS offers the additional advantage of providing not only topographic information about the sample, but also chemical.

Despite the rapidly increasing interest in TERS, progress remains limited by the difficulty of interpreting the resulting experimental images.

In this context, we aim to contribute by presenting ab-initio simulation methods and demonstrating how they can be used to greatly facilitate the interpretation and prediction of TERS images. Moreover, we will study the influence of the substrate on the images, and how different tip geometries and materials affect resolution and induce image asymmetry. We will also compare several simulation methods with different levels of complexity and computational cost.

O 44.5 Tue 14:00 P2

Automatic tip functionalization with CO on Ag(111) using machine learning — •Johanna Schnorrenberg, Jonas Heggemann, Paul Laubrock, and Philipp Rahe — Universität Osnabrück, Institut für Physik, Barbarastraße 7, 49076 Osnabrück, Germany

Functionalization of scanning probe microscopy tips with CO molecules enables high-resolution imaging, sub-molecular contrast and access to charge distributions of adsorbed molecules. [1, 2]

However, the manual functionalization procedure is time-consuming and limits experimental throughput. To address this, tip functionalization can be automated. [3]

Here, we implement a full pipeline for CO tip functionalization on Ag(111). The process includes localizing a CO molecule during scanning the surface, performing the pick-up of this CO molecule and evaluating the resulting tip condition. Tip quality is assessed by imaging CO molecules on the substrate and classifying the achieved resolution as "good" or "bad" for a CO-tip using a convolutional neural network (CNN). The CNN performance is compared to a conventional image analysis algorithm, in this case a template matching algorithm.

We expect this automated approach to significantly improve the efficiency of AFM experiments and thereby enabling faster and more systematic data acquisition on molecular systems.

[1] B. Schulze Lammers et al., Nanoscale, 13, 13617 (2021)
[2] L. Gross et al., Angew. Chemie Int. Ed., 57, 3888 (2018)
[3] B. Alldritt et al., Comp. Phys. Commun., 273, 108258 (2022)

O 44.6 Tue 14:00 P2

Spectral interferometry scanning near-field optical microscopy; investigating resonant tip-sample near-field interactions

— •Tom Jehle, Sam S. Nochowitz, Juanmei Duan, and Christoph Lienau — Institute of Physics, University of Oldenburg, 26129 Germany

Localized phonon polaritons and plasmon polaritons resonantly enhance near-field mediated light matter interactions and are key for strong coupling between single quantum emitters and nanocavities (1). Localized polariton resonances with high oscillator strength show tip-sample distance dependent frequency shifts in scanning probe experiments, requiring spectroscopic analysis at explicit tip-sample distances (2). Here, we introduce a broadband interferometric scattering-type SNOM technique (3) to reconstruct spectral amplitude and phase of visible light scattered from a gold taper. Harmonic sampling with a fast line camera allows reconstruction of spectra with high tip-sample distance resolution. Spectral amplitude, phase and the evaluation of the distance dependence of the near-field interaction allows the retrieval of the temporal near-field dynamics with sub-cycle precision. We demonstrate our technique by measuring the tip-sample distance dependent time dynamics of the near-field at the apex of a resonant gold taper coupled to its image. Our results pave the way towards hyperspectral imaging in the visible with nm spatial resolution and fs temporal resolution of the reconstructed time dynamics. (1) S. Hu et al., Nat. Commun. 15, 6835 (2024); (2) H. Wang et al., Nat Commun. 9, 2005 (2018); (3) J. Zhan et al., Nano Lett. 24 (49),15738 (2024)

O 44.7 Tue 14:00 P2

Cryogenic Band Pass Amplifier for measuring Atomic Shot Noise

— •Benjamin Frölich, Kevin Hauser, Lebin Yu, Gleb Neplyakh, Ajla Karić, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Scanning tunneling microscopy provides access to the texture and correlation of charge carriers in quantum materials by listening to their characteristic shot noise signatures that reveal 1e and 2e charge quantization effects at the atomic scale. Previous studies introduced a band pass amplifier with center frequency of 3 MHz based on their in house made high electron mobility transistor (HEMT) and LC tank circuit to measure such shot noise. Here we build a similar band pass amplifier with a center frequency of 17 MHz based on a comercially available InP HEMT. Another goal is the evaluation of resonating circuits like the LC tank at cryogenic temperatures. We achieve 26 dB single stage amplification at liquid nitrogen temperatures. Simulations suggest a noise figure of < 0.12 dB. Experiments at even lower temperatures present challenges impacting implementation into the cryostat.

O 44.8 Tue 14:00 P2

all-in-one preparation stage of STM/AFM QPlus sensors for ultrahigh vacuum

— •reza habibipour, jakob pelster, marco pratzer, michiel reul, and markus morgenstern — II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Germany

QPlus sensors enable the combination of atomic force microscopy (AFM) and scanning tunneling microscopy (STM) with high resolution. We developed a compact preparation stage for positioning, glueing, annealing and tip etching of wires with diameters down to 7.5 um and length down to 200 um. The QPlus sensors are based on a piezoelectric quartz tuning fork with nominal frequency of 32.6 kHz. A tip wire is attached to one prong with the other prong is fixed to a ceramic block on the ultrahigh-vacuum (UHV) sample holder. Two tuning-fork contacts connect to the sample plate for AFM oscillatory function and for STM current. Sensor preparation utilizes a long-working-distance optical microscope (~6 cm) and micrometer manipulators for precise glue and wire positioning. A heater is used to cure the glue. A tungsten-carbide flush cutter trims the wire to within 0.2 mm of the prong edge. Alternatively, an etching ring is employed for tip shaping. Afterwards contacts can be checked in-situ by a Keithley instrument. Q-factors at room temperature and UHV amount to 16.000. The resulting QPlus sensors will be employed in a 300 mK STM/AFM cryostat mostly for maneuvering towards stacks of 2D materials by AFM prior to STM measurements.

O 44.9 Tue 14:00 P2

Iron Implantation from a Ferrocene Ion Source

— •Urs Boison, Ajla Karić, Berk Zengin, Lebin Yu, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

The scattering of electrons on defects in low dimensional materials provides insight into the electronic structure using quasiparticle interference or tunneling spectroscopy. Since natural defects are mostly spin averaging and obscure magnetic textures, using magnetic impurities would allow a richer inspection of the underlying magnetic properties. At present, magnetic impurities are difficult to produce because chemically active defects are required to chemisorb magnetic atoms, such as hydrogen. We use metal ions in a volatile molecule that can easily and directly be delivered to ion sources commonly used for sample cleaning. Using a conventional sputtering source and heated ferrocene (vapor pressure of 1773 Pa at 400 K), we implant ferrocene molecules between 100 and 3000 eV and use different vapor pressures to investigate the ion implantation efficiency and possible defect generation. We test the optimal dose as a function of these parameters using ion current measurements and mass deposition on a quartz crystal microbalance. To verify successful implantation, we use scanning tunneling microscopy on graphene and superconducting layers. Magnetic defects should exhibit signatures related to Yu-Shiba-Rusinov states, confirming the conservation of their spin upon implantation.

O 44.10 Tue 14:00 P2

Development of a Low-Temperature Scanning Probe Microscope

— •Tingwen Miao — Tsung-Dao Lee Institute, Shanghai, China

We independently designed and constructed a low-temperature ultrahigh-vacuum scanning probe microscope (SPM) system which is equipped with a single-axis 9T magnetic field and can be cooled down to 400mK. The system integrates the functionalities of atomic force microscopy (AFM) and scanning tunneling microscopy (STM) into the scanning head, enabling in-situ measurements of both electrical signals and force signals. The cooling curve, current noise, non-contact AFM and STM imaging and I(V) spectroscopy are characterized to verify that the system achieve the fundamental SPM capabilities. Subsequent magnetic field test and low-temperature test will be performed to confirm that the system can achieve all designed performance.

O 44.11 Tue 14:00 P2

Correlative AFM-SEM-EDS microscopy on nanoparticles and -wires

— Chris Schwalb[1], •Lukas Stühn[1], Hajo Frerichs[1], Sebastian Seibert[1], Darshit Jangid[1], Marion Wolff[1], Kerim Arat[2], Hamed Alemansur[2], Afshin Alipour[2], Andreas Amann[2], Luis Montes[2], Jost Diederichs[2], Jeff Gardiner[2], Will Neils[2], and Stefano Spagna[2] — [1]Quantum Design Microscopy GmbH, Pfungstadt, Germany — [2]Quantum Design Int., San Diego, USA

Correlative AFM-SEM-EDS microscopy enables multimodal nanoscale analysis but is often hindered by complex sample transfers and the lack of a joined coordinate system. Our approach integrates these techniques to allow simultaneous acquisition of topographical, mechanical, electrical, SEM and EDS data from the same region of interest[1]. We illustrate the advantages of such in-situ correlative measurements through several case studies, including hard-to-access structures such as bone lacunae, individual nanowires on 5 nm TEM grids, and nanoparticles relevant for multimodal characterization workflows[2]. In addition, we present first results on individual ZnO nanowires for energy-harvesting concepts, where SEM enables rapid localization and AFM provides mechanical and electrical characterization[3,4]. Overall, the presented in-situ correlative strategy, the FusionScope, expands the analytical capabilities for nanoscale inspection and process control across a wide range of materials and devices. [1] https://doi.org/10.1093/mictod/qaad083 [2] https://doi.org/10.1093/mam/ozae044.233 [3] https://doi.org/10.3390/mi16080927 [4] https://doi.org/10.1002/adfm.202310110

O 44.12 Tue 14:00 P2

Distance dependent of local work function on Pb/Si(111) islands — •Ajay Kumar[2], Thomas Späth[1], Ben Lottenburger[2], Zeineb Ben Tanfous[3], Daniel Rothhardt[2,4], Paul P. Schmidt[2], Manuel Schulze[2], Ralf Metzler[2], Kurt Busch[3], Gino Wegner[3,5], and Regina Hoffmann-Vogel[2] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany — [2]Physikalisches Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Humboldt University of Berlin, 12489 Berlin, Germany — [4]Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland — [5]Max-Born-Institute, 12489 Berlin, Germany

A quantitative description of the measured local contact potential difference (LCPD) as a function of tip-sample separation is essential for a deeper understanding of Kelvin probe force microscopy (KPFM), since it permits a more complete characterization of the sample's electronic properties and of the forces acting on the probe. We employ Pb islands on the Si(111)-7*7 reconstruction as a model system of metallic islands on a semiconducting substrate. Using a frequency-modulation scanning force microscope, we have performed frequency-shift bias-approach measurements at 115 K on these Pb islands and have studied the variation of the LCPD with tip-sample distance.

O 44.13 Tue 14:00 P2

Nonlinearity mapping using adaptive control schemes in scanning force microscopy — •Lukas Böttcher[1], Hannes Wallner[2], Niklas Kruse[2], Franziska Dorn[1], Wolfram Just[2], Ingo Barke[1], Jens Starke[2], and Sylvia Speller[1] — [1]Institute of Physics, Universität Rostock, Germany — [2]Institute of Mathematics, Universität Rostock, Germany

When probing surfaces by scanning force microscopy methods using oscillating cantilevers, bistabilities may occur [1,2]. This is a result of nonlinearities arising due to tip-sample interactions. In this work we focus on the attractive regime. Using an adaptive control scheme we track branches of unstable periodic orbits of the oscillating cantilever, arising between the two stable states [3]. Combining this with a topography scan of a polymer blend surface we explore spatial changes of the unstable branch. Parameters, such as the frequency width of the bistable region or the slope at the unstable branch can serve as nonlinearity parameters and respective maps can be acquired. The aim is to connect such nonlinearity maps to material-related properties such as density and elasticity.

[1] Gleyzes, P. et al.: Bistable behavior of a vibrating tip near a solid surface. Appl. Phys. Lett. 58, 2989 (1991) [2] Misra, S. al.: Event-driven feedback tracking and control483 of tapping-mode atomic force microscopy. Royal Society of London Proceedings484 Series A 464, 2113*2133 (2008) [3] Böttcher, L. et al.: Exposing hidden periodic orbits in scanning force microscopy. Commun Phys 8, 57 (2025)

O 44.14 Tue 14:00 P2

Realizing Spin-Polarized Scanning Tunneling Microscopy for an Atomic-Scale Study — •Leon Bojunga, Felix Otto, Jonas Brandhoff, Maximilian Schaal, Christian Haberland, Lorenz Brill, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS) is a powerful tool for investigating spin structures with real-space resolution down to the atomic scale. By combining a spin-sensitive tip with controlled magnetic fields at cryogenic temperatures, SP-STM/STS enables the study of phenomena such as Kondo resonances, spin excitations, organic radicals, and magnetism. Realizing SP-STM/STS requires, beyond standard low-temperature STM stability, a magnetically sensitive tip and a precisely tunable external magnetic field. In this work, we fabricate Ni tips by electrochemical etching and verify their apex geometry via SEM to ensure high quality. This is achieved using a home-built etching setup that enables a reproducible process with consistent results. Testing of the fabricated tips is carried out using an STM at cryogenic temperatures, which, together with a perpendicular magnetic field of up to 3 T, allows controlled magnetization of the tip. To assess the magnetic sensitivity and spatial resolution of the Ni tips, we employ Co bilayer islands on Cu(111), whose well-defined magnetic structure provides an ideal benchmark for validating tip polarization and imaging performance.

O 44.15 Tue 14:00 P2

Low latency, galvanically isolated data transfer architecture for distributed low-level precision measurements — Toni Marković, Shane O'Neill, Aitziber Herrero, David Zurbriggen, Daniel Uehli, and •Alessandro Pioda — SPECS Zurich GmbH, Technoparkstrasse 1, 8005 Zurich

Many recent achievements in the field of quantum devices, spintronics, novel materials and surface science, have been possible thanks to the ability to cool samples to temperatures significantly below 1 Kelvin and to the use of state of the art measurement electronics. Requirements for signal resolution, precision and quality increase significantly at low temperatures, while the growing complexity of experiments and higher measurement throughput require a growing number of signals, larger bandwidths, and push the cost of measurement electronics upwards.

Here we present a data transfer architecture that enables a low-latency, synchronous transfer of raw DAC and ADC data from multiple signal generation and acquisition interfaces to a central processing core. The architecture allows transfer of very high-resolution data with microsecond resolution, high resolution data with nanosecond resolution or a combination thereof. The use of off-the-shelf optical fiber cables for data transfer allows for decentralized measurements, simultaneous experiments on different experimental set-ups, as well as galvanic isolation between the processing core and the signal interfaces. The architecture can handle hundreds of signals, all synchronous and with no multiplexing. We also discuss state of the art signal interfaces and typical applications for this novel architecture.

O 44.16 Tue 14:00 P2

Development of low noise cryogenic circuitry for shot noise measurements in STM — •Anne-Catherine Oeter, Soumyaranjan Jhankar, Christian Ast, and Klaus Kern — Max Planck Institut for Solid State Research

Tunneling currents of electrons are subject to shot noise. Measuring shot noise in a scanning tunneling microscope (STM) can give more insight into the tunneling dynamics and the properties of the tunneling charges. Our goal is to measure shot noise at low tunneling currents simultaneously with the dc tunneling current. To this end, we are developing a low-noise cryogenic pre-amplification circuit. It is made up of a tank oscillator circuit, to filter and amplify the white noise signal at a frequency beyond flicker noise, as well as a HEMT based cryogenic amplification circuit. We will discuss how we want to improve the shot noise circuitry already used in the literature, for example, how to enhance the quality factor of the inductances used to filter the ac signal.

O 44.17 Tue 14:00 P2

Realization of laser-assisted UHV sample surface preparation for STM — •Clara Marie Nieder, Soumyaranjan Jhankar, David Sousa, and Christian Ast — Max Planck Institute for Solid State Research

Scanning tunneling microscopy (STM) enables the study of the electronic properties of superconductors such as vanadium. To achieve reliable STM measurements, the preparation of clean and well-defined metal surfaces under ultra-high vacuum (UHV) conditions is essential. This requirement becomes particularly demanding for reactive transition metals, where surface oxides can form even under high-quality UHV conditions. In this work, we present a laser-assisted UHV sample preparation approach to obtain clean vanadium surfaces. For this method, we utilize a diode laser directed at the front surface of the sample to achieve high temperatures. To prevent mechanical or electrical complications inside the UHV chamber, we place all optical and diagnostic components, including pyrometric temperature monitoring, outside the chamber. This enables a controlled and localized high-temperature annealing for oxide removal. Therefore the method represents a promising way to reproducibly prepare reactive and superconducting surfaces for subsequent STM measurements.

O 45: Organic molecules on inorganic substrates: Adsorption and growth – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 45.1 Tue 14:00 P2

Domain mixing of coronene and nonahelicene with CuO$_x$ species on Cu(110) — •Max Halbauer, Martin Wolf, and Akitoshi Shiotari — Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany

Various surfaces are known to reconstruct as a result of surface energy minimization (e.g. Pt(110)-(2×1), Si(111)-(7×7)). For certain systems, the surface reconstruction is induced by the adsorption of molecules or atoms (e.g. C$_{60}$/Cu(111) [1]). In this work, we show how the organic molecules, coronene and nonahelicene, interrupt the growth of copper oxide rows of the typical Cu(110)-p(2×1)O reconstruction and mediate the formation of mixed domains instead. The resulting adlayer domains on Cu(110) were imaged by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) under ultrahigh vacuum and cryogenic conditions. Models for the adsorption structures of the molecules and CuO$_x$ species are discussed and confirmed with simulated images. A mechanism for the mixed domain growth is proposed, whereby surface diffusion and favourable lateral interactions between the molecules and oxide species drive the formation of the observed coordination framework. The finding opens prospects for controlling the lateral chemical and electronic interactions between adsorbed molecules by partial oxidation of the Cu(110) surface.

[1] L. Forcieri, S. P. Jarvis, *et.al.*, *Phys. Rev. B* **2021**, *104*, 205428.

O 45.2 Tue 14:00 P2

Importance of Electrostatic Effects for Interpretation of X-ray Photoemission Spectra of Self-Assembled Monolayers — •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

The subject of this contribution is electrostatic effects in X-ray photoemission (XP) from self-assembled monolayers (SAMs), which are application-relevant ultrathin molecular films, coupled to the substrate by a suitable anchoring group. Whereas, in most cases, the standard concept of chemical shift is fully sufficient to describe XP spectra of these systems, consideration of electrostatic effects is frequently necessary for their proper interpretation. Due to the insulating character of the SAM matrix, decoupled electronically from the substrate, the introduction of a dipolar "sheet" at the SAM-substrate interface or within this matrix creates a potential discontinuity, shifting the energy levels above the "sheet" with respect to those below it. This shift is reflected then in the matrix-related spectra, resulting in shifts and splitting of the characteristic photoemission peaks. Representative examples in this context underline the importance of electrostatic effects in photoemission and suggest that they should be considered on equal footing with the chemical shift.

O 45.3 Tue 14:00 P2

Self-assembled quasi-one-dimensional metal-organic framework — Jonas Brandhoff, Jule S. Hölzer, Felix Otto, Torsten Fritz, and •Roman Forker — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We compare condensed monolayers of 4,5,9,10-pyrenetetrone (Py4O) on Cu(111) in two fundamentally different configurations, namely with and without adatoms. To this end, we employ density-functional theory (DFT) calculations to understand the structural configurations as well as the electronic properties. We uncover the coupling between the organic molecule, surface, and possible adatoms. Furthermore, we demonstrate how a quasi-one-dimensional arrangement including a Cu adatom is thermodynamically stable. This interpretation is substantiated by means of scanning-tunneling microscopy (STM) experiments, along with low-energy electron diffraction (LEED) patterns. Additionally, we use photoelectron spectroscopy to assess the electronic structure. Finally, we elucidate the bond formation between the d-orbitals of the Cu adatom and the p-orbitals of the molecular oxygen.

O 45.4 Tue 14:00 P2

Landing-Energy-Controlled Surface Conformation of Electrosprayed Foldamer Molecules on Au(111) — •Jue Wang^1, Dennis Meier^{1,2}, Shengming Zhang^1, Patrick Lawes^1, Pengfei Zhao^1, Jinhua Wang^3, Victor Maurizot^3, Andreas Walz^{1,4}, Annette Huettig^{1,4}, Hartmut Schlichting^{1,4}, Anthoula C. Papageorgiou^{1,5}, Joachim Reichert^1, Ivan Huc^{6,7}, and Johannes V. Barth^{1,7} — ^{1}TU Munich, DE — ^{2}Tufts University, US — ^{3}CNRS, Univ. Bordeaux, FR — ^{4}pureions GmbH, Gilching, DE — ^{5}National and Kapodistrian University of Athens, GR — ^{6}LMU Munich, DE — ^{7}Cluster of Excellence e-conversion, DE

Preserving the structural integrity of biomimetic foldamers upon surface deposition is essential for their integration into functional molecular architectures. In this study, we investigate the electrospray ion beam deposition of foldamer molecules in ultra-high vacuum and examine how their conformation depends on the mean landing energy during deposition. With a low mean landing energy of about 0.6 eV, intact foldamers are observed on the surface. Higher landing energies predominantly result in unfolded molecules. The unfolded conformation are further accessible by annealing of the adsorbed folded molecules. These results highlight the importance of soft-landing conditions to maintain hydrogen bond-stabilized architectures on surfaces, offering a model platform for studying the structure-function relationship of surface-supported thermolabile biomolecules

O 45.5 Tue 14:00 P2

Adsorption, Dissociation and Chain Formation of 2NHC-azo-iPrl on Au(111) — Ebru Cihan^1, Natasha Khera^1, Franz Plate^1, Ningwei Sun^2, Soyoung Park^{2,3}, Franziska Lissel^{2,3}, and •Francesca Moresco^1 — ^{1}Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — ^{2}Institute of Macromolecular Chemistry Leibniz Institute of Polymer Research, Hohe Strasse 6, Dresden, Germany — ^{3}Institute for Applied Polymer Physics, TU Hamburg, Hamburg, Germany

In this study, we investigated 2NHC-azo-iPrl molecules on the Au(111) surface. While the central azobenzene core is clearly visible in STM images, in most cases, only two isopropyl groups are present per molecule. Our results indicate the possibility of a reaction between I- counterions and the isopropyl (iPr) side groups, which may lead to the dissociation of iPrI upon heating. Furthermore, experiments using STM lateral manipulation, which facilitate the separation of chain structures on azobenzene bridges, suggest that the chains are likely connected to each other by weak van der Waals or hydrogen bonds. Additionally, to further investigate the azobenzene core of the molecule, voltage pulses were applied to the molecule using the STM tip. This investigation reveals the potential for cis-trans isomerization in the azobenzene core.

O 45.6 Tue 14:00 P2

Tuning molecular self-assembly of BDA on CsPbBr$_3$(100) — •Hannah Loh, Milan Möller, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

CsPbBr$_3$ is a promising alternative to organic-inorganic perovskites in solar cells and light emitting diodes [1]. In these devices, organic layers are often used as charge transport layers and hence interface properties are of particular interest. Depending on the termination of the CsPbBr$_3$ substrate [2] the adsorption properties can be tuned [3].

In this contribution we invesitgate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial CsPbBr$_3$ thin films on Au(100). Independent of surface termination the BDA molecules lie flat and form compact islands. On the CsBr-terminated surface, molecules follow a head to tail hydrogen-bridge stabilized arrangement. The interaction with the PbBr terminated surface is stronger causing partially a slight tilt of the molecules to adapt to the substrate unit cell and deprotonation.

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Loh H. et al., ACS Nano, **19**, 10199-10206 (2025)

O 45.7 Tue 14:00 P2

Force mapping of a pyridyl-functionalized platform molecule by noncontact atomic force microscopy — •Hyeji Choi^1, Behzad Mortezapour^2, Martin Wolf^1, Richard Berndt^2, and Akitoshi Shitotari^1 — ^{1}Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — ^{2}Institut für Experimentelle und Angewandte

Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Platform molecules based on trioxatriangulenium (TOTA) form triangular adsorption motifs on metal surfaces with a functional group protruding to the vacuum [1]. However, probing the atomic-scale structure of such steric molecules remains challenging. Here, we study pyridyl-TOTA on Ag(111) and perform single-molecule force mapping, using noncontact atomic force microscopy (NC-AFM) at 6 K. We obtained force and potential maps of the pyridyl group interacting with a metal tip by measuring frequency shift as a function of tip height and location. These maps reveal anisotropy depending on the direction relative to the pyridyl ring plane. Simulations using Lennard-Jones potential reproduce the map appearances, enabling estimation of the preferred ring orientation and directional stiffness. We thus demonstrate the high potential of single-molecule force mapping for the structural characterization of steric adsorbate.

[1] Mortezapour, B., et al., ACS Nano 19, 38773-38780 (2025)

O 45.8 Tue 14:00 P2

Decoupling of Organic Monolayers from Cu(111) Using Blue Phosphorene — •Felix Otto, Wiebke Makowski, Jonas Brandhoff, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Two-dimensional (2D) materials are promising for future electronics due to their tunable properties. Since graphene's discovery in 2004, materials like MoS_2, h-BN, and Blue Phosphorene (BlueP) have been synthesized, offering high charge mobility and adjustable band gaps. BlueP can be grown on substrates such as Cu(111), making it suitable for decoupling organic layers. This study investigates whether BlueP can effectively decouple PTCDA monolayers from Cu(111). Two BlueP phases – hexagonal and chiral – were prepared and characterized, revealing structures with hexagonal unit cells but significantly stretched lattices compared to free-standing BlueP. Despite structural differences, both phases exhibited similar chemical and electronic properties. PTCDA was deposited on both phases, forming ordered herringbone structures. On the chiral phase, a single structural model sufficed, while two were necessary for the hexagonal phase. Spectroscopic analyses indicated weak interactions and evidence of integer charge transfer, supporting the idea that BlueP acts as an effective decoupling layer. These findings contribute to understanding how 2D-materials can be used to electronically isolate organic monolayers, advancing their application in nanoelectronics.

O 45.9 Tue 14:00 P2

Density functional study of the geometric and electronic properties of a tetracene-adduct molecule on Ag(110) — •Fabian Dixer[1], Eric Fackelman[2], Veronika Schmalz[3], Monja Stettner[2], François C. Bocquet[2], Andrei C. Matetskii[2], Serguei Soubatch[2], Ulrich Koert[3], Frank Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-3, FZ Jülich and RWTH Aachen University, Germany — [3]Department of Chemistry, Philipps-Universität Marburg, Germany

We present a density-functional theory (DFT) investigation of the adsorption behavior of the tetracene-maleic anhydride Diels-Alder adduct (4A-MAD) on Ag(110). This molecule serves as a model system for studying light induced retro 4+2 cycloadditions on surfaces. Using a repeated-slab approach with a van-der-Waals corrected GGA functional, we explore the adsorption energy landscape by sampling multiple initial configurations and performing local relaxations. The most favorable geometries are examined in terms of work-function changes, charge-density-difference distributions, and projected densities of states. We further simulate photoemission momentum maps of the frontier molecular orbitals within photoemission orbital tomography and compare them with angle-resolved and angle-integrated photoemission data from our experimental collaborators. This combined analysis provides a comprehensive picture of the molecule-substrate interaction and lays the groundwork for future studies of on-surface photochemical cleavage of the Diels-Alder adduct.

O 45.10 Tue 14:00 P2

Theoretical Investigation of Halogenated Polycyclic Aromatic Hydrocarbons on Clean and Coated Metal Surfaces — •Florian Pfeiffer[1], André Schirmeisen[2], Daniel Ebeling[2], and Simone Sanna[1] — [1]Institute for Theoretical Physics, JLU Giessen, Germany — [2]Institute for Applied Physics, JLU Giessen, Germany

Halogenated organic precursors are the building blocks for the on-surface synthesis of complex structures with precisely tuned properties. While chemical synthesis is typically performed on clean metallic surfaces, a NaCl bilayer might be employed to electronically decouple substrate and adsorbates, increasing mobility and thus simplifying manipulation.

To improve our understanding of the fundamental interactions of halogenated precursors on (isolated) surfaces, we examined charge redistribution as well as the adsorption geometry, distance, and energetics for several substrate-adsorbate systems, e.g. Dibromopyrene and Iodotriphenylene on NaCl/Cu and halo-tetracenes on coinage metals.

The Vienna Ab initio Simulation Package [1] implementation of density functional theory was used to calculate potential energy surfaces and nudged elastic bands for modelling adsorption behaviour and diffusion pathways, respectively. Comparability with experimental results [2] was achieved by simulation of atomic force microscopy using the Probe-Particle Model [3].

[1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993)

[2] Q. Zhong et al., Nat. Chem. 13, 1133 (2021)

[3] P. Hapala et al., Phys. Rev. B 90, 085421 (2014)

O 45.11 Tue 14:00 P2

Formation and Electronic Interaction of Donor–Acceptor Heterostructures — •Philipp Janzen, Jonas Brandhoff, Felix Otto, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Combining donating and accepting molecules lies at the heart of many electronic devices. These molecular heterostructures allow for a delicate tailoring of charge-transfer interfaces. In this work, we investigate such heterostructures formed by the adsorption and structural organization of 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) and 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) on Au(111). Owing to their shared symmetry, HHTP and HATCN form a well-matched co-assembly on the surface. Employing scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), we are able to resolve the structural properties of the individual systems, as well as the combined heterostructure. Additionally, X-ray photoelectron spectroscopy (XPS) and photoemission orbital tomography (POT) provide insights into charge-transfer processes and the electronic structure at the interface.

O 46: Organic molecules on inorganic substrates: electronic, optical and other properties – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 46.1 Tue 14:00 P2

Investigation of chiral helicene molecules on the superconducting substrate Pb(111) — •Melvin Grumser[1], Rahel Specht[1], Vincent Herzog[1], Wenhui Niu[2], Narcis Avarvari[3], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]University of Angers, Angers, France

Chiral molecules have recently garnered a lot of attention for their ability to partially spin polarize currents running through them, which is of interest for the emerging field of spintronics. Chirality induced spin selectivity (CISS) typically manifests itself in experiments in which a current passes through a chiral molecule, as has been done down to the single-molecule scale using scanning tunneling microscopy [1]. However, recent studies suggest that the adsorption of chiral molecules might already lead to magnetization in the surface layer which could locally interact with the Cooper-pairs of a superconducting substrate [2]. Here, we investigate the effect of adsorbed chiral molecules on the elemental superconductor Lead. For this, [7]-Helicene and [6]-Helicene derivatives were evaporated onto a Pb(111) surface and investigated via STM and AFM. The molecules form ordered islands with different orientations of the molecules. In addition, we use scanning tunneling spectroscopy and identified the energy of the HOMO and LUMO. However, we do not observe any signatures of an alteration of the local superconducting behavior.

[1] Safari, Mohammad Reza, et al. Small 20.22 (2024): 2308233.

[2] Shapira, Tamar, et al. Phys. Rev. B 98.21 (2018): 214513.

O 46.2 Tue 14:00 P2

On-Surface Reaction of Naphthothiadiazole Derivatives on Au(111) — •Mohsen Ajdari[1], Jakob Steidel[1], Larissa Winkelmann[1], Felix Landwehr[1], Jakob Sawatzki[1], Jakob Roth[1], Christian Huck[1], Hendrik Hoffmann[2], Uwe H. F. Bunz[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute for Organic Chemistry, Heidelberg University, Germany

Naphthothiadiazole (NTD) and its halogenated derivatives (NTD-Br/Cl) are promising electron acceptor candidates for use in (opto)electronic applications.

In a multi-technique approach, this study utilizes scanning tunneling microscopy, two-photon-photoemission spectroscopy, and temperature-programmed desorption to identify on-surface reactions of adsorbed NTD-Br/Cl on Au(111).

Our findings suggest that the halogenated molecules undergo temperature (NTD-Br) and photo-induced (NTD-Br/Cl) dehalogenation reactions. As a result, we found work function changes, differences in the energy-level alignment as well as changes in the adsorption structure.

O 46.3 Tue 14:00 P2

Second Harmonic Generation in Thin Films of Chiral Organic Molecules — •Martin Richter[1], Gayani Liyanage[1], Marjan Krstic[2], Erik Misselwitz[3], Milan Kivala[3], Carsten Rockstuhl[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Theoretical Solid-State Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Organic Chemistry, Heidelberg University, Germany

Nonlinear optical (NLO) techniques enable increased sensitivity to chiroptical features. In contrast to linear circular dichroism (CD), second harmonic generation (SHG) chiroptical features can be explained within the dipole approximation. This includes electric as well as magnetic dipolar contributions. The latter are usually much weaker and specific measurement schemes are required to detect them. Here, we investigated thin films of chiral organic molecules using SHG-CD and SHG-ORD (optical rotatory dispersion) to probe the nonlinear CD and optical rotation. Continuous rotation of a quarter-wave plate generates circular and elliptical light to gain insights into the relative amplitudes of the second-order susceptibilities from electric χ^{eee} and magnetic (χ^{mee} and χ^{eem}) dipolar contributions. Our theoretical modelling allowed us to disentangle electric and magnetic dipole contributions.

O 46.4 Tue 14:00 P2

Electronic structure of spiro-bridged N-heterotriangulenes on Au(111) — •Jakob Roth[1], Jakob Sawatzki[1], Christian Huck[1], Angelina Jocic[2], Milan Kivala[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute of Organic Chemistry, Heidelberg University

N-heterotriangulenes are versatile p-type organic semiconductors combining enhanced planarity with sterically defined bridges, enabling highly stable amine-centered radical cations, making them promising candidates for semiconducting and energy storage applications.

Here, we investigated the adsorption and electronic structure of two model systems - dimethylmethylene-bridged N-heterotriangulene (TN) and spirofluorene-bridged N-heterotriangulene (FTN) - deposited on Au(111). The spiro-annulated fluorenyl groups of FTN are expected to elevate the molecular core and hence reduce the electronic coupling strength to the metal substrate. Scanning tunnelling microscopy reveals that both species form well-ordered monolayers. Two-photon photoemission spectroscopy quantitatively resolves occupied and unoccupied electronic (transport levels) as well as excitonic states (optical gaps). These results highlight how molecular design controls surface coupling and electronic level alignment in Triphenylamine-based materials.

O 46.5 Tue 14:00 P2

Deprotonation of quinacridone on Ag(100) - an NIXSW/XPS study of the phase transition — Lucas Hirschfeld[1], Morris E. L. Mühlpointner[1], Anna J. Kny[1], Sergey Subach[2], and •Moritz Sokolowski[1] — [1]Clausius Institute for Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Germany

Quinacridone (QA) forms two different phases on the Ag(100) surface. When QA is deposited at room temperature, the formation of the α-phase with a point-on-line (*pol*) structure is observed. After annealing, the commensurate β-phase is irreversibly formed [1]. The mechanism, involving the loss of intermolecular hydrogen bonds, was not disclosed so far. Thus we have performed a detailed Normal Incidence X-ray Standing Waves (NIXSW)/XPS study.

The N1s XPS spectra exhibit a second peak shifted by 2.2 eV to lower binding energies when going from the α- to the β-phase. This reveals that the irreversible reaction from the α- to the β-phase is explained by a deprotonation of 50 % of the amine groups. The deprotonated N-atoms form stronger bonds to the Ag(100) surface, indicated by a drastic approach of the respective N adsorption height from 4.3 Å in the α-phase to 3.4 Å in the β-phase. These results show that the reaction is driven by the energy gain related to N/Ag interfacial bonds, which overcompensate the loss of intermolecular hydrogen bonds.

Support by Diamond Light Source is acknowledged.

[1] JPCC 124.45 (2020), 24861-24873.

O 46.6 Tue 14:00 P2

Fluorescence Spectroscopy of Quinacridone Molecules on thin Epitaxial KCl(100) films. — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

Quinacridone forms one-dimensional chains on metal surfaces and thin epitaxial KCl films grown on Ag(100) [1]. TD-DFT predicts the transition dipole moment in the direction of chain growth. The resulting J-like coupling suggests superradiance which can be enhanced by chemical modifications that increase the inter-chain distance. However, no data on the optical properties of QA on KCl surfaces exist.

We have measured the fluorescence at cryogenic temperatures (7 K) of quinacridone (QA) and its fluorinated derivative (FQA) on ultrathin KCl films grown on Ag(100). Isolated QA molecules on KCl have a 0-0 transition at 20200 ± 200 cm^{-1}. The spectral lines have asymmetric shapes with large line widths (400 to 700 cm^{-1}). We relate the broadening to the weak bonding interactions of the molecule and the substrate.

Upon forming a 2D aggregate on the surface, we observe a significant red shift by 1600 cm^{-1} for QA and FQA. This can be understood by the attractive of the transition dipoles.

[1] JPCC **127** (2023): 23814-23826.

Acknowledgements: We thank the DFG for support via the research training group 2591, Mohammad Al Dubel and Sigurd Höger for kindly providing FQA molecules and Harshita Malik and Thomas Bredow for DFT calculations.

O 46.7 Tue 14:00 P2

On-Surface Coupling of Feringa-Type Molecular Motors — •David Le[1], Grant J. Simpson[1], Matthew J. Timm[1], Dongdong Liu[2], James M. Tour[2], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]Rice University, Houston, USA

Artificial molecular motors are fundamental components of nanoscale machines that convert external energy into uni-directional motion. On metallic surfaces, their operation can be probed with sub-molecular precision, allowing observation of rotational pathways and intermediates. In nanomachines, it could be advantageous to have not only one, but several motor units incorporated. However, the synthesis of such complex molecules is very challenging. Here, we studied whether individual Feringa-type motor units can be coupled covalently directly on a Au(111) surface to form bimotors, thus avoiding the complex synthesis and difficult deposition of molecules that contain more than one motor unit. Using low-temperature scanning tunnelling microscopy (STM) under ultrahigh vacuum conditions, we identified individual bimotor molecules after the coupling and could resolve distinct conformations. Moreover, conformational transitions and lateral translation could be induced by STM tip manipulation. The results for bimotors are compared with the mono-motors, i.e. before the coupling. Our results demonstrate controlled reactions and manipulation of molecular motors on a metallic surface, supporting the development of more complex nanomachines.

O 46.8 Tue 14:00 P2

Optical properties of pi conjugated molecule on insulator films supported by metal surface — •harshita malik — Clausius Institute for Physical and Theoretical Chemistry , University of Bonn,Bonn,Germany

Quinacridone (QA) is a pi-conjugated molecule whose optical properties are strongly influenced by hydrogen bonding and by its local environment. To establish consistent reference data, we determined the gas-phase and solution-phase excitation energies of QA using CCSD, TDDFT, and GW-BSE, and compared the results with available experimental spectra. These calculations provide reliable values for the ionization potential, the lowest singlet excitation, and the main vibronic features.

We then examined several structural variants of QA, including tautomers, substituted derivatives, and solid-state polymorphs. Their different packing motifs lead to measurable shifts in excitation energies, which we quantified using periodic GW-BSE.

To investigate QA on insulating surfaces, we used machine-learning potentials (MACE) combined with Bayesian optimization (BOSS) to identify stable adsorption geometries on KCl(100). The monomer and dimer structures obtained from this approach agree with DFT benchmarks and serve as starting points for further excited-state calculations on KCl films supported on Ag(100). I am currently working on computing excitons and other optical properties for QA adsorbed on these KCl/Ag surfaces to understand how substrate screening and adsorption geometry modify its electronic and optical response.

O 46.9 Tue 14:00 P2

Photoemission intermittency from organic quasi-one-dimensional crystals coupled with silver nanoparticles — •Moha Naeimi[1,2], Waqas Pervez[1,2], Frithjof Harmsen[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]Institute of physics, University of Rostock — [2]Department of life, light & matter, University of Rostock

Organic, quasi-one-dimensional crystals are suitable platforms for triplet exciton migration, latter only requiring minimal orbital coupling [1]. In organic molecules, triplet excitons can be generated via singlet fission, where excited singlet states convert into two long-lived triplet states [2]. We recently prepared long quasi-one-dimensional rubrene crystals on silicon substrates with a native thin silicon oxide layer (SiO2) [3]. After depositing Ag nanoparticles, we observe strong photoemission intermittency (blinking) at the interface sites and weak blinking on the rod crystal itself. In this work, we characterize the blinking in terms of its time traces and time-of-flight electron spectra. The blinking is consistent with exciton propagation that becomes trapped at nanoparticle-containing interface sites, where apparent electron binding energies shift to lower values. These molecule-nanoparticle systems offer promising pathways for directed energy transport and guided exciton migration.

[1] S. R. Yost et. al., J. Phys Chem C 116, 17369 2012. [2] T. Zhu et. al., J. Phys. Chem. Lett. 9, 6502 - 6510 2018. [3] Naeimi et. al, Adv. Opt. Mater., 2025 (DOI:10.1002/adom.202502744).

O 46.10 Tue 14:00 P2

Tip-induced hysteretic switching in copper-coordinated bipyridine (BIPY) thin films — •Sunny M P Gautam, Ankita Jaiswal, Thiruvancheril G Gopakumar, and Sandeep Verma — Indian Institute of Technology, Kanpur, India

In this work, we present a rationally designed hypoxanthine-based ligand, 1,9-bis(pyridine-2-ylmethyl) hypoxanthine (BIPY), specifically tailored for constructing functional surface-confined metal-organic networks (SMONs). The ligand integrates a π-conjugated purine core with flexible pyridyl donor arms, creating a nitrogen-rich, tridentate coordination environment ideal for forming robust 2D frameworks. Its conformational adaptability around metal centers enables dynamic metal*ligand interactions, offering a pathway toward SMON-based molecular switching driven by electronic-state transitions rather than geometric changes. Such electronically mediated bistability provides enhanced stability and potentially faster switching compared to conventional conformational molecular switches. Our results highlight BIPY as a promising platform for developing adaptive, switchable SMON architectures with potential applications in sensing, spintronics, data storage, and molecular logic systems.

O 46.11 Tue 14:00 P2

Monolayers of Thiols with Very High Dipole Moments Show Surprisingly Small Work Function Changes — Michael Gärtner[1], Andreas Terfort[1], and •Michael Zharnikov[1,2] — [1]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

The recently introduced concept of distributed dipoles in molecular self-assembly was combined with the standard dipolar tail group decoration in the context of electrostatic engineering of surfaces and interfaces by self-assembled monolayers (SAMs). To this end, thiol-anchored molecules, containing dipolar 2,5-bipyrimidine units within their molecular backbones, were decorated with either nitrile or dimethylamino tail groups and assembled on Au(111). The directions of the distributed and tail group dipoles were aligned either upwards or downwards to the anchor to achieve the maximum effect on the work function (WF) of the substrate. Despite a dense molecular packing and an upright molecular orientation, the decoration of the bipyrimidine thiols with the tail groups not only provided no WF gain but even had a detrimental effect in the dimethylamino case. This behavior is explained by the upside-down orientation of a part of the molecules in the SAMs, driven by the minimization of the energy associated with the strong dipole-dipole interaction between the SAM-forming molecules.

O 47: New methods: Theory

Time: Tuesday 14:30–15:30 Location: HSZ/0201

O 47.1 Tue 14:30 HSZ/0201

Energy-resolved tip-orbital fingerprint in scanning tunneling spectroscopy based on the revised Chen's derivative rule — Ivan Abilio[1,2] and •Krisztián Palotás[1] — [1]HUN-REN Wigner Research Center for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary

The revised Chen's derivative rule for electron tunneling [1] is implemented to enable computationally efficient first-principles-based calculations of the differential conductance dI/dV for scanning tunneling spectroscopy simulations [2]. By taking pristine and boron- or nitrogen-doped graphene sheets as sample surfaces, the reliability of our implementation is demonstrated by comparing its results to those obtained by the Tersoff-Hamann and Bardeen's electron tunneling models. It is highlighted that the energy-resolved direct and interference contributions to dI/dV arising from the tip's electron orbitals result in a fingerprint of the particular combined surface-tip system. The significant difference between the electron acceptor boron and donor nitrogen dopants in graphene is reflected in their dI/dV fingerprints. The presented theoretical method allows for an unprecedented physical understanding of the electron tunneling process in terms of tip-orbital-resolved energy-dependent dI/dV maps that is anticipated to be extremely useful for investigating the local electronic properties of novel material surfaces in the future. References: [1] Phys. Rev. B 91, 165406 (2015). [2] Phys. Rev. B 111, 245425 (2025).

O 47.2 Tue 14:45 HSZ/0201

Innovative Approaches to Semiconductor Surface Oxidation Studies Using Active Learning and MLIP — •Ondrej Krejci[1,2], Shola Adyemi[2], Konstantinos Konstantinou[2], and Milica Todorović[2] — [1]Department of Chemistry and Materials Science, Aalto University, Espoo, Finland — [2]Department of Mechanical and Materials Engineering, University of Turku, Turku, Finland

Oxygen passivation of InAs surfaces critically affects material performance in electronic devices, but the nature of the oxide surface reconstruction is not well characterized. To address this, we employ a machine learning (ML) driven workflow. Starting from the $\zeta(4\times2)$ reconstruction of pristine InAs(100) [1], we use Bayesian Optimization [2] to identify oxygen binding sites. This allows us to populate the surface with increasing number of oxygen atoms. The oxide models serve as input for a ML interatomic potential based on the MACE model [3], trained via the active learning method PALIRS [4]. The potential is used for molecular dynamics simulations to identify promising candidates for the oxidized InAs(100) surface reconstruction. Our workflow enables an efficient exploration of configurational space surpassing traditional computational approaches.

[1] Appl. Phys. A 75, 89 (2002)
[2] Npj. Comput. Mat. 5, 35 (2019)
[3] NeurIPS 35, 11423 (2022)
[4] Npj Comput. Mat. 11, 324 (2025)

O 47.3 Tue 15:00 HSZ/0201

Complete basis limit with hybrid functionals using LAPW — •Janis Uzulis and Andris Gulans — University of Latvia, Riga, Latvia

We present a systematic framework for achieving the complete basis limit (CBL) for molecules and solids in hybrid functional calculations with density functional theory using the linearized augmented plane wave (LAPW) method. Standard LAPW calculations with nonlocal exchange employ radial basis functions and core orbitals obtained from a (semi)local functional, leading to inconsistencies that prevent the calculations from converging to CBL. We address this issue and achieve the same level of precision that previously was attainable only with local functionals. By applying this method, we obtain the Hartree-Fock total energy for crystals with a few μHa precision. Aside from high-quality reference data (reaction energies, cohesive energies and equation of state) for computational-chemistry and band-structure codes, our work provides an insight into the range of applicability of the standard approach to hybrids in LAPW.

O 47.4 Tue 15:15 HSZ/0201

AI-Driven Optimization Techniques for Density Functional Theory Calculations — Álvaro Fraile-Carmena[1], Damián Sánchez-Maqueda[1], Cristian Ramírez-Atencia[1], and •María Camarasa-Gómez[2] — [1]Universidad Politécnica de Madrid, C/ Alan Turing, s/n, Madrid 28031, Spain — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Paseo de Manuel Lardizábal 5, Donostia-San Sebastián 20018, Spain

Accurately determining optoelectronic properties of molecules and solids is an ongoing challenge in first-principles methods. This objective has gained even more relevance, as research on quantum materials evolves rapidly. So far, density functional theory (DFT) has remained the primary computational tool for this task. However, reaching with DFT accuracy levels comparable to many-body perturbation theory still requires significant computational effort [1]. Here we introduce an approach that integrates AI-driven optimization techniques into DFT workflows [2]. Embedding these optimization methods directly in ab initio software enhances both accuracy and efficiency. We present results obtained with surrogate models and state-of-the-art open source optimization libraries [3], showing their potential to accelerate and improve electronic structure simulations. [1] M. Camarasa-Gómez, S. E. Gant, et al., npj Comput. Mater. 10, 288 (2024) [2] Á. Fraile-Carmona, D. Sánchez-Maqueda, C. Ramírez-Atencia, and M. Camarasa-Gómez (2025) [in preparation] [3] J. Blank, and K. Deb, IEEE Access 8, 89497 (2020)

O 48: Metal & Semiconductor substrates: Structure, epitaxy and growth

Time: Tuesday 14:30–16:00 Location: HSZ/0204

O 48.1 Tue 14:30 HSZ/0204

Electric-field induced formation of a two-dimensional adatom gas on cryogenic Li(110) — Shyam Katnagallu[1], Samuel Mattoso[1], Huan Zhao[1,2], Se-Ho Kim[1,3], Jing Yang[1], Baptiste Gault[1,4], •Christoph Freysoldt[1], and Jörg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf Germany — [2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China — [3]Department of Materials Science and Engineering, Korea University, Seoul, Korea — [4]Department of Materials, Royal School of Mines, Imperial College London, UK

The field evaporation behavior of Li at 60 K in atom probe tomography (APT) shows very inhomogeneous distribution on the detector hit map with hot-spot sites accounting for thousands of evaporations, implying an unusual high surface mobility. We therefore investigated the ad-atom energetics and diffusion behavior on the prototypical Li(110) surface in the presence of the very high fields (10^{10} V/m) by density-functional theory. Two key effects are found to jointly explain the experimentally observed behavior. Firstly, free ad-atoms become energetically favorable over kink sites at fields above 10 V/nm, making sizeable ad-atom densities in thermodynamic equilibrium. Secondly, the ad-atom diffusion barrier vanishes at ∼11 V/nm due to a degeneracy of the on-top and bridge sites. We suggest that a highly dynamic adatom gas forms, that enables efficient transport to evaporation hotspot sites. Our static calculations are corroborated by molecular dynamics simulations, that show the spontaneous ad-atom emission from a kink-site enabled by the field.

O 48.2 Tue 14:45 HSZ/0204

Structural analysis of the interaction of H_2S with the FeO_2 chain phase on Ir(100) — •Alexander Wegerich, Eric Engel, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

On the Ir(100) surface, a self-organised growth of oxide chains of the form Ir(100)-(3 × 1)-MO_2 (M = Mn, Fe, Co and Ni) can be observed. These transition metal oxide chains are shifted by half an Ir(100) lattice constant with respect to the iridium rows [1]. Furthermore, it is

possible to reduce these oxide chains to an Ir(100)-(3 × 1)-MIr_2 (M = Mn, Fe, Co and Ni) surface alloy by annealing under H_2 atmosphere, now with the reduced chains aligned to the Ir rows [2].
Using quantitative LEED-IV analyses, STM and DFT, we examine whether the iron oxide chain phase can be structurally changed and/or tuned by reaction with S, the only other non-metallic chalcogen. In contrast to oxygen, sulphur does not create a Ir(100)-(3 × 1)-FeS_2 chain-like phase, but a c(6 × 2) superstructure. Prepared by annealing the FeO_2 chains under a H_2S atmosphere, the oxide chains are reduced and sulphur adsorbes on them. The so-formed c(6 × 2) can be interpreted as a c(2 × 2)-S adphase on the Ir(100)-(3 × 1)-$FeIr_2$ chains.
[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)
[2] P. Ferstl et al., Phys. Rev. B **96**, 085407 (2017)

O 48.3 Tue 15:00 HSZ/0204

STM study of surface evolution and phase stability in Sn/Pt(111) systems — •Qing Shi, Fumio Komori, Masaki Mizuguchi, and Toshio Miyamachi — Nagoya University, Nagoya, Japan

The formation of Pt_3Sn surface alloys on Pt(111) is of considerable interest for applications in catalysis and topological electronics. Depositing Sn on Pt(111) followed by annealing offers a route to realize atomically flat, single-crystalline $Pt_3Sn(111)$ surfaces suitable for detailed surface studies. Here, we reveal how the annealing process directly controls the surface morphology and local electronic structure in Sn/Pt(111) systems by scanning tunneling microscopy and spectroscopy (STM/S).

In the lower-temperature regime ($<$ 400 K), where a Sn overlayer is stabilized, Sn atomic layers preferentially attach to step edges. The STS measurements indicate that the Sn overlayer is metallic due to hybridization with the Pt substrate. Upon annealing to higher temperatures, the surface undergoes Pt-Sn alloying, leading to the formation of a Pt3Sn phase across the surface. This transition is accompanied by pronounced island coarsening, morphological rounding, and an increase in local disorder, driven by thermally activated atom processes. Equilibrium shape analysis of the alloy islands reveals nearly isotropic step free energies, indicating minimal energetic differences between alternating A- and B-type step edges. Spectra acquired on the Pt_3Sn terraces show a high density of states near the Fermi level, corresponding to contributions from both bulk and surface electronic states.

O 48.4 Tue 15:15 HSZ/0204

Enhanced thermal switching of an azobenzene derivative via metal doping on graphitic surfaces. — •Nidhi Rawat[1], Hariom Birla[2], and Thiruvancheril G. Gopakumar[3] — [1]Indian Institute of Technology Kanpur, Kanpur, India — [2]Indian Institute of Technology Kanpur, Kanpur, India — [3]Indian Institute of Technology Kanpur, Kanpur, India

The thermal isomerization (switching) of azobenzene derivatives is often limited by high activation barriers, limiting efficient switching between trans and cis configurations induced by heat. In this study, we first examined the thermal induced switching of pristine azobenzene-based thin films and observed no isomerization upon heating. Upon introducing a metal dopant into the films, several morphological changes are observed, across varying molecular coverages, upon heating confirming that thermal switching is readily induced in the doped films. The analysis of the morphology and microscopic structure of the film is analysed using AFM and STM. These results clearly demonstrate that metal doping can effectively modulate the energy barrier and facilitate thermally driven molecular switching. This approach offers a promising pathway to tailor the isomerization dynamics of molecular systems, providing new opportunities for the development of thermally responsive devices.

O 48.5 Tue 15:30 HSZ/0204

Evolution of surface superstructures on altermagnetic MnTe thin films — •Marco Dittmar, Franziska Beisler, Hannes Haberkamm, Lena Hirnet, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

MnTe has recently attracted significant attention as a workhorse altermagnet, where real space spin arrangements give rise to symmetry-driven, momentum-dependent spin splitting without net magnetization. In terms of basic research as well as for enabling high-quality interfaces in potential devices, the investigation of the surface atomic structure of MnTe becomes very important. In this talk, we present an electron diffraction surface analysis of epitaxially grown MnTe thin films, highlighting the factors that govern their surface atomic structure. In particular, we discuss how variations in Te flux and surface evaporation conditions guide the formation and stability of different surface reconstructions, we have found experimentally.

O 48.6 Tue 15:45 HSZ/0204

Atomic structure of MBE-grown Ta-Ge alloy on Ge(001). — •Suhani Singh[1], David Sommers[1], Patrick Strohbeen[2], Yi-Hsun Chen[1], Javad Shabani[2], Arkady Fedorov[1], and Peter Jacobson[1] — [1]School of Mathematics and Physics, University of Queensland, St. Lucia, Queensland 4072, Australia — [2]Center for Quantum Information Physics, Department of Physics, New York University, New York, New York 10003, USA

Tantalum-germanium (Ta-Ge) alloys are a promising option for superconducting devices.[1] Here, we study the atomic-scale structure and thermal evolution of an MBE-grown Ta-Ge alloy film on Ge(001) using scanning tunnelling microscopy (STM) and synchrotron-based soft x-ray photoemission (XPS). A series of annealing steps between 673 K and 873 K smoothed the initially corrugated surface and enabled atomic-resolution STM. Short anneals at 873 K, reveal three-fold symmetric surface domains. Longer anneals at 873 K led to the appearance of square lattice consistent with Ta(100), coexisting with more corrugated regions. Further temperature increase made the surface progressively rougher and difficult to image. Synchrotron-based XPS shows higher temperature annealing produces a Ge-rich surface, suggesting Ta migrates into the bulk. These preliminary results map out how thermal processing affects the Ta-Ge surface and will guide strategies to obtain cleaner, sharper superconductor-semiconductor interfaces.

[1] Patrick J Strohbeen et al. *Molecular beam epitaxy growth of superconducting tantalum germanide*. Applied Physics Letters 124, 9 (2024).

O 49: Plasmonics and nanooptics: Light-matter interaction, spectroscopy I

Time: Tuesday 14:30–15:45 Location: HSZ/0403

O 49.1 Tue 14:30 HSZ/0403

Beyond-Dipole Approaches to Generating and Applying Twisted Light — •Esra Ilke Albar[1], Franco Bonafé[1], Valeriia Kosheleva[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max-Planck-Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, DE — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA

We perform numerical electrodynamics simulations where a nanoplasmonic Archimedean spiral is targeted with a circularly polarized, 8-cycle plane wave pulse to probe the generation of twisted pulses, i.e., fields with orbital angular momentum(OAM). We identify mismatches between the generated pulse and the ideal OAM beams, which motivates us to discuss the spatiotemporal optical vortices (STOVs). All realistic electromagnetic fields are finite pulses, while the structural properties of plasmonic OAM generators are often adjusted to the central wavelength. As a next step, we employ a two-particle point charge system to map the local OAM density and confirm the space dependence of the generated pulse. This pushes us to expand beyond the known electric dipole approximation(EDA). We introduce our beyond dipole formalism and present high harmonic generation results computed within this approach.

O 49.2 Tue 14:45 HSZ/0403

Electro-Optic Phonon Polaritons — •Michael S. Spencer[1], Olga Minakova[1], Maximilian Frenzel[1], Joanna M. Urban[1], Martin Wolf[1], and Sebastian F. Maehrlein[1,2,3] — [1]FHI Berlin — [2]HZDR — [3]TU Dresden

Ultrafast control of fundamental excitations and order parameters represents a major driving force for the rising field of terahertz (THz) cavity electrodynamics. However, most efforts to date have not taken full advantage of THz sampling capabilities. By using an electro-optic crystal to fill a cavity, we directly measure intra-cavity electric fields, and polarizations arising from dipole-active excitations, all in the time domain. We identify that under cryogenic conditions, and in high-quality cavities, a polaritonic state is formed from the superposition of cavity photons and optical phonons. We explore the relationship between the light-matter coupling strength and temperature, and between the polariton splitting and cavity quality factor. With our novel electro-optic cavity design, we are able to investigate the detuning-dependence of the strong coupling behavior, obtaining the full picture of light-matter interactions. Furthermore, we reveal fluence-dependent polariton dynamics, indicative of significant coupling beyond the harmonic approximation. This identification of strong light-matter interactions in electro-optic cavities opens an important new testing ground for measuring novel, light-matter-entangled states.

O 49.3 Tue 15:00 HSZ/0403

Femtosecond and attosecond correlations in multi-electron pulses — •Rudolf Haindl[1,2], Valerio Di Giulio[1,2], Armin Feist[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany

In femtosecond electron emission from nanoscale field emitters, Coulomb interactions result in structured few-electron states exhibiting strong correlations in energy [1,2], transverse momentum [1], and time [3]. Here, we combine femtosecond-gated, event-based detection with inelastic electron-light scattering to directly map the phase-space distribution of two-electron states [4].

Our experiments reveal a bimodal structure in longitudinal phase space, distinguishing contributions from interparticle interaction and dispersion. Furthermore, we demonstrate that global phase modulation coherently shapes the few-electron distribution to exhibit attosecond temporal correlations. We show how this controlled phasing drives a multi-electron quantum walk, a phenomenon that can be harnessed to produce tailored excitations and super-radiance via two-electron energy post-selection.

[1] R. Haindl et al., Nat. Phys. 19, 1410-1417 (2023).
[2] S. Meier et al., Nat. Phys. 19, 1402-1409 (2023).
[3] J. Kuttruff et al., Sci. Adv. 10, eadl6543 (2024).
[4] R. Haindl et al., Phys. Rev. Lett. 135, 165002 (2025).

O 49.4 Tue 15:15 HSZ/0403

Quantum-electrodynamical density-functional theory for periodic solid-state materials — •Benshu Fan[1], I-Te Lu[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute

Quantum-electrodynamical density-functional theory (QEDFT) has emerged as a powerful first-principles framework for describing properties of materials coupled to quantized electromagnetic fields. While it has been successfully applied to capture cavity-induced modifications of electronic structures mainly for atoms and molecules, a consistent treatment of phonon-related and optical properties for periodic solids remains elusive. In this work, we present a unified QEDFT framework that incorporates collective light-matter coupling in the electronic ground state, density functional perturbation theory for phonons, and real-time time-dependent QEDFT for optical excitations. This approach enables ab initio calculations of cavity-modified electronic and phononic dispersions, Born effective charges, dielectric tensors, and both non-resonant and resonant optical absorption spectra for solids. Using wurtzite gallium nitride (GaN) embedded in an optical cavity as an example, we show how the quantized vacuum field reshapes electronic and phononic properties and gives rise to possible experimentally observable signatures in the dielectric function and absorption spectra. Our results establish QEDFT as a general first-principles framework for exploring and predicting cavity-modified properties of quantum materials.

O 49.5 Tue 15:30 HSZ/0403

Anyonic Chern Insulator in Graphene Induced by Surface Electromagnon Vacuum Fluctuations — •Xinle Cheng[1], Emil Viñas Boström[1], Frank Y. Gao[2], Edoardo Baldini[2], Dante M. Kennes[1,3], and Angel Rubio[1,4] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Department of Physics, The University of Texas at Austin, Austin, Texas, 78712 — [3]Institute for Theory of Statistical Physics, RWTH Aachen University, 52056 Aachen, Germany — [4]Initiative for Computational Catalysis, The Flatiron Institute, Simons Foundation, New York City, NY 10010, USA

Sub-wavelength cavities have emerged as a promising platform to realize strong light-matter coupling in condensed matter systems. Previous studies are limited to dielectric sub-wavelength cavities, which preserve time-reversal symmetry. Here, we lift this constraint by proposing a cavity system based on magneto-electric materials, which host surface electromagnons with non-orthogonal electric field and magnetic field components. The quantum fluctuations of the surface electromagnons drive a nearby graphene monolayer into an anyonic Chern insulator, characterized by anyonic quasi-particles and a topological gap that decays polynomially with the graphene-substrate distance. Our work opens a path to controllably break time-reversal symmetry and induce exotic quantum states through cavity vacuum fluctuations.

O 50: Electronic structure theory II

Time: Tuesday 14:30–16:15 Location: TRE/PHYS

O 50.1 Tue 14:30 TRE/PHYS

Efficient DFPT for 2D Films in the FLAPW Code FLEUR — •Thomas Bornhake[1,2], Alexander Neukirchen[1], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany

Interest in structural instabilities, magnetism, transport, and superconductivity in 2D films is rapidly increasing, and all of these phenomena involve phonons. However, *ab initio* phonon calculations for films typically require large supercells, which include substantial vacuum. As a result, they become computationally expensive. In this talk, we present an efficient and unique DFPT implementation in the context of the all-electron FLAPW code FLEUR [1,2] that treats films as single slabs in a truly 2D geometry perfectly embedded in semi-infinite vacuum [3]. We outline the key features of the method, benchmark it against the commonly employed supercell approach, and show first results on how a homogeneous external electric field modifies the phonon properties.

This work was supported by the CoE-MaX (EuroHPC Joint Undertaking, Grant 101093374) and DFG through CRC 1238 (Project C01).

[1] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de

[2] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).

[3] M. Posternak *et al.*, Phys. Rev. B **21** 5601 (1980).

O 50.2 Tue 14:45 TRE/PHYS

Valence only FLOSIC with pseudo core electrons — •Simon Liebing and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, 09599 Freiberg, Germany

Over the past decade, the FLOSIC method [1, 2] has demonstrated its versatility and applicability to a wide range of systems. However, it has been observed that this method can require significant computational time, particularly when adjusting the core electrons in the case of heavier elements. Previous work has shown that FLOSIC calculations can be effectively carried out using pseudopotentials [3]. In the case of heavier atoms, however it is possible that the valence orbital descriptors may shift too close to the core region due to the limitations of pseudopotentials. In this work, the authors introduce a novel approach to also account for the repulsive interactions between the core and valence electron FLOSIC descriptors in case of pseudopotentials. This method has the potential to significantly reduce the computational cost typically associated with SIC calculations compared to standard DFT methods. References: [1] M. R. Pederson et al., J. Chem. Phys., 140, 121103 (2014) [2] S. Schwalbe, et al., J. Chem. Phys., 153, 8, 2020. [3] S. Liebing et al., DPG Verhandlungen Berlin, O, Session 82, Contribution 8, 2018.

O 50.3 Tue 15:00 TRE/PHYS

Spectroscopy of chemisorped systems from a first-principles local-orbital representation — •Simiam Ghan and Jens Nørskov — Technical University of Denmark DTU

We present a local-orbital representation of density functional theory (DFT) which elucidates the properties of chemisorped systems. A direct calculation of orbital overlap and coupling matrix elements between the adsorbate and surface allows us to construct the hybridization function, familiar from e.g. Anderson-Newns-Grimley models, which encodes rich orbital phase interactions[1]. Beyond a qualitative tool, we demonstrate the quantitative correspondence of this object to observables in ultrafast spectroscopy and scanning-tunneling spectroscopy. The scheme is generally useful to assess the coupling between a local state and its environment from first principles.

[1] S. Ghan *et al.*, J. Chem. Phys. 158, 234103 (2023).

O 50.4 Tue 15:15 TRE/PHYS

Quantum-mechanical analysis of the 4H-SiC surface — •Kateřina Dočkalová[1,2], Martin Friák[2], and Jana Pavlů[1] — [1]Dept. Chem., Masaryk Uni., Brno, Czech Rep. — [2]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Rep.

Silicon carbide (SiC) is a key wide-bandgap semiconductor employed in high-power and high-voltage electronic devices. Among its polytypes, 4H-SiC is particularly promising for next-generation power electronics. We investigated the atomic and electronic structure of the 4H-SiC (0001) surface with a specific focus on the challenges of modelling polar orientations. To accurately capture the intrinsic surface properties, we evaluate the planar-averaged electrostatic potential and the electron localisation function (ELF) using various models (differing in bottom-surface termination, passivation with pseudohydrogens, and vacuum thickness) and applying electrostatic corrections. These strategies suppress artificial dipole moments and eliminate spurious internal electric fields that often compromise surface calculations. We find that either carbon termination at the bottom surface or pseudohydrogen passivation can individually introduce a spurious internal electric field manifested in the vacuum potential. Interestingly, applying electrostatic corrections does not improve the electrostatic-potential profile for models in which the vacuum region is already sufficiently thick. Financial support from the Czech Academy of Sciences (Praemium Academiae, M.F.) and Masaryk University (MUNI/A/1691/2024) is acknowledged. Computational resources were provided via e-INFRA CZ (ID:90254).

O 50.5 Tue 15:30 TRE/PHYS

Quantifying conductance variations in single molecule junctions using machine learning — •Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

In single molecule circuits, conductance (the inverse of resistance) is strongly dependent on the junction geometry. Break-junction experiments are often carried out at room temperature, where many molecular conformations are sampled during the measurements. In contrast, the computational cost of DFT-NEGF calculations restricts them to only a few geometries.

We recently developed a computationally efficient method to calculate molecular conductance within DFT for thousands of geometries, based on small Au-molecule-Au clusters [1,2]. Their geometry is taken from MD simulations of the junction at room temperature. We can thus compute within DFT the conductance for tens of thousands of thermally-accessible molecular geometries.

We study typical conjugated and alkane molecules and interpret these large conductance datasets with machine learning methods including regression models, feature importance techniques, and SHAP analysis. Our work identifies which of the bond lengths, angles, or dihedral angles in the molecule, all of which are changing continuously and simultaneously, have a larger impact on conductance.

[1] H. Vazquez, J. Phys. Chem. Lett. 13 9326 (2022)

[2] E. Montes, W.Y. Rojas and H. Vázquez, J. Phys. Chem. C 129, 9947 (2025)

O 50.6 Tue 15:45 TRE/PHYS

Towards Accurate Surface Adsorption Through a Numeric-Orbital FDET Framework — •Danjo De Chavez[1] and Reinhard J. Maurer[1,2,3] — [1]Department of Chemistry, University of Warwick, UK — [2]Department of Physics, University of Warwick, UK — [3]Faculty of Physics, University of Vienna, AT

Multiscale embedding methods balance accuracy and computational efficiency in modeling extended materials by combining high-level treatments of active regions with lower-level descriptions of their environments. We implemented Frozen Density Embedding Theory (FDET) with Freeze-and-Thaw (F&T) cycles in the numeric atomic orbital code FHI-aims, enabling consistent cluster and periodic calculations. Initial electron densities are constructed from free-atom superpositions, with one subsystem kept frozen while the other is optimized. The implementation leverages the efficient parallelization of FHI-aims. Embedding potential and subsystem density are decomposed using an auxiliary basis set via an RI framework, facilitating reconstruction in the real space. This method enables accurate predictions with high-level theory for adsorption, bond dissociation, optical excitation, and charge-transfer phenomena relevant to surface catalysis and spectroscopy.

O 50.7 Tue 16:00 TRE/PHYS

Brillouin zone sampling in ONETEP — •Chengcheng Xiao, Peter Haynes, and Arash Mostofi — Department of Material, Imperial College London, London SW7 2AZ, United Kingdom

ONETEP is a parallelised linear-scaling density-functional theory (DFT) simulation software package designed for large-scale calculations of properties of materials. It was engineered under the premise that, for self-consistent calculations of systems with thousands of atoms, the Brillouin zone only needs to be sampled at its centre - the Gamma-point.

Whilst this is a suitable approximation for large systems, it often leads to the unnecessary use of large supercells of structures where periodicity can be exploited. For those systems, a more suitable method is to sample the Brillouin zone along the periodic directions.

In this work, we introduce a new Brillouin zone sampling technique in ONETEP where the localisation constraint imposed on the basis functions is selectively lifted along the periodicity directions, making it possible to perform a "hybrid" calculation where the best scaling can be achieved by incorporating both Brillouin zone sampling and linear-scaling techniques. Furthermore, if the unit cell is small along all directions, all localisation constraints can be lifted, which effectively turns ONETEP into a plane-wave code. This enables us to compare the algorithmic accuracy of ONETEP to other DFT codes on the same footing. These developments enable much more efficient calculations on short and intermediate-scale periodic systems, such as bulk crystals, nanowires, surfaces, and interfaces.

O 51: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Tuesday 14:30–15:45 Location: TRE/MATH

Invited Talk O 51.1 Tue 14:30 TRE/MATH
Ultrafast aqueous electric double-layer dynamics — •Mischa Bonn — Max Planck Institute for Polymer Research

The formation of electric double layers (EDLs) at solid-liquid interfaces is universal, yet their molecular structure and dynamics remain incompletely understood. Building on recent advances in interface-specific spectroscopy and nanofluidic model systems, this talk will address how interfacial polarization, geometric confinement, and charge density collectively shape the structure and dynamics of water at electrochemical interfaces. We will highlight new femtosecond-resolved optical spectroscopy measurements that access the genuine ultrafast response of the aqueous EDL, revealing that field-driven ionic rearrangements and solvent reorganization occur on time scales of only a few tens to hundreds of picoseconds - significantly faster than expected from classical diffusion-limited models. These results demonstrate that collective many-body interactions and short-range correlations dominate the EDL response long before macroscopic diffusion sets in. Taken together, the studies provide a molecularly consistent picture in which interfacial polarization and charge act in concert to control water structure and dynamics across electrochemical interfaces, with direct implications for energy conversion, ion transport, and operando spectroscopies of electrified surfaces.

O 51.2 Tue 15:00 TRE/MATH
Second-order nonlinear vibrational spectroscopy: from depth-resolved studies at charged aqueous interfaces towards determining excitonic-vibrational coupling in hybrid heterostructures — •Debojyoti Roy, Sarabjeet Kaur, Álvaro Díaz Duque, Martin Wolf, Alexander P. Fellows, and Martin Thämer — Fritz-Haber-Institut of the Max Planck Society, 14195 Berlin, Germany

The properties of charged aqueous interfaces are governed by interfacial electric fields that influence ion distributions in the liquid phase, forming an electric double layer. While the evolution of the electric potential is relatively well described by theoretical models, much less is known about the influence of the DC fields on the interfacial molecular structure of water and its evolution with depth. Using our recently developed combined sum- and difference-frequency generation spectroscopy (SFG/DFG), we investigate the depth-dependent water structure at charged interfaces as a function of ionic strength, obtaining deep insight into the anisotropic orientational distribution of water and detailed information on the properties of the hydrogen bond network at different distances from the phase boundary.

Besides depth-resolution, the complementary information from SFG and DFG responses can also be used to isolate coupling terms in doubly-resonant studies. Here we also explore this possibility conceptually and propose such studies on exciton-vibrational coupling in 2D material/organic interfaces, which have various applications in solar cells but still lack understanding of their physicochemical properties.

Invited Talk O 51.3 Tue 15:15 TRE/MATH
Interface-specific nonlinear THz spectroscopy — •Chuanshan Tian — Department of Physics, Fudan Univ. China

Quantum confinement and proximity effects at material interfaces give rise to a range of novel physical and chemical phenomena, substantially advancing our ability to understand and control material properties. The development of in situ and interface-sensitive characterization techniques is therefore critical for uncovering the microscopic mechanisms governing interfacial systems and for improving device performance. This presentation will outline recent advances in interface nonlinear optical spectroscopic techniques, with a particular focus on their extension into the (multi-)terahertz spectral regime. Applications of these methods in probing interfacial microstructures and dynamic processes will be discussed, highlighting their potential for resolving complex interfacial phenomena with high specificity.

O 52: Oxide and insulator surfaces: Structure, epitaxy and growth I

Time: Tuesday 14:30–16:00 Location: WILL/A317

Invited Talk O 52.1 Tue 14:30 WILL/A317

Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope

— •Friedrich Esch — TU Munich, Garching, Germany

Reducible oxides are versatile supports for catalytically active particles. Their reducibility offers the possibility to steer fundamental properties such as cluster stability and shape, charge transfer, lattice oxygen reverse spillover, or encapsulation. In this talk, I present our fundamental studies on the dynamics of atomically precise Pt clusters on two complementary supports, Fe_3O_4(001), where reduction leads to interstitial diffusion and hole formation, and CeO_2(111), where it leads instead to the formation of surface-near vacancies. As a local probe, we employ scanning tunneling microscopy (STM) at elevated temperatures and under reactive gas environments, upgraded with sophisticated tools for fast movie acquisition and cluster tracking. We complement this structural characterization with integral pulsed valve molecular beam "sniffer" activity and x-ray photoemission measurements. While on magnetite stabilization of even very small clusters via encapsulation is observed [1,2], on ceria, a dimensionality crossover from 3D to 2D clusters occurs, triggered by the degree of surface reduction [3].

[1] S. Kaiser et al., ACS Catal. 11 (2021) 9519.
[2] S. Kaiser et al., ACS Catal. 13 (2023) 6203.
[3] J. Reich et al., ACS Catal. 15 (2025) 18369.

O 52.2 Tue 15:00 WILL/A317

Segregation effects in 2D mixed oxide nano-islands: edge structure and composition in V(2-x)FexO3 monolayer islands

— Ying Wang[1], Piotr Igor Wemhoff[1], Ghada Missaoui[1], Niklas Nilius[1], Jacek Goniakowski[2], and •Claudine Noguera[2] — [1]Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne Université, Institut des Nanosciences de Paris, Paris, France

Low-coordinated atoms located at the surface or edges of oxide nanostructures play a crucial role in adsorption and reaction processes in heterogeneous catalysis. Contrary to binary compounds, there is a significant lack of information on their nature and behavior available for ternary materials. In this study, high-resolution scanning tunneling microscopy, DFT calculations and Monte Carlo simulations have been used to decipher the edge structure and composition of mixed V(2-x)FexO3 honeycomb monolayer islands grown on Pt(111).

DFT calculations and MC simulations demonstrate that, in contrast to a clear preference for VO-terminated edges in the pure V2O3 system, Fe segregation to the edges of mixed films tends to produce undercoordinated edge Fe cations, with a ratio of Fe/VO edge species highly sensitive to the oxygen environment. We show that the different oxygen affinity of V and Fe cations, yielding different bonding strengths of terminal vanadyl and ferryl groups are the main cause of the segregation pattern. The sensitivity of edge composition to the oxygen environment thus represents a lever for manipulating the edge configurations and tuning their catalytic response.

O 52.3 Tue 15:15 WILL/A317

Ultra-high THz-confinement in $LaAlO_3$ twin-walls

— •Jakob Wetzel[1], Javier Taboada-Gutiérrez[2], Susanne C. Kehr[1], Alexey B. Kuzmenko[1,3], Lukas M. Eng[2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]University of Geneva, Department of Quantum Matter Physics (DQMP), Geneva 1211, Switzerland — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Recent advancements in polaritonics and nano-photonics have focused on the confinement of optical modes in ultra-thin films, 2D materials, and interfaces in order to uncover pathways toward ultra-compact nanophotonic circuits and sub-diffraction imaging technologies. Such approaches to THz-confinement face fundamental challenges such as inherent strain, defects, and lattice mismatches.

Here we present the experiment- and simulation-based investigations of ferroelastic twin-walls in $LaAlO_3$, which provide a *perfect* strain-free interface to explore optical effects emergent from the coincidence of two equal but directionally rotated optical axes. Scanning near-field optical microscopy (s-SNOM) in combination with the HZDR free electron laser FELBE shows an ultra-high confinement (>250) of THz-fields at these twin-wall. Experimental results are reproduced by COMSOL-simulations and understood with an adapted dipole model.

O 52.4 Tue 15:30 WILL/A317

Atomic-scale effects of surface modifications on mixed conducting oxides

— •Matthäus Siebenhofer, Claudia Steinbach, and Jürgen Fleig — TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria

Mixed ionic and electronic conducting (MIEC) oxide surfaces play a critical role in various technologies due to their high catalytic activity for processes such as oxygen reduction, oxygen evolution, and (photo)electrochemical water splitting. Recent advances have shown that even minute amounts of surface modifications can dramatically alter the work function and the catalytic performance but the detailed mechanisms behind these effects remain poorly understood.

This contribution discusses our efforts to understand the fundamental processes that occur during modification of MIEC oxide surfaces with ultra-thin oxide layers and acidic contaminants. We employ in-situ impedance spectroscopy during pulsed laser deposition (i-PLD) to monitor changes in the oxygen exchange activity of pristine thin film surfaces; X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) provide insights into atomic-scale processes induced by these modifications.

Our results demonstrate that surface modifications introduce charge redistribution between the modification and the MIEC oxide. These effects are governed by the ionic potential and acidity of both the host material and the modifying species. Based on these observations, we provide design strategies to tailor optimized material combinations for targeted catalytic applications.

O 52.5 Tue 15:45 WILL/A317

Probing electron-transfer between layers of a CrOx/Pt(111) thin film via workfunction and adsorption measurements in the STM

— •Ghada Missaoui[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

Low-temperature tunneling spectroscopy has been employed to probe the workfunction of atomically flat Cr-oxide single- and double-stack films grown on Pt(111). The single-stack Cr3O6 trilayer exhibits an exceptionally high workfunction of more than 7.0 eV, decreasing to 5.0 eV for Cr6O11 double-stacks. The charge redistribution behind this workfunction drop was analyzed by density functional theory. The high workfunction of Cr3O6 trilayers originates from a massive electron transfer from the Pt(111) support into empty Cr-states that reduces 2/3 of the oxide cations from their formal 4+ to a 3+ charge state. The negative surface dipole diminishes upon growing a Cr-O honeycomb plane on top of the trilayer, forming a Cr6O11 double-stack. The ad-layer acts as electron donor, allowing the charge transfer from the platinum to decrease substantially. The charge redistribution not only triggers the detected workfunction drop but also leads to a different reactivity of single- versus double-stack CrOx films, as demonstrated with MgPc adsorption experiments performed with the STM.

O 53: Topical Talk Parkinson

Time: Wednesday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 53.1 Wed 9:30 TRE/PHYS
Single-Atom Catalysis: Insights From Model Systems — •Gareth S. Parkinson — Institute of Applied Physics, TU Wien, Vienna, Austria

Single-atom catalysis promises maximal atom efficiency, tunable active sites and improved selectivity, and is now a key concept in the design of sustainable catalysts. Yet many of the central claims about what single-atom catalysts are, how they operate, and whether they remain truly isolated under reaction conditions are still under debate. In this overview talk I will use oxide-supported single atoms as case studies to examine what can really be established about structure, stability and mechanism, and where the evidence remains ambiguous. I will show how atomically well-defined model surfaces, probed by STM, noncontact AFM, XPS and vibrational spectroscopy, in tight integration with theory, can test key assumptions about single-atom catalysis. I will close with a perspective on outstanding challenges, from adsorbate induced restructuring and water to the transfer of insight from model systems to working catalysts.

O 54: Nanostructured surfaces and thin films

Time: Wednesday 10:30–12:30 Location: HSZ/0201

O 54.1 Wed 10:30 HSZ/0201
Advanced Characterization of Black Silicon via AFM and XPS: Geometric and Chemical Insights for better characterization of PV materials — •Jens Neurohr[1], Hendrik Hähl[1], Karin Jacobs[1], Michael Klatt[2], and Frank Müller[1] — [1]Experimental Physics and Center for Biophysics, Saarland University, Campus E2 9, 66123 Saarbrücken, Germany — [2]German Aerospace Center (DLR), Institute for Material Physics in Space, 51170 Köln, Germany

Understanding the link between surface geometry and chemical properties is crucial for photovoltaic (PV) applications, especially in nanostructured materials like black silicon (b-Si). RMS roughness is commonly used to describe nanorough surfaces, but it cannot capture their complexity or predict behaviors such as bacterial adhesion [1] or chemical composition.

On steep, irregular surfaces, chemical analysis techniques such as X-ray photoelectron spectroscopy (XPS) becomes challenging. To overcome this, we use Minkowski functionals and tensors [2,3] to relate XPS data to detailed Atomic Force Microscopy (AFM) topography.

Our results show that nanoscale geometry strongly influences chemical surface analysis and that geometric descriptors provide a powerful framework for studying complex surfaces.

[1] C. Spengler et al., Nanoscale, 11 (2019) 19713.
[2] R. Schneider, W. Weil, Springer (2008).
[3] G. E. Schröder-Turk et al., Advanced Materials, 23 (2011) 2535.

O 54.2 Wed 10:45 HSZ/0201
Systematic Investigation of Colloidal Au Nanoparticles for High-Density III-V Nanowire Growth — •Pavithira Manoharan, Chris Yanic Bohlemann, Peter Kleinschmidt, Thomas Hannappel, and Juliane Koch — Fundamentals of Energy Materials,Technical University of Ilmenau, 98693 Ilmenau, Germany

Over the past two decades, nanoscale structures such as III-V nanowires (NWs) have become versatile components for electronic and photonic applications, including high-performance photovoltaic and photoelectrochemical systems. Many simulation studies show that the density and lateral arrangement of NWs play a decisive role in optimizing light absorption, charge separation, and surface reactions. However, growing ordered NW arrays remains technologically challenging and costly. In this work, we present a simple and cost-effective method for producing high-density, disordered III-V NW using commercially available Au colloid solutions as a source of the catalyst particles. We perform a systematic study on how experimental parameters, such as surface preparation and substrate deposition conditions, affect the resulting nanowire density and diameter. This comprehensive approach provides insight into catalyst behavior prior to the vapor-liquid-solid growth and enables controlled modification of the NW structures. We also evaluate the limitations and potential of this method for NW-based energy conversion architectures.

O 54.3 Wed 11:00 HSZ/0201
Imaging the transition from diffusive to Landauer resistivity dipoles — •Serhii Kovalchuk[1,2], David Kämpfer[1,3,4], Jonathan K. Hofmann[1,3,4], Timofey Balashov[1,3,5], Vasily Cherepanov[1], Bert Voigtländer[1,3,4], Ireneusz Morawski[2], F. Stefan Tautz[1,3,4], and Felix Lüpke[1,6] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Experimental Physics, University of Wrocław, 50-204 Wrocław, Poland — [3]Jülich Aachen Research Alliance (JARA), Fundamental of Future Information Technology, 52425 Jülich, Germany — [4]Lehrstuhl für Experimentalphysik IV A, RWTH Aachen University, 52074 Aachen, Germany — [5]Lehrstuhl für Experimentalphysik II A, RWTH Aachen University, 52074 Aachen, Germany — [6]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

A point-like defect in a current-carrying conductor produces an electrochemical potential dipole that opposes the applied field. When the carriers mean free path is shorter than the defect size, the dipole reflects diffusive transport; when it is longer, ballistic scattering leads to a size-independent residual resistivity dipole as predicted by Rolf Landauer.

We investigate this behaviour around nanoscale holes in thin Bi films on Si(111) using scanning tunneling potentiometry. The measured dipole amplitudes show a clear crossover from linear to constant scaling with decreasing hole size, marking the transition from diffusive to Landauer-type dipoles. This crossover allows us to extract the Fermi wave vector and estimate the carrier mean free path in the Bi films.

O 54.4 Wed 11:15 HSZ/0201
Current-driven Rb$^+$ intercalation for on-chip tuning of superconductivity in Rb$_x$C$_{60}$ thin films — •Konstantin Shchukin[1,2], Oliver Gallego Lacey[3], Baptiste Coquinot[4], Jacek Jakowski[5], Jingsong Huang[5], Patrik Staudenmayer[1], Yannic Falke[2], Ram Prakash Pandeya[1], and Alexander Grüneis[1] — [1]Institut für Festkörperelektronik, Technische Universität Wien, Gußhausstraße 25, 1040 Vienna, Austria — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CEA, Université Grenoble Alpes, IRIG-Pheliqs, 38000 Grenoble, France — [4]Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria — [5]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA

Superconducting fullerides are usually synthesised by thermal or solution intercalation of alkali ions, which limits control of stoichiometry. We use electro-intercalation to drive Rb$^+$ into C$_{60}$ thin films. Our on-chip setup combines *in-situ* growth, Raman spectroscopy and four-terminal transport, so that the stoichiometry x of Rb$_x$C$_{60}$ is obtained from the $A_g(2)$ mode and linked to the superconducting transition temperature Tc. By varying the Rb/C$_{60}$ ratio, we tune the films to superconducting Rb$_3$C$_{60}$ and change T$_c$ from 7 K to 26 K. Time-dependent Raman and transport data show that the Rb$^+$ electro-intercalation follows Butler-Volmer-type kinetics. Electro-intercalation enables precise, on-chip control of superconductivity in ultrathin fulleride films and is extendable to other porous and layered materials.

O 54.5 Wed 11:30 HSZ/0201
Mesoporous Cobalt Ferrite Thin Film Oxygen Evolution Electrocatalysts: The Role of Fe-Content on Structure, Activity and Stability — •Ann-Kristin Stief, Barbara Gonzalez-Navarrete, Stefan Lauterbach, Jan Philipp Hofmann, and Marcus Einert — TU Darmstadt, Darmstadt, Germany

Cobalt Ferrite is a promising alkaline Oxygen Evolution Reaction (OER) catalyst to replace state-of-the-art but expensive Ir- and Ru-based acidic OER catalysts in green hydrogen production. Given the limited and contradictory literature on the optimum stoichiometry of $Co_{3-x}Fe_xO_4$, we conducted a systematic stoichiometry study from x = 1.0 - 2.0 in increments of 0.2. To this end, mesoporous thin films were synthesized via dip-coating combined with soft-templating, using the commercially available polymer Pluronic F-127 for the first time. Electrochemical testing revealed that the x = 2.0 composition achieved the lowest iR-corrected overpotential (342 mV at 10 mA/cm^2), the smallest Tafel slope, and the lowest charge transfer resistance. Structural characterization disclosed enhanced crystallinity, reduced grain size and higher degree of inversion upon Fe-enrichment. X-ray Photoelectron Spectroscopy (XPS) further indicated that Fe-rich precatalysts form higher surface concentrations of hydroxide or defective oxide. Together, these findings contribute to the understanding of composition-structure-activity relations of Cobalt Ferrite OER catalysts, thereby laying a foundation for tailoring their catalytic performance. This work was supported by BMFTR within SINATRA (TWOB, Award Nr. 033RC036).

O 54.6 Wed 11:45 HSZ/0201

Probing Electromagnetic Chirality in Nanoresonators Using Scanning Reflection Anisotropy Microscopy — •Fabian Haake — ETH Zurich, Switzerland

We report on the application of a Scanning Reflection Anisotropy Microscope (SRAM) to study metasurfaces consisting of chiral nanoresonators. SRAM is a polarization-modulated optical method previously applied to strain mapping in crystalline materials and, more recently, demonstrated for amorphous systems (Sendra *et al.*, 2023; APL. 124, 171102, 2024). The structures were fabricated on Si_3N_4 TEM membranes using electron-beam lithography and metal deposition. Arrays of left- and right-handed resonators were fabricated and probed, showing a wavelength-dependent RAS contrast between the two enantiomorphic forms. Finite-element simulations under circularly polarized illumination reproduce the observed handedness-dependent responses. The results demonstrate that SRAM sensitively resolves enantiomer-specific optical signals at the microscopic scale, enabling direct characterization of electromagnetic chirality in metasurfaces.

O 54.7 Wed 12:00 HSZ/0201

Self-assembly of linear three-ring aromatic thiols on Au(111) and their conversion into 2D molecular materials — •Verena Müller[1], Anna-Laurine Gaus[2], Daniel Hüger[1], Julian Picker[1], Christof Neumann[1], Max von Delius[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstrasse 10, 07743 Jena, Germany — [2]Ulm University, Institute of Organic Chemistry, Albert Einstein Allee 11, 89081 Ulm, Germany

Self-assembled monolayers (SAMs) allow surface modification at the molecular level and moreover have the ability of crosslinking with low-energy electrons to form mechanically stable and transferable 2D materials, so-called carbon nanomembranes (CNMs).

We investigate the self-assembly of linear, three-ring aromatic thiols on Au(111) and their subsequent electron-induced conversion into carbon nanomembranes (CNMs). Our study examines terphenylthiol (TPT) derivatives with distinct terminal groups (-F, -CF_3, -NO_2) as well as a pyridinebiphenyl compound. Utilizing complementary surface science techniques - X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning tunneling microscopy (STM) - we elucidate the structural properties of the resulting self-assembled monolayers (SAMs) and investigate their transformation into CNMs. The resulting CNMs exhibit tunable gas permeation characteristics, governed by the chemistry of the precursor molecules and the SAM structure.

O 54.8 Wed 12:15 HSZ/0201

Liquid Flame Spray Enables Durable, Transparent, and Super-repellent Silica Coatings — •Suhad Sbeih — German Jordanian University, Amman, Jordan

Developing coatings that are simultaneously transparent, durable, and highly water-repellent remains a long-standing challenge in materials science. In this work, we show that the liquid flame spray (LFS) technique offers a fast and scalable solution. In this process, a silica precursor is combusted to generate nanoparticles that deposit on moving substrates, forming a hierarchical surface texture in a single step. By carefully adjusting the burner-substrate distance, precursor concentration, and coating velocity, we produced coatings that combine optical clarity with extreme water repellency, reaching contact angles above 150° and roll-off angles below 10°.

Beyond these surface properties, the coatings exhibited outstanding durability and retained their performance after rinsing, condensation, tape, and scratch tests. The results highlight LFS as a versatile approach for engineering multifunctional surfaces that bring together transparency, robustness, and super-repellency. Such coatings open new opportunities for large-area applications in optics, energy devices, and biomedical technologies.

O 55: Oxide and insulator surfaces: Structure, epitaxy and growth II

Time: Wednesday 10:30–12:30 Location: HSZ/0204

O 55.1 Wed 10:30 HSZ/0204

Modulated structures in complex 2D oxides — •Muriel Wegner, Loi V. Tran, Oliver Krahn, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

Crystalline materials are typically characterized by a set of lattice vectors that reflect the materials dimensionality. In surface science we are used to two vectors spanning the lattice. However, systematic lattice modifications, which can be displacive in nature or connected to a different periodicity in a given materials property like magnetism, can call for the need of additional modulation vectors for a proper interpretation of the diffraction pattern. Such modulated structures are rarely discussed in surface science. Here we present the structure of a Ba-Ti-O monolayer film grown on Pd(111) and Pt(111). On Pd(111) this structure is commensurate and fully determined by two lattice vectors. In contrast, on Pt(111) four vectors are needed, two describing the average structure and two additional modulation vectors. This Ba-Ti-O structure is a complex network of Ti-O rings, in which 53% of the rings are decorated with Ba atoms. On Pd(111) it forms a rhombic structure with a periodicity of 23.2 Å and an inner angle of 129.7°. On Pt(111) it grows with the identical lattice parameters. However as a consequence of the modified substrate spacing, the domain size is restricted by systematic inclusions of defects, which cause a modulation period of about 100 Å.

O 55.2 Wed 10:45 HSZ/0204

How coordination preferences dictate the mixing behavior of 2D oxide films: Fe/Cr spinel-type oxides on Pt(111) — Ghada Missaoui[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

Fe/Cr mixed oxide films, prepared by reactive co-deposition of both elements on Pt(111), are analyzed by STM and DFT calculations. The mixed oxide grows into bi- (h=0.5 nm) and tri-stack films (h=0.7 nm) terminated either by open (2x2) (bi-stacks) or dense (1x1) atomic patterns (bi- and tri-stacks). The former is identified as Cr6O11 phase composed of an interfacial O-Cr-O trilayer and a Cr2O3 honeycomb plane. The latter develops upon substituting Fe into the surface plane, where it forms a hexagonally dense-packed Fe-O bi-layer. Two polymorphs with different mixing enthalpy occur as a function of mixing ratio. At high Fe content, X6O9-type bi-stacks prevail (X = Fe,Cr) with Cr preferentially accumulating in octahedral sites at the interface and Fe filling tetrahedral sites at the surface. At low Fe content, the Cr interface stack reconstructs to stabilize more oxygen, while the surface stack remains Fe-dominated. The resulting film has X6O11 stoichiometry and deviates from the X6O9 structure not only by the oxygen content but also by its workfunction and surface buckling, in agreement with STM data. The observed cationic stacking, with alternating Fe and Cr planes resembles the bulk ilmenite structure (FeCrO3).

Invited Talk O 55.3 Wed 11:00 HSZ/0204

Cationic Mixing in Ultrathin Oxide Films: How substrate and oxygen conditions control nanoalloying. — •Jacek Goniakowski — Institut des NanoSciences de Paris, CNRS & Sorbonne

Université, Paris, France

While alloying is a powerful strategy for tuning material properties, the fundamental physics and chemistry of cation mixing in metal-supported ultrathin oxide films, including those relevant to inverse catalysts, remain poorly understood, and only a few doped or mixed phases have been characterized at the atomic scale. Here, density functional theory, combined with recent surface science experiments, is used to elucidate how oxygen conditions and substrate properties govern the formation of mixed two-dimensional oxide phases through a subtle interplay of structural and electronic effects.

The study shows that, although bulk V-Fe-O mixed oxides are rare, reduced V-Fe-O monolayers on Pt(111) are stable across a wide range of cation compositions. However, oxidation of the film strongly narrows the accessible compositional window. Likewise, substrate passivation (e.g., oxidized Ru(0001)) restricts the range of stable compositions. For somewhat thicker films, exemplified by V-Cr-O bistacks, the presence of crystallographically distinct cation sites further promotes mixing, enabling the stabilization of spinel-like V-Cr phases with no direct bulk counterparts. Our results highlight key effects governing compositionally complex supported ultrathin oxide films and suggest pathways to explore novel mixed phases.

O 55.4 Wed 11:30 HSZ/0204

Surface reconstruction of the polar spinel $MgAl_2O_4$(001) surface — David Kugler[1], Andrea Conti[1], Johanna I. Hütner-Reisch[1], Soumyajit Rajak[2], Matthias Meier[1], Nan Jiang[2], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], Gareth S. Parkinson[1], and •Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Department of Chemistry, University of Illinois Chicago, USA

The atomic-scale surface structure governs the surface chemistry of materials. Magnesium aluminate ($MgAl_2O_4$) spinel, a wide-gap insulator, poses considerable challenges for experimental surface characterization. Using noncontact atomic force microscopy (nc-AFM), we resolve the atomic structure of the $MgAl_2O_4$(001) surface. The surface adopts a c(2×4) reconstruction accompanied by altered surface stoichiometry. The reconstructed surface is enriched in aluminum and contains ordered pairs of octahedrally coordinated Mg atoms that, in bulk, occupy tetrahedral sites. This cation redistribution stabilizes the otherwise polar $MgAl_2O_4$(001) termination. The resulting structure closely resembles reconstructions observed on other spinel oxides, suggesting a common mechanism for polarity compensation across the spinel group.

O 55.5 Wed 11:45 HSZ/0204

Size Matters: Size-dependent non-equilibrium dynamics of fluxional subnanoclusters — •Patricia Poths[1], King Chun Lai[2], Christoph Scheurer[1], Sebastian Matera[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der Max-Planck Gesselschaft, Berlin — [2]Max Planck Computing and Data Facility, Garching

Sub-nanoclusters are known to be fluxional, thermally populating multiple structural isomers, and to have size-dependent catalytic behavior. Due to computational limitations, only quasi-static equilibrium properties could be addressed by first-principles methods so far. Here, we investigate the kinetic evolution underlying isomer fluxionality by coupling machine-learned interatomic potentials (MLIPs) with our recently introduced automatic process explorer (APE) [1]. With this methodology, we construct comprehensive isomerization networks of Pdn (n=3-11) clusters deposited on the MgO(100) surface, and evaluate the corresponding state-to-state dynamics. Using methods from Markov State Modeling, we find that the intrinsic timescales for equilibration can vary by several orders of magnitude based on cluster size. Furthermore, intrinsic timescales for each cluster isomer can vary by multiple orders of magnitude, indicating the existence of metastable sets with quasi-liquid behavior, i.e. rapid conversion between isomers within the set but only slow transition to isomers outside. These simulations reveal that the prevalent quasi-static picture is of limited use for nonequilibrium problems like catalysis, but also that relaxation dynamics should be observable on experimental timescales.

[1] K.C. Lai et al., Phys. Rev. Lett. 134, 096201 (2025).

O 55.6 Wed 12:00 HSZ/0204

Structural and electronic evolution of noble metal-deposited CeO2 catalysts: from model to powder systems — •Zairan Yu, Shuang Chen, Wangtao Li, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

The interaction between noble metals and oxide supports is crucial in heterogeneous catalysis, governing key reactions such as CO oxidation and the water-gas shift. Pt- and Pd-ceria systems show particularly strong electronic and structural metal-support interactions among these reactions. Despite extensive investigation, the atomic-scale structure and reactivity of these interfaces remain incompletely understood. Here, we combine polarization-resolved IRRAS on single-crystal surfaces and in situ UHV-FTIR transmission studies on ceria nanoparticles, using CO as a probe to elucidate surface structural dynamics and active sites. For Pt/CeO2(111), IRRAS and DFT results reveal that isolated Pt single atoms are not stabilized on the surface, but instead migrate into subsurface interstitial sites at low coverages, giving rise to a characteristic blue-shifted CO band at 2169 cm-1. In the Pd/CeO2/γ-Al2O3 system, highly dispersed Pd cations embedded in the ceria matrix with nearby interfacial oxygen vacancies are identified, correlating with superior catalytic performance in STD reactions. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-Project-ID 426888090-SFB 1441.

O 55.7 Wed 12:15 HSZ/0204

Titanium intermixing into cuprous oxide thin films: An STM and XPS study — •Bo-Yi Zhong and Niklas Nilius — Carl-von-Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany

According to DFT calculations, gap size and p-type conductivity of binary Cu2O can be tuned over wide ranges by doping the material with transition metal ions. To test this assumption, we have prepared Cu/Ti mixtures and exposed them to different oxidation conditions. Mixing is only revealed at low temperature and gives rise to amorphous oxide films without diffraction pattern. Annealing in oxygen triggers a gradual phase separation, with TiOx moving to the surface and CuOx remaining at the interface to the Pt(111) support. The phase separation produces a distinct intensity behavior of the Ti 2p and Cu 2p XPS peaks as a function of temperature. Morphologically, the Ti ions get embedded into the surface reconstruction of Cu2O(111) at low Ti content, as observed in atomically resolved STM images. With rising Ti level, the surface Ti-O forms large crystallites exposing distinct stripe-patterns on their surface, suggesting a TiO2(110)-type morphology. Moreover, STM spectroscopy finds a gap state at 1.5 eV in Ti-poor preparations, compatible with the empty-state resonance of the Ti impurities. At higher Ti content, the gap state broadens and evolves to the TiO2 conduction band. The electronic response of the phase-separated system, with Cu2O at the interface and TiO2 at the surface, resembles the one of a pn-junction.

O 56: Scanning probe techniques: Method development II

Time: Wednesday 10:30–12:15 Location: HSZ/0401

O 56.1 Wed 10:30 HSZ/0401

Simulation of coupled AFM and constant current STM images — •Marvin Krenz[1,2], Miguel Wiche[1,3], Daniel Ebeling[1,3], and Simone Sanna[1,2] — [1]Center for Materials Research, Justus-Liebig University, Giessen, Germany — [2]Institute of Theoretical Physics, Justus-Liebig University, Giessen, Germany — [3]Institute of Applied Physics, Justus-Liebig University, Giessen, Germany

We present a simulation method for AFM images with a constant current STM feedback loop. In contrast to regular AFM constant height images, those images can picture the features of bulky or corrugated molecules, as shown by experiment [1].

The method is based on the electronic density of the molecules, and thus applicable to virtually any DFT code. We apply this method to two test systems, the 6F-Pentacene molecule at Cu(111) and the iodotriphenylene at Ag(111), at different level of approximation.

Both systems compare well to the experimental images; at the highest level of approximation nearly all features of the experiment are reproduced.

[1] Martin-Jimenez, D.; Ahles, S.; Mollenhauer, D.; Wegner, H. A.; Schirmeisen, A.; Ebeling, D. Physical Review Letters 2019, 122, 196101.

O 56.2 Wed 10:45 HSZ/0401

High spatial resolution of Si(111)-7x7 using LFM with a CO-tip — •Shinjae Nam[1,2], Thomas Holzmann[1], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]Center for Quantum Nano Science, Seoul, South Korea

The Si(111) 7x7 reconstructed surface has long served as an iconic benchmark for proving the capabilities of scanning probe microscopes. Since STM first resolved the 7x7 pattern in 1983, advances in frequency-modulation AFM have enabled true atomic resolution and quantitative access to short-range chemical and frictional interactions. In this work, we report unprecedented atomic resolution and quantitative mapping of site-dependent lateral forces on the Si(111) 7x7 surface using a qPlus-based lateral force microscope. The tip is terminated with a CO molecule, and oscillating laterally with an amplitude of 50 pm. Unlike reactive Si tips, the CO tip provides a chemically inert and well-defined probe apex, enabling exceptionally sharp contrast and resolving subtle differences between faulted and unfaulted half-cells. The measured lateral force maps agree quantitatively well with theoretical models. These results establish CO-tip LFM as a powerful technique for probing lateral interactions with single-atom precision.

O 56.3 Wed 11:00 HSZ/0401

Spatially Resolved Mode Analysis of Ultra-Long qPlus Probes for STM/AFM — •Aleksander Bogucki[1,3], Yeon-Ji Kim[1,2], Yewon Kim[1,2], Sarah Yi[1,2], German Orlov[1,3], Lei Fang[1,3], Wonjun Jang[1,3], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [3]Ewha Womans University, Seoul 03760, Republic of Korea

Combined scanning tunneling and atomic force microscopy (STM/AFM) based on quartz tuning forks (qPlus) typically relies on short tip lengths ($<$0.5 mm) for optimal performance. However, restricted sample environments such as liquid cells or setups requiring significant clearance for high-numerical-aperture optical elements demand probe geometries far exceeding standard dimensions. While tips in the 1-3 mm range have been recently explored [1], the dynamics of significantly longer tips are less well characterized.

We present a systematic study of qPlus sensors with ultra-long tips ($>$8 mm). We correlate electrical response spectra with spatially resolved optical vibrational analysis to map eigenmodes and identify non-vertical components. Supported by FEM simulations, we demonstrate that tip material and geometry can be optimized to tune the spectral response. Finally, we assess the potential of these ultra-long designs for specialized SPM setups.

References: [1] T. Yamada et al., Nanoscale Adv. 5, 840-850 (2023).

O 56.4 Wed 11:15 HSZ/0401

Comparative Analysis of SPM-Based Work Function Measurement Techniques with Application to Work Function Engineering of Superconducting Nb(110) — •Daryoush Nosraty Alamdary, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Lehrstuhl für Experimentelle Physik 2, Julius-Maximilians-Universität Würzburg, Germany

The engineering of the work functions at the interface of complex materials for energy band tuning [1] requires precise and reliable measurement methods, sensitive to atomic monolayer thin films. While there are handful of established methods that allow a precise determination of the work function, scanning probe microscopy-based methods constitute a class of their own since they are based on a local probe. In this work, we present a comparative study of three techniques, i.e., $I(z)$ spectroscopy, field emission resonances, and Kelvin probe force spectroscopy, regarding their complexity and reliability to determine the local work function. For a few well-studied model systems we analyze the respective benefits and challenges. Using the most reliable methods, established by the comparative analysis, we systematically study the coverage-dependent crystal structure and work function of epitaxial Ir films on superconducting Nb(110) [2] and discuss the suitability for work function engineering towards induced superconductivity.

[1] P. Rüßmann *et al.*, Proximity induced superconductivity in a topological insulator, arXiv:2208.14289 (2022)

[2] P. Beck *et al.*, Structural and superconducting properties of ultrathin Ir films on Nb(110), Phys. Rev. Mater. **6**, 024801 (2022)

O 56.5 Wed 11:30 HSZ/0401

Towards Atomically Precise Fabrication through STM with Flat, Crystalline Probes — •Marc Savoie, Eduardo Barrera Ramirez, Bheeshmon Thanabalasingam, and Marco Taucer — CBN Nanotechnologies Inc, Ottawa, Canada

Scanning Tunneling Microscopy (STM) enables the fabrication of atomically precise structures. Traditionally, STM probes manipulate atoms on the sample surface, but this presents challenges for fabricating covalently bonded structures. The high strength of covalent bonds means that detailed knowledge and control over both the probe and sample sides of the tunneling junction is required to form the desired bond and avoid unwanted changes. We introduce inverted-mode STM, an approach that reverses the roles of probe and sample to enable mechanically controlled chemical reactions for atomically precise fabrication. We have developed flat, crystalline Si(100) STM probes that act as the substrate for atomic manipulations. The flat probe is imaged by tailored, 3D molecules deposited on a surface. By determining the orientation of the molecule, the challenge of knowing the atomic configuration on both sides of the junction is effectively resolved. Treating the two sides of the tunnel junction as reagents whose relative positions can be controlled with sub-angstrom precision, we show that hydrogen atoms can be reproducibly abstracted from a locally flat, crystalline region of the probe apex at zero volts using a novel molecule terminated in an alkynyl radical. Multiple surface-bound reagents can sequentially address the same build site on a probe apex. The approach is expected to apply to abstraction and donation of other elements and moieties.

O 56.6 Wed 11:45 HSZ/0401

Atomically Precise Si Abstraction by Inverted-Mode STM — •Rosemary Cranston, Zehra Ahmed, Eduardo Barrera, Brandon Blue, Adam Bottomley, Christian Imperiale, Alex Inayeh, Mathieu Morin, Marco Taucer, and Bheeshmon Thanabalasingam — CBN Nano Technologies Inc., Ottawa, Canada

Direct 3D manipulation of covalently bonded atoms remains a challenge for atomically precise fabrication. Here, we introduce inverted-mode scanning tunneling microscopy (STM) as a new approach for controlled atomic-scale reactions and demonstrate its application to individual Si atom abstraction. A Si probe chip (SPC) with an atomically clean Si(100)-2x1 crystalline terrace at the apex serves as the probe, while a Si wafer bearing isolated, custom-synthesized, surface-bound molecular tools act as the sample. These molecules function both as imaging agents and as tools for chemical manipulation. As the sample is scanned with the SPC, each protruding molecule provides a mirror image of the probe apex and can immediately participate in surface reactions. For subtractive Si patterning, we employ tripodal molecules featuring an ethynyl iodide moiety. After bias-induced cleavage of the iodine, the resulting radical is aligned with a target Si dimer of the SPC. A controlled approach-retraction process transfers a

Si atom to the molecule, leaving unique Si vacancies at the target site. Imaging with new iodinated molecules elsewhere on the sample surface confirms changes to the SPC lattice, and allows iterative targeting for the next abstraction, thus enabling a new method for atomically precise fabrication, and the manipulation of Si atoms in 3D.

O 56.7 Wed 12:00 HSZ/0401

Graphene Coated Nanoprobes for Local Conductivity Measurements — •Maria Saavedra-Fredes, Valeria del Campo, and Tomas P. Corrales — Universidad Técnica Federico Santa María, Valparaíso, Chile.

Here we explored the fabrication of AFM cantilevers coated with graphene (Gr) with the aim of detecting local electrical currents. The fabrication process begins with the growth of Gr on copper foils via Chemical Vapor Deposition (CVD). Subsequently, the copper substrate is dissolved using a ferric nitrate solution and then replaced with water, leaving a Gr film floating at the water air interface. This film is transferred onto an AFM cantilever using a three-axis hydraulic micromanipulator. Raman spectroscopy and SEM confirm the presence of graphene on our Gr-coated nanoprobes This technique differs from traditional methods because the Gr is collected directly from the air water interface without the use of polymer films in the process (10.3390/cryst7090269). Then, to detect currents using conductive mode AFM (10.1002/adma.201200579) and study the conduction between our Gr-coated nanoprobe and a graphene layer deposited on silicon.

O 57: Plasmonics and nanooptics: Light-matter interaction, spectroscopy II

Time: Wednesday 10:30–12:30 Location: HSZ/0403

Invited Talk O 57.1 Wed 10:30 HSZ/0403

From Plasmonic Near-Fields to Electron Dynamics - A Photoemission Perspective — •Pascal Dreher — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany — Present Address: Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Electromagnetic near-fields are ubiquitous in solid-state physics. At surfaces, interfaces, and in nanostructures they control dynamical processes and shape optical and electronic material properties. By concentrating electromagnetic energy to subwavelength volumes, near-fields enable tailored nanoscale light-matter interactions relevant to plasmonics, nanophotonics, and ultrafast carrier dynamics. A detailed understanding of these interactions, however, requires experimental access to the full three-dimensional, time-dependent vectorial structure of near-fields, ideally in conjunction with direct probes of the electronic excitations they launch.

In this talk, I will address these needs using two complementary experimental approaches: polarimetric photoemission microscopy that maps vectorial near-fields at surfaces, and time- and angle-resolved photoemission that probes the resulting charge-carrier dynamics. Using surface plasmon polaritons as a prototypical platform, it will be demonstrated how these methods allow to relate near-field dynamics and light-matter interactions at the native length, momentum, time, and energy scales.

O 57.2 Wed 11:00 HSZ/0403

Steps Towards Excitation of Quantum Emitters with Switchable Nonlinear Near Fields — •Valentin Dichtl, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth

The third-order nonlinear material response of noble metals enables the formation of the third-harmonic near field around a plasmonic nanostructure. The corresponding spatial emission pattern of the third-harmonic hot spots changes drastically when the fundamental wavelength is slightly tuned over a linear resonance of the nano antenna [1]. This effect can be used to spatially tailor the near field for excitation of various emitters – such as molecules or quantum dots – beyond the diffraction limit.

We identified distinct differences in the nonlinear scattering behavior between the complentarry plasmonic structures rod and slit [2]. Building on this insight we compare these geometries in terms of their suitability for single emitter excitation.

We demonstrate non-destructive third-harmonic generation in close proximity to fluorescent dyes. Finally, we discuss spectral and temporal strategies for discriminating photons originating from fluorescence versus those from harmonic generation.

[1] Wolf, D. *et al.* Shaping the nonlinear near field. *Nat. Commun.* 7:10361 (2016). doi: 10.1038/ncomms10361

[2] Dichtl, V. *et al.* The Nonlinear Limit of Babinet's Principle. *Nano Lett.* 2025, 25, 11084-11088. doi: 10.1021/acs.nanolett.5c02210

O 57.3 Wed 11:15 HSZ/0403

Intrinsic plasmon canalization in the natural biaxial van-der-Waals material $MoOCl_2$ — •Farid Aghashirinov[1], Andrea Manchini[2], Lin Nan[2], Giacomo Venturi[2], Nicola Melchioni[2], Florian Mangold[1], Bettina Frank[1], Antonio Ambrosio[2], and Harald Giessen[1] — [1]4-th Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]Vectorial Nano-Imaging, Istituto Italiano di Tecnologia, Milano, Italy

We investigate directional near-infrared plasmon polaritons in exfoliated $MoOCl_2$ flakes on SiO_2 substrates, excited using gold disk nanoantennas and probed with scattering-type scanning near-field optical microscope (s-SNOM). $MoOCl_2$ is a natural van der Waals material that supports low-loss, in-plane hyperbolic plasmons and exhibits strong optical anisotropy: polarization along the short axis yields metallic behaviour, while alignment with the long axis produces a dielectric response [1]. Using a widely tunable broadband laser from Stuttgart Instruments, we map the polariton dispersion across a broad spectral range and identify distinct propagation regimes. In our work, we observe plasmon-polariton canalization for the first time, where wavefronts propagate without divergence. These measurements highlight $MoOCl_2$ as a broadband, highly directional natural polaritonic platform.

[1] G. Venturi et al., Nat Commun 15, 9727 (2024)

O 57.4 Wed 11:30 HSZ/0403

Toward Plasmonic Neuronal Architectures at the Nanometer Scale — •Christopher Weiss[1], Tobias Eul[2], Emily Kruel[1], Mario Pfeiffer[1], Bert Lägel[1], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Experimentalphysik II, Institute of Physics, University of Augsburg, Germany

Classical von-Neumann computers face severe energy and speed limitations when operating large artificial neural networks, motivating alternative computing concepts beyond the traditional architecture. Plasmonic nanostructures offer a promising route toward ultrafast and highly integrated neuromorphic systems by enabling strong optical confinement at the nanoscale. We present a concept for a plasmonic neuronal cell that combines multiplexed signal reception, static weighting, and nonlinear activation within a single device. Optical inputs encoded in the orbital angular momentum of light are directed into separate dielectric-loaded surface-plasmon-polariton waveguides. Synaptic weighting is implemented through nanoscale gaps, whose attenuation characteristics are analyzed using finite-difference time-domain simulations and experimentally validated by photoemission electron microscopy. Nonlinear activation is provided by plasmon-enhanced two-photon photoemission. These results establish the essential functional components required for ultrafast plasmonic neuromorphic architectures.

O 57.5 Wed 11:45 HSZ/0403

Optical resonance tuning of single polystyrene microspheres using the phase-change material In_3SbTe_2 **as a switchable mirror** — •Rebecca Rahmel, Hristiyana Kyoseva, Lukas Conrads, Thomas Taubner, and Gero von Plessen — I. Institute of Physics (IA), RWTH Aachen University

The optical resonances of dielectric nanoparticles and microparticles can be modified via their size, shape and configuration [1]. Dielectric particles in particle-on-mirror (PoM) geometries show rich optical responses due to their low losses and electric and magnetic multipolar Mie modes [2]. Cueff et al. introduced the concept of a switchable mirror to tune the resonances of dipole emitters using the phase-transition material VO$_2$ [3]. Here we tune the infrared multipolar Mie resonances of dielectric polystyrene (PS) microspheres using a switchable mirror made of the phase-change material In$_3$SbTe$_2$ (IST). IST exhibits a phase change between an amorphous dielectric and crystalline metallic phase in the infrared [4,5] and can be locally switched under the PS microspheres, creating a PoM geometry. Measuring the scattering spectra of the PS microspheres before and after switching, we achieve huge shifts of the resonance wavelength from 5.2 to 8.9 μm. Our work is a first step towards the controlled tuning of multipolar Mie modes of various particles using reprogrammable IST mirror structures.

[1] Kuznetsov et al. *Science* **354**, aag2472 (2016) [2] Yao et al. *ACS Nano* **18**, 26, 16545-16555, (2024) [3] Cueff et al. *Nat. Com.* **6**, 8636 (2015) [4] Heßler et al. *Nat. Com.* **12**, 924 (2021) [5] Conrads et al. *Opt. Mat. Ex.* **15**, 2664-2687 (2025)

O 57.6 Wed 12:00 HSZ/0403

Spectral tuning of hyperbolic shear polaritons in monoclinic gallium oxide via isotopic substitution — •G. Carini[1], M. Pradhan[2], E. Gelzinyte[1], A. Ardenghi[3], S. Dixit[4], M. Obst[5,6], A. S. Senarath[4], N. S. Mueller[1], G. Alvarez-Perez[1,7], K. Diaz-Granados[4], R. A. Kowalski[4], R. Niemann[1], F. G. Kaps[5], J. Wetzel[5], R. B. Iyer[2], P. Mazzolini[8], M. Schubert[9,10], J. M. Klopf[11], J. T. Margraf[12], O. Bierwagen[3], M. Wolf[1], K. Reuter[1], L. M. Eng[5,6], S. Kehr[5,6], J. D. Caldwell[4], C. Carbogno[1], T. G. Folland[2], M. R. Wagner[3], and A. Paarmann[1] — [1]FHI, Berlin, Germany — [2]University of Iowa, Iowa City, IA, USA — [3]PDI, Berlin, Germany — [4]Vanderbilt University, Nashville, TN, USA — [5]TUD, Dresden, Germany — [6]EXC 2147 (ct.qmat), Dresden, Germany — [7]IIT, Lecce, Italy — [8]University of Parma, Parma, Italy — [9]University of Nebraska, Lincoln, NE, USA — [10]Lund University, Lund, Sweden — [11]HZDR, Dresden, Germany — [12]University of Bayreuth, Bayreuth, Germany

This contribution reports a significant spectral tuning of hyperbolic shear polaritons (HShPs) in monoclinic gallium oxide (bGO) via isotopic substitution. HShPs are imaged in real-space with near-field optical microscopy, allowing for a model-free estimation of the frequency shift. Complementary far-field measurements and *ab initio* calculations - in good agreement with the near-field data - confirm the effectiveness of this estimation. This combined study demonstrates the possibility to support such highly directional polaritons in a hitherto inaccessible range, with great promise for future applications.

O 57.7 Wed 12:15 HSZ/0403

Vibrationally Induced Resonances in Nanolasers based on Plasmonic Cavities — •Kai Müller[1], Kimmo Luoma[2], and Christian Schäfer[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Department of Physics and Astronomy, University of Turku, 20014 Turku, Finland — [3]Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10/134, Vienna, 1040, Austria

Optical circuits and light sources, such as lasers, undergo continuous miniaturization. In recent years, this trend has been taken to its extreme with lasers comprising only a few molecules confined in plasmonic nanocavities. Here, we use a novel method that combines the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy with the hierarchical equations of motion (HEOM) to provide theoretical predictions for the quantum dynamics of this few-emitter lasing system. Our approach is informed from first principles and explicitly accounts for the entire vibrational manifold of each molecule in addition to the cavity. We show how the form of the vibrational spectrum influences the lasing process and uncover resonant enhancements in the lasing intensity, which are absent if the coherent drive and vibrational relaxation are combined into the commonly used effective incoherent drive.

O 58: Organic molecules on inorganic substrates: Adsorption and growth III

Time: Wednesday 10:30–12:30 Location: TRE/PHYS

O 58.1 Wed 10:30 TRE/PHYS

Probing weak chemical interactions of metal surface atoms with CO-terminated AFM tips identifies molecular adsorption sites — Jalmar Tschakert[1], Qigang Zhong[1], Alexander Sekels[1], Pascal Henkel[2], Jannis Jung[2], K. Linus H. Pohl[2], Hermann A. Wegner[3], Doreen Mollenhauer[4], André Schirmeisen[1], and •Daniel Ebeling[1] — [1]Inst. of Applied Physics, Justus Liebig University Giessen — [2]Inst. of Physical Chemistry, Justus Liebig University Giessen — [3]Inst. of Organic Chemistry, Justus Liebig University Giessen — [4]Inst. for Technical and Environmental Chemistry, Friedrich Schiller University Jena

Understanding reaction mechanisms of adsorbed organic molecules is key to neat on-surface synthesis of functional nanomaterials. Low temperature atomic force microscopy has become an invaluable tool for studying on-surface reaction mechanisms as it allows to visualize the chemical structure of the reactants and products. However, directly accessing the molecule-surface interactions that are responsible for the pathway of on-surface reactions is difficult. Here, we measure chemical interactions between CO-terminated tips and coinage metal surface atoms in all spatial directions with picometer resolution. Identifying the small covalent bonding contributions in the background of the dispersion-dominated interaction enables revealing insights into the nature of chemical bond formation with metal surface atoms and a reliable determination of molecular adsorption sites. The latter can serve as a starting point and for a comparison with theoretical studies.

[1] Tschakert et al., *Nature Communications* **16**, 7874 (2025)

O 58.2 Wed 10:45 TRE/PHYS

Rare earth modified silicon surfaces: A promising template for ordered organic growth — •Milan Kubicki, Philipp Gruber, Marie-Louise Fraser, Mario Dähne, and Martin Franz — Technische Universität Berlin, Institut für Physik und Astronomie, Berlin, Germany

The formation of self-assembled layers of organic molecules on solid surfaces is an important research field because of their possible application in advanced (opto)electronic devices. While the formation of self-assembled layers is well established on metal surfaces, the growth on silicon surfaces, which are still the material of choice in present semiconductor technology, is much less studied. On pure silicon, however, the formation of ordered organic films is usually hindered by its high dangling bond density, so that an appropriate surface modification is required.

Here we demonstrate the high potential of a rare-earth modification of the Si(111) surface for promoting ordered growth. Using scanning tunneling microscopy, the adsorption of different organic molecules on rare-earth modified silicon surfaces was examined, exemplarily for highly reactive N-heterocyclic carbenes and less reactive transition metal phthalocyanines. Our data demonstrate that single molecules remain mobile on the surface at room temperature. At a coverage of one full monolayer highly ordered films can be formed, demonstrating the great potential of rare-earth modified silicon surfaces as template for organic film growth.

[1] M. Kubicki *et al.*, J. Phys. Chem. C **128**, 13347 (2024).

O 58.3 Wed 11:00 TRE/PHYS

N-Heterocyclic Carbenes on GaAs: From Chain Formation to Ordered Monolayers — •Martin Franz[1], Ankita Das[2], Sandhya Chandola[3], Milan Kubicki[1], Mowpriya Das[2], Andrea Sette[4], Domenico Corona[4], Maurizia Palummo[4,5], Letizia Chiodo[6], René Schöder[1], Preeti Chahar[2], Benjamin Fuhrmann[1], Jonathan Engelhardt[1], Oskar Düren[1], Mario Dähne[1], Conor Hogan[4,7], Norbert Esser[1,3], and Frank Glorius[2] — [1]Technische Universität Berlin, Institut für Physik und Astronomie, 10623 Berlin, Germany — [2]Organisch-Chemisches Institut, Universität Münster, 48149 Münster, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [4]Dipartimento di Fisica, Università di Roma "Tor Vergata", Rome 00133, Italy — [5]CNR Centro S3, CNR-Istituto Nanoscienze, Modena 41125, Italy — [6]Department of Engineering, Università Campus Bio-Medico, Rome 00128, Italy — [7]CNR-Istituto di Struttura della Materia (CNR-ISM), Rome 00133, Italy

N-Heterocyclic carbenes (NHCs) have emerged as well-established ligands for metal surfaces. First studies on silicon exist as well, while III-V compound semiconductors are the materials of choice for optoelectronic devices. Here, the adsorption behavior of NHCs on GaAs is studied in detail [1]. A covalent binding to the surface and a formation of well-ordered monolayers is found, accompanied by exceptionally large work function reductions. The monolayers consist of NHC chains being the result of an attractive interaction between the molecules.

[1] M. Franz et al., Angew. Chem. Int. Ed., 64, e202511094 (2025).

O 58.4 Wed 11:15 TRE/PHYS

Tuning the adsorption of Subphthalocyanine molecules on Au(111) by peripheral and axial functionalization — •Franz Plate[1], Soyoung Park[2,3], Ebru Cihan[1], Natasha Khera[1], Ningwei Sun[2,3], Dmitry A. Ryndyk[1], Franziska Lissel[2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute of Macromolecular Chemistry Leibniz Institute of Polymer Research, Hohe Strasse 6, Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, 21073 Hamburg, Germany

Subphthalocyanine (SubPc)-based molecules have been shown to be chemically versatile and tunable molecules, which can be functionalized with a variety of different chemical groups. This makes them promising candidates for designing single molecule machines to store and convert energy. Examples include vertical molecular rotors on surface. Although SubPc is nonplanar, SubPc-based molecules have been shown to form well-ordered molecular assemblies on surfaces, enabling them to function as modular rotor bases. Their chemically stable and rigid core, allows for a functionalization with different axial ligands as well as extensions at the peripheral positions of the π-conjugated base, which leads to different orderings on the surface. We have studied different SubPc based molecules with different axial and peripheral functionalizations on Au(111) using low-temperature scanning tunneling microscopy, supported by simulations. Depending on the peripheral functionalization with methoxy and thiophene groups, we found different adsorption behaviors, ordering, and intermolecular interactions.

O 58.5 Wed 11:30 TRE/PHYS

From Inert Nitrogen to Reactive Metal Nitrene: An On-Surface Route to N-Heterocycles — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Shadi Fatayer[2], and Laerte Patera[1] — [1]Department of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Applied Physics Program, Division of Physical Science and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

Nitrenes are highly reactive intermediates in organic chemistry and play a key role in the synthesis of nitrogen containing compounds. In solution, nitrenes are typically generated from chemically activated precursors (e.g., azides), whereas direct conversion of primary amines remains challenging due to the inherent strength of N-H bonds. On surfaces, reactive nitrenes have likewise been formed from organic azides [1]; however, azides are thermally and photochemically labile and can decompose violently upon exposure to heat, light, or mechanical shock, posing safety risks. Here, using combined scanning tunneling microscopy (STM), non contact atomic force microscopy (nc AFM), and density functional theory (DFT), we demonstrate the thermally activated formation of a surface stabilized metal-nitrene intermediate from a chemically inert amine, which mediates the on-surface formation of a nitrogen-containing heterocycle. Our findings establish non activated nitrogen functionalities as viable nitrene precursors and reveal new mechanistic pathways for on-surface synthesis of N-heterocyclic compounds.

[1] Hellerstedt et al., Angew. Chem. 131, 2288-2293 (2019).

O 58.6 Wed 11:45 TRE/PHYS

Mirror domains and adsorption induced dipoles in organic semiconductor films revealed by LEEM and μLEED — •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

We apply low-energy electron microscopy (LEEM) and microspot low-energy electron diffraction (μLEED) to study the film growth of non-polar para-sexiphenyl (p-6P) molecules on natively oxidized silicon. In their second monolayer, the molecules form μm-sized, 2D-crystals with a bulk-like unit cell. LEEM reveals dark lines that split individual islands along their long axis into two domains of roughly equal size. The corresponding diffraction patterns are laterally shifted relative to each other, allowing for dark-field imaging of each domain. We attribute this apparent shift in k-space to the presence of lateral electric fields pointing in opposite directions on either side of an island. Given p-6P's large polarizability, we ascribe these fields to induced electric dipole moments in the tilted molecules. Thus, the observed dark lines represent boundaries between adjacent domains of mirrored tilt. Since the shift in k-space is independent of the LEEM extractor field, the dipoles must be inherent to the adsorbed molecules on the Si substrate. We observe an increased work function for the second-layer islands compared to the substrate. This and temperature-dependent measurements support our conclusion that adsorption-induced charge transfer causes the polarization of the molecules.

O 58.7 Wed 12:00 TRE/PHYS

The Role of Metal Ions in Metal-Phthalocyanine Adsorption on Oxide Surfaces — Matthias Blatnik[1], Fabio Calcinelli[2], Andreas Jeindl[2], Michael Schmid[1], Ulrike Diebold[1], Peter Jacobson[3], Oliver T. Hofmann[2], and •Margareta Wagner[1] — [1]TU Wien, Austria — [2]TU Graz, Austria — [3]University of Queensland, Australia

The interaction of conjugated organic molecules with surfaces is of fundamental interest and also important in many applied areas. Surface science investigations have advanced understanding of organic/metal interfaces, but the second electrode in organic optoelectronic devices – typically the transparent conductive oxide In_2O_3 – remains largely unexplored. Our work aims at closing this gap by examining the model system phthalocyanines on indium oxide surfaces.

Phthalocyanines adsorbed on the $In_2O_3(111)$ surface were studied experimentally with low temperature STM and AFM, combined with DFT calculations. A key aspect is the comparable size of the molecules and the surface unit cell, which allows a (1×1) arrangement despite the differing symmetries. Various metal phthalocyanines (MPc: CuPc, CoPc, etc.) are investigated to reveal the influence of the metal ion in the selection of adsorption sites, 2D condensation, and the formation of the first layer. We identify a common, robust adsorption site for different MPc that forces the molecules to overlap in the (1×1) structure of the first layer, and a less common site, where a (1×1) packing without overlap is realized.

O 58.8 Wed 12:15 TRE/PHYS

***In Situ* Field-Induced Switching of Global Chirality in Halogen-Bonded Kagomé Networks** — •Nico Kubetschek, Jana Dietrich, and René Matzdorf — Institute of Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We used small organic molecules to construct a chiral Kagomé lattice on the Ag(111) and Au(111) surfaces. The chirality arises from triple halogen bonds that form windmill-like structures. Under certain conditions, we observe a switching in the rotational sense of whole terraces while scanning with STM. The total molecular coverage was used to tune the switching probability between the two chiral states. We demonstrate a bias-dependent attraction or repulsion of the molecules relative to the STM tip position, explaining the observed perturbation leading to the switching events.

O 59: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

O 59.1 Wed 10:30 TRE/MATH

Polarons in epitaxial single-layer $MnBr_2$ — •Affan Safeer, Oktay Güleryüz, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We investigate polaron formation in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates: graphene on Ir(110), graphene on Ir(111), and Au(111). The polaron number densities and species depend strongly on the underlying substrate, underscoring the crucial role of the substrate. Our findings show that modeling of polarons in such single-layer insulators in contact with conducting substrates must explicitly include the substrate. For $MnBr_2$ grown on graphene/Ir(110), we identify four distinct polaron species, three of which closely resemble those reported for $CoCl_2$ on graphite. These polarons can be created, converted, and laterally manipulated by the STM tip when a tunneling current flows at suitable bias voltages. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided by the periodic potential imposed by the supermoiré pattern arising from the interaction of $MnBr_2$ with graphene and Ir(110).

O 59.2 Wed 10:45 TRE/MATH

Chirality in the Kagome Metal CsV_3Sb_5 — •Tom P. Lammerskötter[1], H.J. Elmers[2], G. Schönhense[2], O. Tkach[2], Y. Lytvynenko[2], H. Agarwal[2], S. Chernov[3], M. Hoesch[3], D. Kutnyakhov[3], M. Scholz[3], K. Rossnagel[4], A. Gloskovskii[3], C. Schlueter[3], A. Winkelmann[5], A. Haghighirad[6], M. Schmitt[7], T. Lee[7], R. Claessen[8], M. Le Tacon[6], J Demsar[2], and O. Fedchenko[1] — [1]Goethe-Universität Frankfurt (Germany) — [2]JGU Mainz (Germany) — [3]DESY Hamburg (Germany) — [4]Universität zu Kiel (Germany) — [5]AGH University of Krakow (Poland) — [6]KIT Karlsruhe (Germany) — [7]DIAMOND (UK) — [8]Universität Würzburg (Germany)

Kagome metals AV_3Sb_5 (A = Cs, K, Rb) exhibit flat bands, Dirac points, and van Hove singularities that drive unconventional charge-density-wave (CDW) order and topological states. We study chirality in CsV_3Sb_5 using angle-resolved photoemission spectroscopy (ARPES) and x-ray photoelectron diffraction (XPD) with circularly polarized photons. XPD reveals a local crystal chirality in the CDW phase. ARPES shows pronounced magnetic circular dichroism (MCD), demonstrating a chiral electronic structure and indicating orbital moments possibly linked to loop-current order. To probe orbital-moment coupling, we study Nb-doped CsV_3Sb_5, where band broadening and enhanced Dirac-like gaps occur. In the CDW phase, the strongly increased MCD indicates time-reversal-symmetry breaking and couples to the three van Hove singularities at the M points.

O 59.3 Wed 11:00 TRE/MATH

Ab initio and group theory ananlysis of monolayer BiTeI — •Josep Mas-Garcia, Jorge Cervantes-Villanueva, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV - University of Valencia - Spain

Monolayer BiTeI is a prototypical polar semiconductor whose remarkable Rashba spin splitting, rooted in strong spin-orbit coupling and non-centrosymmetric structure, offers a fertile landscape for advancing two-dimensional spintronics. This work presents and ab initio and group-theoretical analysis of BiTeI. Employing fully relativistic density functional theory and GW calculations, we obtain electronic structures that serve as benchmarks for the group-theory based Hamiltonian model. Leveraging the systematic method of invariants, we construct symmetry-constrained k-p Hamiltonians near the Γ point. Our implementation of the method of invariants enables precise fitting of the Hamiltoninan eigenvalues to ab initio band dispersions for the obtention of the parameters, and yields a highly compact analytic model that reproduces Rashba splitting and symmetry-dependent features. This framework facilitates straightforward evaluation of key physical quantities, such as effective masses or spin textures, and perturbative responses including electric and magnetic fields and strain effects within a unified and transparent formalism. Moreover our methodology establishes a versatile template for the symmetry-guided modeling of nonmagnetic semiconductors with strong spin-orbit coupling.

O 59.4 Wed 11:15 TRE/MATH

Production of Interstitials in 2D Transition-Metal Dichalcogenides (TMDs) by Ion Irradiation: ab-initio Simulations — •Silvan Kretschmer[1], Joel Davidsson[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark — [2]Department of Physics, Linköping University, Sweden

Defects critically shape the properties of two-dimensional (2D) materials and can be purposefully introduced to tune magnetic, electronic, and optical behavior. Low-energy ion irradiation has recently emerged as an effective route for generating specific defect types via direct implantation [1,2].

First-principles simulations are essential for understanding irradiation-induced defect formation [3], but DFT-based molecular dynamics (MD) is computationally costly and limits broad exploration of materials and irradiation conditions. Machine-learning (ML) interatomic potentials provide a high-accuracy, low-cost alternative, enabling efficient screening of large datasets such as the Impurities in 2D Materials Database [4].

Here, we benchmark a ML potential against ab-initio MD, emphasizing accurate treatment of the short interatomic distances occurring during ion impacts. We apply the fine-tuned ML to study interstitial defect formation in TMDs under low-energy ion irradiation, providing defect formation probabilities and identifying suitable ion-beam parameters for targeted defect engineering in 2D materials.

[1] 10.1038/s41699-022-00318-4 [2] 10.1021/acsnano.4c03475

[3] 10.1103/PhysRevMaterials.8.114003 [4] 10.11583/DTU.19692238

O 59.5 Wed 11:30 TRE/MATH

Long-living metastable electronic states in substituted 1*T*-TaS_2 — •Gaël Reecht[1], Jesumony Jayabalan[1], Ričards Knipšis[2], Florian Diekmann[3], Friedemann Queisser[2], Ping Zhou[1], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]University Duisburg-Essen, Germany — [2]HZ Dresden-Rossendorf, Germany — [3]CAU of Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]DESY, Hamburg, Germany

1*T*-TaS_2 is a prototypical correlated material whose low-temperature phase exhibits a commensurate charge density wave forming Star-of-David (SOD) clusters. Each SOD hosts a single electron close to E_F and, due to strong on-site Coulomb repulsion, the system enters a Mott insulating state. Adding or removing an electron creates doublon or holon excitations, which typically relax within few femtoseconds [1]. Here, we manipulate the lifetime of the quasiparticle excitations by substituting some Ta with an electron richer element. Using LT-scanning tunnelling microscopy and spectroscopy (STM/STS) and time-resolved photoemission spectroscopy, we observe metastable doublons with lifetimes ranging from fs to hours. STM/STS further shows that these excitations are locally confined. The experimental observations are corroborated by a theoretical description based on a Fermi-Hubbard model. The disorder induced by the random substitution leads to a spatial localization of holon and doublon wavefunctions at the origin of the long lifetimes observed experimentally.

[1] M. Ligges et *al.*, Phys. Rev. Lett., **120**, 166401 (2018)

O 59.6 Wed 11:45 TRE/MATH

Fingerprints of Excitonic Collective Modes in the Two-Dimensional Electron Gas — •Jakob Wolff[1,2,3], Silvana Botti[2,3], Lucia Reining[4,3], and Matteo Gatti[4,3,5] — [1]Institut für Festkörpertheorie- und Optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems, University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]LSI, CNRS, CEA/DRF/IRAMIS, École polytechnique, Institut Polytechnique de Paris, France — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

We investigate the collective charge excitations of the two-dimensional homogeneous electron gas in the low density regime within the framework of time-dependent density functional theory. We show that beyond the well-known plasmons new collective excitonic modes emerge, which leave characteristic fingerprints in experimentally accessible quantities, such as asymmetric peak structures in the loss function and enhanced Friedel oscillations. Further, at sufficiently low densities the collective modes become imaginary, indicating an instability towards the formation of a charge-density-wave phase with excitonic origin.

O 59.7 Wed 12:00 TRE/MATH

Moir'e modulated quantum spin liquid candidate 1T-TaSe2 — Ziying Wang, Adolfo O. Fumega, Ana Vera Montoto, Mohammad Amini, Büsra Gamze Arslan, Ales Cahlik, Yuxiao Ding, Jose L. Lado, •Robert Drost, and Peter Liljeroth — Aalto University, Department of Applied Physics

Quantum spin liquids continue to fascinate with their highly entangled quantum states and promises of fractional many-body excitations. Yet there are few tools to probe these materials, and none sensitive enough for applications in 2D materials. This seriously hampers the study of monolayer QSL candidates such as α-RuCl3 and 1T-TaSe2. Scanning tunneling microscopy and spectroscopy may overcome this challenge, as they can access the fundamental excitations of 2D samples through inelastic tunneling spectroscopy. These low-energy excitations can be compared against theoretical models and provide fingerprints of QSL states. We employ this approach against the quantum spin liquid candidate 1T-TaSe2. We observe the emergence of a root 3 reconstruction driven by the substrate, equivalent spectroscopy across all spin sites, and the coexistence of zero and finite energy excitations. These observations are consistent with a QSL ground state. Our results demonstrate that IETS provides a powerful route to obtain atomic-scale insight into the magnetic excitations of two-dimensional materials. Spectral fingerprints may help to identify exotic phases of matter that are otherwise difficult to detect.

O 59.8 Wed 12:15 TRE/MATH

Long-Range Interactions in Twisted Bilayer Materials with Machine Learning for the Electronic Density — •Zekun Lou[1], Alan Lewis[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of York, York, U.K.

Moiré superlattices in twisted bilayer (TB) 2D materials exhibit extraordinary quantum phenomena, but first-principles understanding remains limited by computational costs. While most machine learning (ML) methods for density functional theory (DFT) acceleration are based on the locality assumption, we demonstrate that accurate moiré electronic structure prediction requires long-range encoding due to charge rearrangement, orbital hybridisation, and moiré potential modulation. Using long-range representations [1] for electronic-density prediction [2,3], we achieve low-energy band-structure predictions with <15 meV errors across twisted bilayer graphene (TBG), hBN, and transition-metal dichalcogenides (TMDCs), while ∼100 times faster than DFT. Descriptor requirements are material-dependent: homoatomic systems (e.g., TBG) are well-described by local descriptors, while hBN and TMDCs require long-range encoding. We summarise the physical implications of these findings that marry machine learning and the fundamental physics that governs the electronic density of twisted bilayer materials.

[1] A. Grisafi, M. Ceriotti, JCP 151, 204105 (2019)

[2] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, JCTC 17, 7203 (2021)

[3] A. Grisafi, A. Lewis, M. Rossi, M. Ceriotti, JCTC 19, 4451 (2023)

O 60: Focus Session: Unoccupied States by Inverse Photoemission I

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Wednesday 10:30–12:30 Location: WILL/A317

Invited Talk O 60.1 Wed 10:30 WILL/A317

Disentangling the origins of spin polarization in (inverse) photoemission from solid surfaces — •Jürgen Henk — Martin Luther University Halle-Wittenberg, Halle, Germany

The spin polarization of electronic states in solids can be probed by various photoemission-based techniques. We discuss how optical excitation modifies the spin polarization of the initial electronic states. Illustrative examples include Rashba-type surface states observed in photoemission (PE) from Au(111), the Dirac-like surface state in inverse photoemission (IPE) from W(110), and magnetic contrast in photoemission electron microscopy (PEEM) from Fe(001). Instead of employing a full group-theoretical analysis, we introduce a simplified symmetry-based approach that enables a clear separation of the different contributions to the photoelectron spin polarization—arising from light polarization, spin-orbit coupling, and intrinsic spin textures. This framework facilitates the interpretation of spin-resolved measurements at surfaces without relying on fully relativistic photoemission calculations.

O 60.2 Wed 11:00 WILL/A317

Inverse photoemission - just the inverse of photoemission? — •Markus Donath — University of Münster, Germany

Photoemission (PE) is known as the most powerful experimental technique to investigate the occupied energy levels of electrons in matter. The photoelectric effect, where electrons are detected after excitation with light, was first observed by H. Hertz and W. Hallwachs in 1887/1888. The reverse effect, the emission of Bremsstrahlung after irradiation of electrons was discovered by W.C. Röntgen in 1895. Bremsstrahlung spectroscopy provides access to unoccupied states. The first Bremsstrahlung spectroscopy experiment in the vacuum ultraviolet (VUV) range was performed by V. Dose fifty years ago [1]. In 1980, J.B. Pendry named this technique inverse photoemission (IPE) [2]. By using light in the VUV spectral range, PE and IPE became valuable complementary tools for studying the energy vs momentum dispersion of electron states below and above the Fermi level, even with spin resolution. After some historical remarks, this talk will review strengths and challenges as well as future perspectives of IPE.

[1] V. Dose, Appl. Phys. **14**, 117 (1977).

[2] J.B. Pendry, Phys. Rev. Lett. **45**, 1356 (1980).

O 60.3 Wed 11:15 WILL/A317

A Retrospective on Spin-Resolved IPES in Milan — •Alberto Calloni, Gianlorenzo Bussetti, and Franco Ciccacci — Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

For over thirty years, the Milan group led by Franco Ciccacci has been a key contributor to the development of spin-resolved Inverse Photoemission Spectroscopy (SR-IPES), advancing both the experimental methods and the study of empty electronic states in solids and interfaces. The activity began in the early '90s, when a dedicated system for spin- and angle-resolved measurements was conceived and built in Milan, drawing on the experience gained earlier with one of the first IPES setups using a UV grating. The new apparatus, featuring a spin-polarized GaAs electron source and a solid-state photon detector that ensured efficient detection of the weak IPES signal, enabled the direct investigation of spin-dependent unoccupied states at a time when such studies were still in their infancy. Building on this capability, the group has carried out a broad range of SR-IPES studies on metallic surfaces, magnetic thin films and multilayers, addressing phenomena such as spin-polarized quantum-well states and surface- or interface-induced spin polarization. More recently, together with studies on systems in which spin-orbit effects define the spin texture of the unoccupied states, the IPES setup has also been applied to hybrid organic/inorganic and molecule/ferromagnet interfaces, offering insight into the stability of the unoccupied states and their possible modifications upon interaction with the surrounding environment.

O 60.4 Wed 11:30 WILL/A317

Spin-Orbit Effects in Atomic-Layer Materials: Tl on Ag(111) — •Sven Schemmelmann[1], Peter Krüger[2], Patrick Härtl[3], Matthias Bode[3], Yuichiro Toichi[4], Kazuyuki Sakamoto[4], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany — [3]Experimentelle Physik II, Universität Würzburg, Germany — [4]Department of Applied Physics, The University of Osaka, Japan

Growing Tl on Ag(111) results in several structures of the Tl adlayers. For low coverage a TlAg$_2$ surface alloy is formed [1]. The Tl monolayer and bilayer exhibits moiré superstuctures with a continuous rotation of the Tl adlayer. Interestingly, all these structures exhibit characteristic spin-orbit-induced effects in their unoccupied electronic structure revealed by spin- and angle-resolved inverse photoemission. The surface alloy is predicted to exhibit states with a Rashba-type spin splitting. In experiment, the intensity of these states is too low for a spin analysis [1]. In the Tl monolayer, spin-dependent hybridization of different overlayer states is observed [2]. Surprisingly, also an image-potential state located in front of the surface is found to hybridize with Tl states. The Tl bilayer, in contrast, exhibits a non-Rashba-like spin-polarized Fermi surface whose origin is found in the dispersion of the unoccupied states.

[1] Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)

[2] Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)

O 60.5 Wed 11:45 WILL/A317

Surface state on Au(111): Shockley vs topology — •Patrick Geers, Fabian Schöttke, and Markus Donath — University of Münster, Germany

The L-gap surface state on Au(111) is the famous prototype for a Rashba-split Shockley surface state (SS). In 2015, Yan *et al.* posed the question whether Shockley-type SSs may be interpreted as variation of SSs in topological insulators, as both states exist in inverted band gaps [1]. The behaviour of the SS away from $\overline{\Gamma}$ is important to answer this question. It is crucial to know whether the SS potentially closes the inverted band gap between $\overline{\Gamma}$ and $\overline{\text{M}}$. An analysis of not only the existence of SSs but also their spin textures is necessary to show a potential topologically nontrivial character of such SSs.
Inverse photoemission (IPE) as a technique to study the unoccupied electronic states is capable to measure these SSs with spin resolution at expected energies of about 4 eV above the Fermi level. In this talk, we present spin-resolved IPE results for Au(111) showing the energy vs momentum range between $\overline{\Gamma}$ and $\overline{\text{M}}$, where the SS merges into the bulk bands.

[1] Yan *et al.*, Nat. Commun. **6**, 10167 (2015).

O 60.6 Wed 12:00 WILL/A317

Combining Spin Polarized Inverse Photoemission Spectroscopy with Angle-resolved X-ray Magnetic Circular Dichroism — •Takashi Komesu[1], Arjun Subedi[1], Bharat Giri[1], Ather Mahmood[1], Will Echtenkamp[1], Mike Street[1], Alpha N'Diaye[2], Xiaoshan Xu[1], Christian Binek[1], and Peter Dowben[1] — [1]University of Nebraska-Lincoln, Lincoln, NE, U.S.A — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, U.S.A

While angle-resolved magnetometry and angle-resolved X-ray Magnetic Circular dichroism (XMCD) might provide hints of spin or moment canting at a surface, even XMCD taken in the total electron yield (TEY) mode cannot convincingly implicate the surface. Spin Polarized Inverse Photoemission Spectroscopy (SPIPES) is hugely surface sensitive, which is an advantage for characterizing boundary polarization of materials. With in-plane SPIPES, we have convincing proof of deviation from the expected perpendicular anisotropy for boron (B) doped Cr$_2$O$_3$(0001) and at the surface of NiCo$_2$O$_4$(001). For NiCo$_2$O$_4$(001), the Ni magnetic moments are canted slightly off the surface normal, as evident in elemental specific angle-resolved XMCD and consistent with the very surface sensitive SPIPES. In this presentation, we will show the great value of combining SPIPES with XMCD and magnetometry. Furthermore, we can provide an example where an exponential decay of spin polarization is not evidence of a finite paramagnetic correlation length, as in the case of thickness dependent Pd over layers on Cr$_2$O$_3$(0001), where Pd is no longer paramagnetic.

O 60.7 Wed 12:15 WILL/A317

On the sign of the Rashba parameter in image-potential states — •Fabian Schöttke[1], Kaishu Kawaguchi[2], Kenta Kuroda[3], Peter Krüger[1], Thorsten Deilmann[1], Sven Schemmelmann[1], Ayumi Harasawa[2], Shuntaro Tani[2], Yohei Kobayashi[2], Takeshi Kondo[2], and Markus Donath[1] — [1]Universität Münster, Germany — [2]Institute for Solid State Physics, The University of Tokyo, Japan — [3]Hiroshima University, Hiroshima, Japan

Image-potential surface states are simple model systems, where spin-dependent effects can be studied in view of spintronic applications. The Rashba effect in surface states at high-Z materials is related to both the strong spin-orbit interaction in heavy atoms and the orbital angular momentum arising from the inversion-symmetry breaking at the surface. Our studies with spin- and angle-resolved inverse photoemission and three-photon photoemission on image-potential states at Re(0001), Bi$_2$Se$_3$ and Bi$_2$Te$_3$ show a clear correlation between orbital angular momentum and spin directions. A key factor of our analysis is spin resolution, which enhances the effective resolution to separate spectral features considerably, provided they have different spin character.

O 61: Organic molecules on inorganic substrates: electronic, optical and other properties II

Time: Wednesday 15:00–17:45 Location: HSZ/0201

O 61.1 Wed 15:00 HSZ/0201

Circular dichroism in the photoelectron angular distribution of achiral molecules — Christian Simon Kern[1], Xiaosheng Yang[2], Giovanni Zamborlini[1,3], Simone Mearini[3], Matteo Jugovac[3], Vitaliy Feyer[3], Umberto De Giovannini[4], Angel Rubio[4], Serguei Soubatch[2], Michael G. Ramsey[1], •Frank Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-3, FZ Jülich & RWTH Aachen University, Germany — [3]PGI-6, FZ Jülich & Universität Duisburg-Essen, Germany — [4]MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Circular dichroism in the angular distribution (CDAD) is the effect that the angular intensity distribution of photoemitted electrons depends on the handedness of the incident circularly polarized light. CDAD has been reported also for achiral organic molecules at the interface to metallic substrates. For this latter case, we investigate two prototypical pi-conjugated molecules, namely tetracene and pentacene, whose frontier orbitals have a similar shape but exhibit distinctly different symmetries. By comparing experimental CDAD momentum maps with simulations within time-dependent density functional theory, we show how the final state of the photoelectron must be regarded as the source of the CDAD in such otherwise achiral systems. We gain additional insight into the mechanism by employing a simple scattering model for the final state, which allows us to decompose the CDAD signal into partial wave contributions.

O 61.2 Wed 15:15 HSZ/0201

Many-body electronic structure of acenes on an MoS2 monolayer — •Jan-Phillip Topmöller and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

TMDCs show great potential in terms of their applicability in optical electronics. Due to their large surface, molecules can easily bind to the TMDC and affect its electronic properties. Here we investigate acenes as a prototypical class of molecule.

We use DFT (GGA) and DFT-D3 to determine the most stable adsorption position of acenes like benzene, naphthalene and anthracene on MoS2. Subsequently, we use many body perturbation theory to calculate the electronic structure of the adsorbate system and its individual components (MoS2 and the molecule) in order to investigate the effect of the molecule on the MoS2 electronic and optical spectrum.

O 61.3 Wed 15:30 HSZ/0201

Azimuthal-Scanning SFG Microscopy for Mapping Packing Motifs and In-Plane Disorder in Molecular Films — •Nasim Mirzajani, Ben John, Alex Fellows, and Martin Thaemer — Fritz-Haber-Institut, Berlin, Germany

Phase-resolved vibrational sum-frequency generation (SFG) microscopy is a powerful tool for probing anisotropic and heterogeneous structure of molecular films. As a second order nonlinear technique, SFG is uniquely sensitive to disorder in film morphology but it has not been yet used to quantify order in molecular film assemblies. Here, we introduce an azimuthal-scanning SFG microscopy approach that extracts detailed information on structure as well as in-plane orientational order by analyzing the full set of rotational frequencies arising from azimuthal dependence. Applying the method to a lipid monolayer, we determine the full 3D structure of the lipids, the packing motif as well as the degree of its in-plane disorder. This technique provides a general framework for probing packing structure in thin films and is broadly applicable to diverse molecular and phononic materials.

O 61.4 Wed 15:45 HSZ/0201

Synthesis and Characterization of a Polyradical Hexaazacycloarene — •Zilin Ruan, Olaf A. Kleykamp, Tim Naumann, Faming Kang, Jörg Sundermeyer, and J. Michael Gottfried — Department of Chemistry, Philipps University Marburg, 35037 Marburg, Germany

Cycloarenes have drawn considerable research interest owing to their unique electronic and topological features. The synthesis of large zigzag-edged cycloarenes, which are predicted to exhibit exotic polyradical ground states, has remained elusive. Here, we report the synthesis of a zigzag-edged hexaazacycloarene incorporating six graphitic nitrogen atoms within its macrocyclic backbone, achieved through a combined in-solution cyclization and on-surface cyclodehydrogenation on a Au(111) surface. The structural and electronic properties of the resulting macrocycle were investigated by STM/STS, nc-AFM and KPFM. DFT and multireference CASSCF calculations reveal that the isolated molecule has an open-shell singlet ground state with six unpaired electrons and undergoes a spontaneous symmetry breaking from C6 to C2, driven by strong electron-electron correlations and a pseudo-Jahn-Teller instability. Notably, the expected low-energy spin excitations are absent on Au(111), which is rationalized by the hybridization between the molecular π-system and the substrate, effectively quenching the intrinsic magnetism. These results provide crucial insight into correlation-driven magnetism and represent a significant advance toward the realization of cycloarenes with π-magnetism.

O 61.5 Wed 16:00 HSZ/0201

Vibrational Spectra of Materials and Molecules with Path Integrals and Machine Learning — •Jorge Castro, Krystof Brezina, and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Vibrational spectroscopy provides fundamental insight into molecular structure and dynamics. Nuclear quantum effects (NQEs) can critically modulate vibrational peak positions, shapes, and intensities. Recently, we showed that the partially adiabatic elevated-temperature centroid molecular dynamics (PA-T_e-CMD) [1] accurately reproduces vibrational spectra across molecular and condensed-phase systems, including low-temperature regimes where NQEs are strongest. This approach enables the simulation of quantum infrared and Raman responses in diverse spectroscopic settings. Tip-Enhanced Raman Spectroscopy (TERS) [2] achieves sub-nanometer spatial resolution and is uniquely sensitive to single-molecule vibrational motion and surface defects. Building on first-principles finite-field formulations of TERS [3], we combine this framework with PA-T_e-CMD to quantify the role of nuclear quantum motion and anharmonicity in near-field Raman observables. As a first application, we investigate hydrogen-bonded chains of 2,5-diamino-1,4-benzoquinonediimine (DABQDI) and discuss how NQEs imprint on vibrational signatures in simulated TERS images.

[1] J. Castro et al., J. Chem. Phys. 163, 204102 (2025). [2] J. Lee et al., Nature 568, 78*82 (2019). [3] K. Brezina et al., arXiv:2509.13075 (2025).

O 61.6 Wed 16:15 HSZ/0201

Quasiparticle level alignment in anthracene-MoS$_2$ heterostructures — •Hsin-Mei Ho, Michael Lorke, and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Stacking atomically thin materials through van der Waals (vdW) interaction has opened a new paradigm for fundamental and applied sciences. While preserving the advantages of individual components, heterostructures are predicted to exhibit emergent properties at the interfaces. In the presence of external perturbations, since the behavior of a hybrid system is strongly related to the electronic band structure, it is of interest to find a methodology beyond the ground-state formalism of density functional theory (DFT). In this work, we begin with DFT calculations and consider the organic-inorganic heterostructures composed of anthracene molecules on monolayer MoS$_2$. Motivated by studies on the crystallinity of organic films, interfacial configurations with different coverage and orientation of anthracene are investigated. We find that both the bandgap values and band offsets are sensitive to whether the molecules are closely packed and whether they adopt perpendicular or parallel orientations on MoS$_2$. Whereas DFT predicts type-II level alignment, inclusion of quasi-particle corrections via the GW approximation yields type-I alignment. These findings highlight the importance of level-alignment predictions for interpreting experiments and for guiding the design of organic-TMDs heterostructures.

O 61.7 Wed 16:30 HSZ/0201

Magnetic interactions between spins in the Metallacrown CuCu4: bulk vs adsorbed molecule on Au(111) — •Ariyan Tavakoli[1], Stefan Lach[1], Frederik Pütz[1], Dominic Stephan[1], Anne Lüpke[2], Dominik Laible[2], Siegfried Kaidisch[3], Andreas Winidischbacher[3], Eva Rentschler[2], Peter Puschnig[3], Christiane Ziegler[1], and Hans Christian Schneider[1] — [1]RPTU University Kaiserslautern-Landau, Germany — [2]Johannes Gutenberg University Mainz, Germany — [3]University of Graz, Austria

Metal-organic complexes featuring multiple metal ions with unsaturated spin structures are intriguing because of their potential to tune molecular magnetic properties. In this study, we compare the magnetic and electronic properties of the CuCu4 metallacrown [1] in bulk, gas-state, and adsorbed on an Au(111) surface. Using the broken-symmetry approach, we benchmark various (range-separated) hybrid functionals against the computationally efficient GGA+U method to evaluate exchange coupling constants in different states [2]. We compare ultraviolet photoemission spectroscopy (UPS) combined with ab-initio calculations to show how the exchange interactions between Cu spins shift significantly, resulting in a transition from a low-spin state ($S = 1/2$) in the bulk to a higher-spin state ($S = 3/2$) on Au(111).

[1] Happ, P.; et al. Phys. Rev. B, 93, 174404 (2016).

[2] Pavlyukh, Y. et al., Phys. Rev. B. 99, 144418 (2019).

O 61.8 Wed 16:45 HSZ/0201

Vectorial spin-to-charge conversion by supramolecular chirality — •Sophie Knewitz[1], Guillaume Schweicher[2], Ashish Moharana[1], Yves Geerts[2], and Angela Wittmann[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Université Libre, Bruxelles, Belgium

The chiral-induced spin selectivity (CISS) effect describes how electrons get spin-polarized due to the presence of chiral molecules. The high polarization efficiency makes it promising for future sustainable hybrid chiral molecule magnetic applications. While there are many experimental reports of different aspects of the CISS effect, a complete understanding of the fundamental mechanisms remains an open challenge. In this work, we investigate the role of supramolecular chirality and atomic spin-orbit coupling on the CISS effect in hybrid metal thin film / chiral organic crystal heterostructures. Using spin pumping to inject a pure spin current in the metal thin film, we probe the spin-to-charge conversion at the chiral interface. Based on our recent finding that CISS is a vectorial effect [1], we use a molecular chiral crystal to probe the CISS effect in a well-ordered system in order to maximize the polarization efficiency. Our angle-dependent measurements confirm that the spin selectivity of the chiral supramolecular crystal is highly sensitive to its orientation relative to the spin direction in the metal thin film under the applied magnetic field. These results open new ways for the vectorial manipulation of hybrid spintronic devices by chirality.

[1]: Moharana, A. et al., Sci. Adv. 11, eado4285 (2025).

O 61.9 Wed 17:00 HSZ/0201

Chiral recognition of enantiomers on a superconducting surface — •Lorenz Meyer, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The adsorption of a racemic mixture of heptahelicene on Pb(111) gives rise to enantiopure domains, in which left-handed and right-handed variants are spatially resolved with submolecular structure. For molecules inside the domains the molecular spiral is oriented along the surface normal, while at domain boundaries the spiral axis is tilted. Both enantiomers leave the Bardeen-Cooper-Schrieffer energy gap of the substrate invariant and exhibit an elevated energy difference between the occupied and unoccupied frontier orbitals. Funding by the Deutsche Forschungsgemeinschaft through KR 2912/21-1 and the Bundesministerium für Bildung und Forschung is acknowledged.

O 61.10 Wed 17:15 HSZ/0201

Unveiling the precise configuration of a molecular junction — Joshua Scheidt[1,3], Jonas Lederer[3], Mong-Wen Gu[1,2], Hadi Arefi[1,2], Jose M. Guevara[1,2], Amin Karimi[1,2], Rustem Bolat[1,2], Marvin Knol[1,2], Klaus-Robert Müller[3], F. Stefan Tautz[1,2], and •Christian Wagner[1,2] — [1]PGI-3, Forschungszentrum Jülich, Germany — [2]JARA, Fundamentals of Future Information Technology, Germany — [3]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, Germany

Exploring structure-property relationships of molecular junctions is crucial for future single-molecule applications. While, e.g., a strong scattering of conductance values is found in break-junctions, the responsible structural variations cannot be identified. Here, we describe NC-AFM/STM-based two-contact manipulation experiments on PTCDA (3,4,9,10-perylene-tetracarboxylic dianhydride) on Ag(111) and analyze them using a DFT-based machine learning model of the junction. Our approach allows solving the inverse problem of configuration identification from force gradient data[1] and reveals the origin of the 3-4 fold conductance variations observed upon sub-Angstrom changes in the junction geometry.

[1] J. Scheidt et al., J. Phys. Chem. C 127, 13817 (2023)

O 61.11 Wed 17:30 HSZ/0201

Low-temperature scanning tunneling microscopy and spectroscopy of 1,10-phenanthroline molecules on Au(111) surface — •Yuya Kaneko[1], Takaya Shimokawa[1], Hinata Aso[1], Erlina Tik Man[1], Kenji Hayashida[2], Koutarou Takeyasu[3], Junji Nakamura[4], and Yasuo Yoshida[1] — [1]Dept. of Phys. Kanazawa Univ., Kanazawa, Ishikawa 920-1192, Japan. — [2]Graduate School of Pure and Applied Sciences, Univ. of Tsukuba, Ibaraki 305-8577, Japan. — [3]institute for Catalysis, Hokkaido Univ., Hokkaido 001-0021, Japan. — [4]International Institute for Carbon-Neutral Energy Research, Kyushu Univ., Fukuoka 819-0395, Japan.

Fuel cells are considered a key technology for achieving a low-carbon society. However, current fuel cells rely on precious platinum for the oxygen reduction reaction (ORR). Nitrogen-doped carbon catalysts have attracted attention as promising alternatives due to their low cost and high durability, yet the detailed reaction mechanism remains unclear. Here, we report a scanning tunneling microscopy and spectroscopy (STM/S) study of in situ deposited 1,10-phenanthroline molecules, which serve as ideal model catalytic molecules for ORR activity [1]. [1]Takeyasu K., Furukawa M., Shimoyama Y., Singh S. K., Nakamura J., (2020) Role of Pyr-idinic Nitrogen in the Mechanism of the Oxygen Reduction Reaction on Carbon Electro-catalysts. Angew. Chem. Int. Ed.,60,5121-5124..

O 62: Graphene: Electronic structure, excitations, etc. (joint session O/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0204

O 62.1 Wed 15:00 HSZ/0204

Magneto-photoelectric effect in graphene via tailored potential landscapes — •Friedemann Queisser[1], Joris Josiek[1,2], Stephan Winnerl[1], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider the propagation of charge carriers in planar graphene under the combined influence of a constant transversal magnetic field and an in-plane varying electric potential. By suitably designing the potential landscape, we may effectively steer charge carriers generated by photo-excitation, for example, in order to achieve an efficient charge separation. These finding may pave the way for transport schemes or photoelectric/photovoltaic applications. Funding by the DFG through the SFB 1242 is gratefully acknowledged.

O 62.2 Wed 15:15 HSZ/0204

Topological obstruction in twisted bilayer graphene — Florie Mesple[1], Pierre Mallet[2], •Guy Trambly de Laissardière[3], Clement Dutreix[4], Gérard Lapertot[5], Jean-Yves Veuillen[2], and Vincent T. Renard[5] — [1]Dept. Physics, Univ. of Washington, Seattle, USA — [2]CNRS, Univ. Grenoble Alpes, Inst. Néel, Grenoble, France — [3]CY Cergy Paris Univ., CNRS, LPTM, Cergy-Pontoise, France — [4]Univ. Bordeaux, CNRS, LOMA, Talence, France — [5]Univ. Grenoble Alpes, CEA, IRIG, PHELIQS, Grenoble, France

The rich physics of magic angle twisted bilayer graphene (TBG) results from the Coulomb interactions of electrons in nearly flat bands of nontrivial topology [1]. Here [2], we perform STM/STS measurements on a moiré pattern generated in a TBG tilted by 4.3°, focusing on a point-like defect. We observe quasi-particle interferences (QPIs) resulting from intravalley backscattering between Dirac cones of graphene layers 1 and 2. Rationalized by tight binding calculations and T-matrix

theory, our work shows that the QPIs are strongly impacted by the relative chirality of the Dirac cones of layer 1 and 2 in each valley. It establishes that, within a given moiré valley, the two Dirac cones have the same electronic chirality, as expected in the usual continuum model [3]. This peculiar topology leads to a topological obstruction.
[1] B. A. Bernevig, D. K. Efetov, Physics Today **77**, 38 (2024)
[2] F. Mesple, et al., arXiv:2506.08913 (2025)
[3] R. Bistritzer, A. H. MacDonald, PNAS **108**, 12233 (2011)

O 62.3 Wed 15:30 HSZ/0204

Quasiparticle Interferences in 30°-twisted graphene quasicrystal — •Jean-Maxime Schlachter[1], Ahmed El Alouani[2], Vincent S Renard[2], Abhishek Karn[1], Ileana Florea[2], Stéphane Vézian[2], Adrien Michon[2], Clemens B Winkelmann[1], and Vincent T Renard[1] — [1]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France — [2]CNRS-CRHEA, Université Côte d'Azur, rue B. Grégory, 06560 Valbonne, France

Quasicrystals are materials that have clean diffraction pattern but no translational symmetry. The advent of van der Waals stacking has opened the possibility to engineer quasicrystals. For example, the moiré pattern in 30°-twisted graphene bilayers has 12-fold rotational symmetry which is not compatible with translation symmetry in 2D, hence it is a quasicrystal (1). Studying this system gives insight into the behavior of Dirac fermions in 2D quasicrystals. ARPES experiments (2) demonstrated the existence of multiple Dirac cone replicas, originating from the incommensurate interlayer coupling. The goal of this study is to determine to what extend these Dirac cone replicas influence the electronic properties of the Dirac fermions. Our low temperature scanning tunneling microscope (STM) experiments evidence the replicated Dirac cones by specific patterns in the local density of states patterns associated with scattering between them, contrary to previous STM experiments (3).
(1) P. Moon et al., Phys. Rev. B, **99**, 16, :165430 (2019) ; (2) S. J. Ahn et al., Science, **361**, 6404, :782-786 (2018) ; (3) C. Yan et al., 2D Mater., **6**, 4, :045041 (2019)

O 62.4 Wed 15:45 HSZ/0204

Machine Learning for Bandstructure-Structure Relationships in Doped Graphene — •Benedict Saunders[1], Lukas Hörmann[1,2], Valdas Vitartas[1], Chen Qian[1], and Reinhard J Maurer[1,2] — [1]University of Warwick, Coventry, United Kingdom — [2]University of Vienna, Vienna, Austria

The introduction of topological defects or dopants to graphene's honeycomb lattice is a common approach to tuning the electronic and transport properties of the material to suit a specific application. Nitrogen is a widely investigated dopant, which can be introduced into the lattice in various configurations, each with a distinct effect on the material's bandstructure. However, due to the combinatorial explosion of possible dopant configurations, conventional first-principles screening of the electronic bandstructure for all possible configurations is not feasible. Here, we address this limitation by employing the recently developed MACE-H machine learning model to predict the electronic Hamiltonian of nitrogen-doped graphene configurations directly for a series of previously generated defect configurations. This allows us to rapidly generate accurate bandstructures and densities-of-states for large numbers of configurations, enabling the identification of structure-property relationships as a function of temperature and composition.

O 62.5 Wed 16:00 HSZ/0204

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil

Two-dimensional materials such as graphene are particularly intriguing due to their exceptional mechanical and electronic properties. A natural next step involves combining different 2D materials to form heterostructures with enhanced functionalities. In epitaxial graphene on silicon carbide (SiC), intercalation provides an effective means to tune the electronic, optical, and transport properties of graphene while preserving its honeycomb lattice. Moreover, intercalation enables the synthesis of otherwise unstable 2D layers. In particular, the intercalation of heavy elements such as Pb [1] and Bi [2] is especially promising, as these can introduce strong spin-orbit coupling (SOC) effects [3] (e.g. Rashba effect, gap opening) in graphene. In this work, we use first-principles calculations to investigate the electronic properties of heterostructures formed by Pb and Bi intercalation.
[1] Schölzel, Franziska, et al. ,Small Structures (2024), 2400338
[2] Tilgner, N., et al. Nat Commun 16, (2025), 6171.
[3] Unigarro A., et al. J. Phys. Chem. C (2025), 129, 11, 5617-5624

O 62.6 Wed 16:15 HSZ/0204

Domain-resolved electronic structure of AgTe-intercalated graphene on SiC(0001): From semiconducting Te-rich interlayer bands to metallic AgTe alloy states — •Vibha Reddy[1], Sawani Datta[1], Bharti Matta[1], Philipp Rosenzweig[2], Ulrich Starke[1], and Kathrin Küster[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, — [2]Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Intercalation at the graphene/SiC(0001) interface provides a powerful route towards engineering the electronic properties of both the graphene and the intercalant. Here, we present the first realization of a transition-metal chalcogen alloy intercalated into the graphene/SiC(0001) interface via AgTe intercalation. The nominally AgTe-intercalated system segregates into multiple microscale intercalation phases, namely, Te-rich, Ag-rich and AgTe alloyed domains. Spatially-resolved and angle-resolved photemission spectroscopy (ARPES) reveals that each domain exhibits distinct graphene doping levels and interlayer band dispersions, highlighting the strong interplay between local intercalation chemistry investigated by X-ray photoelectron spectroscopy (XPS) and electronic band structure. Given the intrinsic spin-orbit coupling and topologically non-trivial states associated with Te- and Ag-based 2D materials, the AgTe alloy-intercalated graphene represents a promising platform for realizing domain-specific emergent quantum phenomena, underscoring the chemical versatility and tunability of alloy-based heterostructures in interface engineering.

O 62.7 Wed 16:30 HSZ/0204

Proximity-induced electronic states in epitaxial graphene/SiC (0001) via Sn intercalation — •Huu Thoai Ngo[1], Zamin Mamiyev[1], Niklas Witt[2,3], Tim Wehling[2], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of Theoretical Physics & Centre for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Intercalation of heavy elements at the buffer layer/SiC interface is an effective route to decouple it from the substrate while tailoring its electronic properties, for example, energy gap opening [1] and Mott insulating states [2]. In this work, we investigate the Sn-intercalated buffer layer using low-temperature STM/STS, supplemented by SPA-LEED, and DFT calculations. By precisely controlling the intercalation process, we obtain two distinct Sn phases beneath graphene: Sn(1x1) that induces Kekulé-O distortion, and honeycomb-Sn structure that gives rise to Moiré patterns. Remarkably, our STS results reveal a gap opening in Kekulé-O graphene due to Sn-induced sublattice symmetry breaking. In contrast, the honeycomb-Sn phase exhibits Mott insulating states. These findings demonstrate how Sn intercalants modify the structural and electronic properties of graphene at both nano- and microscale. [1] Ghosal, Tegenkamp, C. et al. Phys. Rev. Lett. 129, 116802 (2022). [2] Ghosal, Tegenkamp, C. et al. Phys. Rev. B 111, 235426 (2025).

O 62.8 Wed 16:45 HSZ/0204

Doping monolayer graphene to the Van Hove singularity — •Guangyao Miao[1], Daniel Jansen[1], Bilal Hawashin[2], Julian Kleeschulte[2], Katharina Offermann[1], Christian Krämer[1], Affan Safeer[1], Abdallah Karaka[1], Jeison Fischer[1], Thomas Michely[1], Michael M. Scherer[2], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Tuning correlated states in graphene is an intriguing topic, particularly since the experimental realization of superconductivity, correlated insulator states, and magnetic states in twisted-angle bilayer graphene near the magic angle, along with Van Hove singularities (VHSs) tuned to the Fermi level. Such correlated phenomena have also been predicted in monolayer graphene doped to its van Hove singularity. Motivated by this, we study the effect of Cs doping on a graphene monolayer on Ir(111) using MBE. A $\sqrt{3}\times\sqrt{3}$ superstructure is observed due to the Cs intercalations between graphene and Ir(111). Further deposition of Cs on top of graphene leads to the formation of several surface structures with varying Cs concentrations, including adatoms, stripes, and compact islands. Their morphology and electronic structures are revealed by scanning tunneling microscopy and spectroscopy at low temperature. By optimizing the dosage, we successfully tune the VHS to the vicinity of the Fermi level and observe a $2\sqrt{3}\times2\sqrt{3}$ superstructure with respect to the graphene lattice. Possible origins of the superstructure related to many-body interactions will be discussed.

O 62.9 Wed 17:00 HSZ/0204

Optimizing quantum transport in multi-barrier graphene systems using differential evolution — •Leon Browne and Stephen R. Power — School of Physical Sciences, Dublin City University, Ireland

Potential and mass barriers in graphene introduce electron scattering, modulating transmission probabilities. Complex multi-barrier setups allow electron transmission to be controlled with high precision, but have a huge design space of possible barrier geometries. This work presents a framework to optimize electronic transport in such systems using differential evolution algorithms. First, transfer matrix methods are employed to efficiently compute quantum transport through multi-barrier structures, before optimization is applied to find barrier configurations whose transmission profiles closely match a predefined target profile. To address the trade-off between the accuracy and complexity of resulting barrier configurations, regularization techniques are incorporated into the optimization process. Our approach demonstrates the potential for highly tunable electronic transport in graphene-based systems by exploiting evolution-inspired optimization techniques.

O 62.10 Wed 17:15 HSZ/0204

Comparative study of plasmons in half-filled graphene via Quantum Monte Carlo and kinetic theory — Maksim Ulybyshev[1], •Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok

A quantitative description of hydrodynamic electronic transport in strongly correlated materials requires accurate knowledge of collective excitations such as plasmons, which can notably influence viscosity. In free-standing graphene, where long-range interactions are important, standard Dirac-cone perturbation theory misses important finite Brillouin-zone and strong-coupling effects. We investigate plasmons in half-filled free-standing graphene using unbiased Quantum Monte Carlo simulations. Our results reveal well-defined plasmon peaks near the Gamma-point, map their dispersion, and extract the momentum dependence of their quasiparticle residue. Comparing to perturbative predictions, we find substantial deviations arising from the interaction and lattice effects captured only beyond the Dirac approximation. These results underscore the need to incorporate such corrections in analytical theories of electronic transport in graphene.

O 62.11 Wed 17:30 HSZ/0204

NanoARPES Facility in Shanghai Synchrotron Radiation Facility and Investigation of the Moiré bands in Graphene Devices — •Zhongkai Liu — Shanghaitech University

Spatially resolved angle-resolved photoemission spectroscopy (NanoARPES) is an indispensable tool for probing the electronic structure of exfoliated sample flakes, fabricated devices, and more. In this presentation, we describe the construction, specifications, capabilities, and operation of BL07U-the NanoARPES endstation at the Shanghai Synchrotron Radiation Facility (SSRF) [1]. We will showcase our research on the electronic structure of emerging graphene devices, with a focus on moiré and flat bands. For example, our ARPES studies on magic-angle twisted trilayer graphene clearly reveal the coexistence of moiré flat bands and Dirac bands [2]. In aligned bilayer graphene/hBN heterostructures, we demonstrate that in-situ back gating enables precise tuning of the moiré electronic structure [3]. We directly observe the characteristic topological electronic structures of rhombohedral multilayer graphene, from a 3D generalization of the 1D Su-Schrieffer-Heeger (SSH) chain in thin layers to a topological Dirac nodal spiral semimetal in bulk rhombohedral graphite [4]. Finally, we present our work on the moiré band in bulk alternating twist graphene, which becomes flat at "magic momenta".

Reference: [1] H. Gao et al., Synchrotron Radiation News 37, 12-17 (2024) [2] Y. W. Li et al., Advanced Materials 202205996 (2022) [3] H. B. Xiao et al., Advanced Science 202412609 (2025) [4] H. B. Xiao et al., Science Bulletin 70, 1030-1033 (2025)

O 63: Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0401

O 63.1 Wed 15:00 HSZ/0401

Majorana or Not? An Insight from Atomic-Scale Shot-Noise — •Abhishek Maiti[1], Genda Gu[2], and Freek Massee[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France — [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA

The search for non-abelian states of matter has become a central theme of modern quantum material research. Notably, Majorana zero modes are of special interest, as they can serve as the foundation for topological qubits. A robust zero-bias conductance peak, observed in scanning tunneling spectra, is often regarded as the primary signature of a Majorana zero mode. Yet similar features can also arise from trivial bound states, raising a long-standing challenge of how to distinguish a genuine Majorana from imposters. In my talk, I will address this problem with a new approach, atomic-scale shot-noise spectroscopy, that goes beyond conductance measurements. Through a detailed investigation on multiple defect- and vortex-bound zero-bias states in the widely studied (putative) topological superconductor Fe(Se,Te), I will show that while differential conductance measurements might sometimes fail to detect an imposter Majorana state locally, noise measurements consistently provide a conclusive diagnostic, offering a powerful complementary probe. Looking ahead, this technique can be applied to other reported platforms to verify whether their Majorana-like signature in tunneling conductance can pass the shot-noise test.

O 63.2 Wed 15:15 HSZ/0401

Intrinsic topological superconductivity revealed by surface-extended Andreev bound states in $PtBi_2$ — •Xiaochun Huang[1], Lingxiao Zhao[2], Sebastian Schimmel[3,4], Julia Besproswanny[3,4], Patrick Härtl[1], Christian Hess[3,4], Bernd Büchner[4,5], and Matthias Bode[1] — [1]Experimentelle Physik 2, Physikalisches Institut, Universität Würzburg, Germany — [2]Quantum Science Center of Guangdong, Shenzhen, China — [3]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Germany — [4]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [5]Technische Universität Dresden, Germany

Intrinsic topological superconductivity remains a central question in condensed-matter physics. The three-dimensional Weyl semimetal $PtBi_2$ was recently shown by angle-resolved photoemission spectroscopy to host a superconducting gap that opens exclusively on its Fermi-arc surface states with a nodal structure, establishing it as a prime candidate for intrinsic topological superconductivity [1]. Using scanning tunneling microscopy and spectroscopy, we directly visualize surface-extended Andreev bound states (ABSs) across atomically pristine terraces within a sizable superconducting gap ($\Delta > 10\,\mathrm{meV}$) in $PtBi_2$. Quantitative analysis of the tunneling spectra within an anisotropic chiral pairing framework identifies these ABSs as signatures of an emergent Majorana-cone dispersion. Our findings provide a definitive real-space spectroscopic fingerprint of intrinsic topological superconductivity in $PtBi_2$.

[1] A. Kuibarov *et al.*, Nature **626**, 294 (2024)

O 63.3 Wed 15:30 HSZ/0401

Probing chiral symmetry with a topological domain wall sensor — •Artem Odobesko[1], Glenn Wagner[2], Titus Neupert[2], Ronny Thomale[1], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, University of Zurich, Zürich, Switzerland

Chiral symmetry is a fundamental property with profound implications

for the properties of elementary particles, that implies a spectral symmetry (i.e. E -> -E) in their dispersion relation. In condensed matter physics, chiral symmetry is frequently associated with superconductors or materials hosting Dirac fermions such as graphene or topological insulators. There, chiral symmetry is an emergent low-energy property, accompanied by an emergent spectral symmetry. While the chiral symmetry can be broken by crystal distortion or external perturbations, the spectral symmetry frequently survives. As the presence of spectral symmetry does not necessarily imply chiral symmetry, the question arises how these two properties can be experimentally differentiated. Here, we demonstrate how a system with preserved spectral symmetry can reveal underlying broken chiral symmetry using topological defects. Our study shows that these defects induce a spectral imbalance in the Landau level spectrum, providing direct evidence of symmetry alteration at topological domain walls. Using high-resolution STM/STS we demonstrate the intricate interplay between chiral and translational symmetry which is broken at step edges in topological crystalline insulator Pb$_{1-x}$Sn$_x$Se.
[1] G. Wagner et al., Newton **1**, 100009 (2025)

O 63.4 Wed 15:45 HSZ/0401

Quantifying quasiparticle chirality in a chiral topological semimetal — •Jiaju Wang[1], Amit Kumar[1], Markel Pardo-Almanza[1], Jaime Sanchez-Barriga[2], Jorge Cardenas-Gamboa[3], Maia Vergniory[3], Vladimir Strokov[4], Moritz Hoesch[5], Chandra Shekhar[6], Claudia Felser[6], Stuart Parkin[1], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, electron chirality has been proposed as an order parameter to quantify chirality. In chiral topological semimetals with the B20 structure, electron chirality is linked to parallel spin-momentum locking (SML) and spin deviations from SML, which affects numerous physical properties. However, experimental quantification of spin deviation still remains a big challenge. To achieve this, we have used spin and angle-resolved photoemission spectroscopy to directly probe the spin texture of Weyl cones in RhSi, a chiral topological semimetal with strong spin-orbit coupling (SOC). The spin-resolved spectra at different azimuthal angles are intricately fitted to extract numerical values of spin deviation for Weyl cones, allowing us to calculate the normalized electron chirality density (NECD). It was found that deviations can decrease the NECD from 1 down to 0.8. This observation may help interpret physical phenomena in chiral topological semimetals.

O 63.5 Wed 16:00 HSZ/0401

Topology and Real-Space Obstruction: The Phase Diagram of the Triangular p-Orbital Lattice — •Jonas Erhardt[1,2], Sven Schemmelmann[3], Fabian Schöttke[3], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,4], Markus Donath[3], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ctd.qmat — [3]Physikalisches Institut, Universität Münster — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Triangular p-orbital monolayers (MLs) host a rich topological phase diagram governed by the competition between spin-orbit coupling (SOC) and substrate-induced inversion-symmetry breaking (ISB). The SOC-dominated quantum spin Hall insulator (QSHI) phase arises from a band inversion in the $p_{\pm}$ manifold and was first realized in indenene, a triangular ML of In atoms on SiC [1]. Real-space interference shifts the associated Wannier centers away from the atoms to interstitial sites A/B, which for the QSHI phase produces an alternating ABAB energy sequence in the charge localization, as demonstrated by scanning tunneling microscopy (STM) [1]. Using the same STM approach, we identify the complementary ISB-dominated regime in a Tl ML on Si(111), where strong adsorption-induced ISB exceeds Tl's SOC. The charge likewise shifts off the atoms but evidences a non-alternating AABB sequence, characterizing Tl/Si(111) as a trivial obstructed atomic insulator. These results complete the experimental validation of the topological phase diagram for triangular p-orbital MLs.
[1] Nat. Commun. **12**, 5396 (2021).

O 63.6 Wed 16:15 HSZ/0401

Majorana-metal transition in a disordered superconductor: percolation in a landscape of topological domain walls — Vladimir A Zakharov[1], Ion Cosma Fulga[2,3], •Gal Lemut[4], Jakub Tworzydło[5], and Carlo W. J. Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, PO Box 9506, 2300 RA Leiden, The Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany — [4]Dahlem Center for Complex Quantum Systems and Physics Department, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [5]Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warszawa, Poland

Most superconductors are thermal insulators. A disordered chiral p-wave superconductor, however, can make a transition to a thermal metal phase. Because heat is then transported by Majorana fermions, this phase is referred to as a Majorana metal. Here we present numerical evidence that the mechanism for the phase transition with increasing electrostatic disorder is the percolation of boundaries separating domains of different Chern number. We construct the network of domain walls using the spectral localizer as a "topological landscape function", and obtain the thermal metal-insulator phase diagram from the percolation transition.

O 63.7 Wed 16:30 HSZ/0401

fabrication and characterization of the Moiré surface state on a topological insulator — •yi zhang — Shanghai Jiao Tong University, Shanghai, China

A Moire* superlattice on the topological insulator surface is predicted to exhibit many novel properties but has not been experimentally realized. Here, we developed a two-step growth method to successfully fabricate a topological insulator Sb2Te3 thin film with a Moire* superlattice, which is generated by a twist of the topmost layer via molecular beam epitaxy. The established Moire* topological surface state is characterized by scanning tunneling microscopy and spectroscopy. By application of a magnetic field, new features in Landau levels arise on the Moire* region compared to the pristine surface of Sb2Te3, which makes the system a promising platform for pursuing next-generation electronics. Notably, the growth method, which circumvents contamination and the induced interface defects in the manual fabrication method, can be widely applied to other van der Waals materials for fabricating Moire* superlattices.

O 63.8 Wed 16:45 HSZ/0401

Backscattering in topological edge states despite time-reversal symmetry — Jonas Erhardt[1,2], •Mattia Iannetti[3,4], Fernando Dominguez[2,5], Ewelina M. Hankiewicz[2,5], Björn Trauzettel[2,5], Gianni Profeta[3,4], Domenico Di Sante[6], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [4]CNR-SPIN C/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [6]Department of Physics and Astronomy, University of Bologna

Quantum Spin Hall Insulators (QSHI) are promising materials for many applications based on Dirac fermions and topologically-protected edge states. Indium adatoms on a silicon carbide surface, the so-called Indenene, was the first material in which a topological classification solely based on an inspection of the bulk wave functions has been demonstrated. In this work, we present a combined experimental and theoretical study of finite-sized Indenene systems, using STM/STS measurements and a quantitative tight-binding model revealing the rich physics of edge states. We find that a strongly non-linear edge dispersion leads to inter-Kramers pair backscattering, thereby extending the conventional understanding of backscattering protection in topological edge states.

O 63.9 Wed 17:00 HSZ/0401

Quantized Subband Tunneling from Topological Insulator Nanowire Scanning Probe Tips — •Abhisek Kole[1,2], Felix Münning[3,4], Xiaosheng Yang[1,5], Jia G. Lu[6], Oliver Breunig[4], F. Stefan Tautz[1,2], Yoichi Ando[4], and Felix Lüpke[1,4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Experimental Physics IV A, RWTH Aachen University, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Institute of Physics I, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [4]Institute of Physics II, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [5]School of Optical and Electronic Information, Huazhong University of Science and Technol-

ogy, Wuhan 430074, China — [6]Department of Physics/Electrophysics, University of Southern California, Los Angeles, CA 90089, USA

In topological insulator nanowires, the interplay between size quantization and the surface states wrapping the nanowire circumference gives rise to a magnetic-flux-tunable band structure. We demonstrate the controlled fabrication of (Bi_(1-x) Sb_x)_2 Te_3 (BST) topological insulator nanowires into scanning tunneling microscopy tips. Tunneling spectroscopy reveals a series of distinct peak-like features that exhibit a characteristic 1D DOS, indicating tunneling into the quantized 1D subbands of the BST nanowire tips. Furthermore, a magnetic-field-induced gap-closing and reopening transition is observed, consistent with the Dirac-like gap-closing transition expected for such wires. Moreover, we find indications of spin-selective helical tunneling between the nanowire tip and the Rashba surface states of Au(111).

O 63.10 Wed 17:15 HSZ/0401

Simultaneous Characterization of Dispersion and Orbital Character of the Topological Surface State on the Topological Insulator Bi$_2$Te$_3$ — •Christoph Stephen Setescak, Adrian Weindl, and Franz Josef Giessibl — Universität Regensburg, D-93053 Regensburg

Scanning probe microscopy (STM and AFM) allows one to locally probe properties of topological insulators (TIs). On the compound Bi$_2$Te$_3$, atomic-scale electronic standing waves can be observed at crystalline step edges, which are associated with the hexagonal warping of the Dirac cone. These real-space oscillations provide a direct means to study the dispersion relation of the topological boundary mode. The interpretation relies on comparing the experimental data to calculations including not only the properties of the TI but also of the tip. In this framework, the tunneling current and differential conductance is modelled using Chen's derivative rule. Bending of the CO molecule at the tip apex due to lateral tip-sample forces is also included in the model. The relevant Bloch functions of the sample are obtained from Wannier-interpolated tight-binding Hamiltonians using maximally localized Wannier functions derived from first-principles DFT + *GW* computations. In combination with the high spatial resolution obtained with CO-terminated tips, not only the dispersion, but also the orbital character of the band structure can be probed.

O 63.11 Wed 17:30 HSZ/0401

Defect-induced displacement of topological surface state in magnetic topological insulator MnBi$_2$Te$_4$ — •Felix Lüpke[1,2], Marek Kolmer[3,4], Hengxin Tan[5], Adam Kaminski[3,4], and Binghai Yan[5,6] — [1]Peter Grünberg Institute (PGI-3) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Ames National Laboratory, Ames, Iowa 50011, USA — [4]Iowa State University, Ames, Iowa 50011, USA — [5]Weizmann Institute of Science, Rehovot 7610001, Israel — [6]The Pennsylvania State University, University Park, Pennsylvania 16802, USA

The gapped topological surface states of MnBi$_2$Te$_4$ (MBT) are an attractive platform for the realization of quantum anomalous Hall and Axion insulator states. However, experimentally observed surface state gaps fail to meet theoretical predictions, with the exact mechanism behind the gap suppression still being debated. We report on the effect of intrinsic anti-site defects on the MBT surface states, which we study using scanning tunneling microscopy (STM), angle-resolved photoemission (ARPES), and density functional theory (DFT). Our results show that high defect concentrations lead to a displacement of the surface states into the interior of the MBT crystal, consistent with theoretical predicitons [PRL 130, 126702 (2023)].

O 64: Surface Magnetism

Time: Wednesday 15:00–17:45 Location: HSZ/0403

Invited Talk O 64.1 Wed 15:00 HSZ/0403

Cantilever based Scanning Force Microscopy: Ultimate Sensitivity and Quantitative Imaging of Nanoscale Spin Textures — •Hans J. Hug — Empa, Ueberlandstrasse 129, 8600 Dübendorf, Switzerland — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel

Cantilever-based scanning force microscopy operated under vacuum or ultra-high-vacuum (UHV) conditions is a powerful and versatile technique for surface characterization with atomic resolution. Beyond topographic imaging, multimodal and multifrequency approaches enable the simultaneous mapping of Kelvin potential differences and magnetic stray fields with exceptional sensitivity. These advanced methodologies have been applied to quantitatively determine skyrmion diameters in both ferromagnetic and synthetic antiferromagnetic multilayers, revealing skyrmions with diameters down to 25 nm. Furthermore, local tip sample distance control allows MFM imaging on curved substrates, uncovering curvature-induced modifications of the Dzyaloshinskii*Moriya interaction. Finally, we demonstrate the capabilities of UHV multimodal scanning force microscopy by resolving the atomic-scale structure, local Kelvin potential, and magnetic stray fields of NiBr* monolayers grown on Au substrates, highlighting the potential of these techniques for exploring emergent magnetic phenomena in low-dimensional materials.

O 64.2 Wed 15:30 HSZ/0403

Intra-atomic s-f correlation in a single Sm atom probed by ESR-STM — Masahiro Haze[1], Saba Taherpour[2,3], Christoph Wolf[2,3], Jaehyun Lee[2,3], Yaowu Liu[2,3], Andreas Heinrich[2,3], Fabio Donati[2,3], •Yasuo Yoshida[4], and Soo-hyon Phark[2,3] — [1]ISSP Univ. Tokyo, Kashiwa, Japan — [2]Center for Quantum Nanoscience, Seoul, Korea — [3]Ewha Womans University, Seoul, Korea — [4]Kanazawa Univ, Kanazawa, Japan

Correlations between s- and f-electrons are a fundamental topic in condensed matter physics, as they can give rise to exotic phases such as heavy-fermion or non-Fermi-liquid states. Recent work has shown that isolated Sm atoms adsorbed on MgO adopt a monovalent configuration with an S=1/2 spin originating from the 6s orbital, making a single Sm atom an ideal platform for studying s-f correlations at the atomic level. Here, we performed ESR-STM measurements on individual Sm atoms adsorbed on MgO films grown on an Ag(100) substrate. We find that the excitation energy varies strongly with the orientation of the external magnetic field, even though STM probes an S=1/2 spin, which is in principle free from single-ion magnetic anisotropy. The extracted g-values from the ESR measurements range from 1.3 to 6.4. This pronounced anisotropy indicates strong coupling between the s- and f-electrons within a single Sm atom, suggesting that surface-adsorbed Sm atoms may serve as promising building blocks for artificial Kondo lattices.

O 64.3 Wed 15:45 HSZ/0403

Elliptical skyrmions in a hydrogenated Fe double-layer on Ir(110) — Timo Knispel[1], Vasily Tseplyaev[2,3], •Gustav Bihlmayer[2], Stefan Blügel[2,3], Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — [2]Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich — [3]Institut für Theoretische Physik, RWTH Aachen University, D-52074 Aachen

Spin-polarized scanning tunneling microscopy (SP-STM) experiments demonstrate that the magnetic ground state of two pseudomorphic Fe layers on Ir(110) is a Néel-type spin spiral with a unique sense of rotation. Employing density functional theory (DFT) calculations, we show that this spin-spiral is stabilized by frustrated exchange interactions, but the rotation direction is fixed by the Dzyaloshinskii-Moriya interaction [1]. Hydrogen adsorption on the 2Fe/Ir(110) surface significantly modifies the spin-spiral minimum, shifting it to a longer wavelength and causing it to flatten energetically out with increasing H coverage. Using DFT calculations, we can trace back this behavior to electron doping of the surface and atomistic spin-dynamics simulations show that it is possible to induce elliptic skyrmions with an external magnetic field. These spin-textures can also be observed using SP-STM with a perpendicular B-field [2].

We acknowledge funding from the CRC 1238 of the Deutsche Forschungsgemeinschaft.

[1] T. Knispel et al., Phys. Rev. B **111**, L020405 (2025)
[2] T. Knispel et al., Nano Lett. **25**, 14565 (2025)

O 64.4 Wed 16:00 HSZ/0403

Light-driven modulation of proximity-enhanced functionalities in hybrid nano-scale systems — •Mattia Benini[1,2], Umut Parlak[3], Jaka Strohsack[4], Andrea Droghetti[5], Tomaz Mertelj[4], Valentin Alek Dediu[2], and Mirko Cinchetti[1] — [1]Department of Physics, TU-Dortmund, Dortmund, Germany — [2]ISMN-CNR, Bologna, Italy — [3]Department of Physics, Univesity of Konstanz, Konstanz, Germany — [4]Jozef Stefan Institute, Ljubljana, Slovenia — [5]Universitá Ca' Foscari, Venezia, Italy

Recent research on Co thin films surface-hybridized with π-conjugated organic molecules demonstrated that interfacial p-d hybridization[1] leads to the establishment of an exotic magnetic configuration, called *Correlated Ferromagnetic Glass* (CFG). It features a glassy-like arrangement of the magnetization and vortex topological defects[2], a strongly enhanced coercivity, and an unexpected complex magnetization dynamics[3]. In this work, we demonstrate that the interface-driven magnetic properties can be actively controlled by optical means, using Co/C$_{60}$ heterostructures as a prototypical system. By generating excitons in the molecular layer with resonant ultrashort light pulses, we achieve up to a 60% reduction of the magnetization precession frequency, ultimately due to a quenching of the interface-induced magnetic anisotropy[4]. References [1] Cinchetti, M. et al., Nat. Mater. 2017, 16 (5), 507*515. [2] Benini, M. et al., Nat Commun 2025, 16 (1), 5807. [3] Strohsack, J. et al., Science Advances 2025, 11 (31), eadw2243. [4] Benini, M. et al., Nat Commun 2025, 16 (1), 7297.

O 64.5 Wed 16:15 HSZ/0403

Layer-dependent magnetic and electronic properties of 2D vdW magnet FeCl$_2$ on Bi(111) — •Shigemi Terakawa[1], Jianqiang Liu[1], Hikaru Ishikawa[1], Ryota Inoue[1], Isamu Yamamoto[2], Amilcar Bedoya-Pinto[3], Niels B. M. Schröter[4], and Kazuyuki Sakamoto[1] — [1]Department of Applied Physics, The University of Osaka, Osaka, Japan — [2]Synchrotron Light Application Center, Saga University, Saga, Japan — [3]Institute of Molecular Science, University of Valencia, Paterna, Spain — [4]Max Planck Institute of Microstructure Physics, Halle, Germany

Two-dimensional (2D) van der Waals (vdW) magnets are promising for future spintronic applications. Recently, transition metal dihalides (TMDHs) have received increasing attention as a new class of 2D vdW magnets. In this study, we report the layer dependence of the magnetic and electronic properties of ultrathin FeCl$_2$, a layered antiferromagnetic insulator, films on Bi(111) from monolayer to four layers. X-ray magnetic circular dichroism (XMCD) measurements revealed that the monolayer film exhibits an in-plane easy axis, while the thicker films have an out-of-plane easy axis with a spin-flip transition, which is consistent with the antiferromagnetic order of bulk FeCl$_2$. The transition field increases with increasing thickness. Angle-resolved photoelectron spectroscopy (ARPES) revealed insulating electronic structure irrespective of the thickness. Layer-dependent change is found as the increase in the width of the bands with large Cl 3p contributions. These results show that both the magnetic and electronic coupling through the vdW interfaces become stronger as the thickness increases.

Invited Talk O 64.6 Wed 16:30 HSZ/0403

Single-spin sensing: A molecule-on-tip approach — •Laurent Limot — Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Magnetometry plays a pivotal role in advancing ultra-dense data-storage technologies and addressing the challenges that arise as spin qubits are downscaled. A promising route toward atomic-scale single-spin sensing is the use of a magnetic molecule as a spin sensor, although practical implementations of this concept remain at an early stage. To demonstrate its feasibility and potential, we combine a nickelocene molecule with scanning tunneling microscopy to achieve versatile, spin-sensitive imaging of magnetic surfaces.

We investigate model Co islands of varying thickness on Cu(111), which exhibit distinct magnetic properties. Our approach proves robust and reproducible, offering atomic-scale sensitivity to both spin polarization and magnetization orientation through the direct exchange coupling between the nickelocene-terminated tip and the Co surface. This capability enables the acquisition of magnetic exchange maps, whose characteristic magnetic corrugation patterns show excellent agreement with computed spin-density distributions. Building on this foundation, we will apply the method to probe the influence of hydrogen on magnetization, a topic of significant relevance in spintronics. Collectively, these advances substantially enhance our ability to probe and visualize magnetism at the atomic scale.

O 64.7 Wed 17:00 HSZ/0403

Tailoring Robust 1D Atomic and Electronic Textures in Mn Ultrathin Films on Fe(110) via Antiferromagnet-Ferromagnet Interfaces — •Toyo Kazu Yamada[1,2], Eiichi Inami[3], and Peter Krueger[1,2] — [1]Dept. Materials Science, Chiba Univ., Chiba, Japan — [2]Molecular Chirality Res. Centre, Chiba Univ., Chiba, Japan — [3]School of Systems Engineering, Kochi Univ. Tech., Kochi, Japan

Controlling the dimensionality of electronic states on two-dimensional (2D) surfaces has remained a significant challenge over decades. In particular, achieving one-dimensional (1D) electronic ordering on 2D surface could enable anisotropic quantum transport and support quantum-confined functional units for nanoscale device integration. In this study, we demonstrate that even conventional 3d transition metals, ferromagnetic (FM) Fe and antiferromagnetic (AFM) Mn, can give rise to 1D atomic stripe patterns in the local density of states (LDOS) on a 2D surface. This study investigates the emergence of one-dimensional (1D) atomic and electronic ordering in ultrathin manganese (Mn) films grown on atomically flat Fe(110) substrates. By combining scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT), we demonstrate that the interplay between antiferromagnetic and ferromagnetic interactions at the interface leads to robust 1D stripe electronic textures that remain stable even at room temperature, persisting in the presence of atomic-scale defects.

O 64.8 Wed 17:15 HSZ/0403

Influence of the light polarization on magnetic dichroism in threshold photoemission — •Frank O. Schumann[1] and Jürgen Henk[2] — [1]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Incoming normal incidence light which is neither purely s- or p-polarized will become in general elliptically polarized inside a metallic surface. We ask how the magnetic dichroism is affected if the incoming light is changed from circularly to linearly polarized, with equally large s- and p-components. This is further compared if the incoming elliptically polarized light is tuned such that it becomes circularly polarized inside the surface. Initial theoretical work on normal emission demonstrated for in-plane magnetized samples a sizeable difference in the dichroism spectra for different light polarizations.[1]

We performed an one-step photoemission calculation for threshold photoemission from a Fe(100) and capture the emission into the full half sphere. The photon energy was 5.2 eV and the angle of incidence was set to 65° as realized in PEEM instruments. We are interested in domain imaging and we determine the relevant asymmetry for magnetic domains.[2] The spectra for a given magnetization direction and polarization state are very different whereas the magnetic dichroism signal displays a weak dependence.

[1] J. Henk and R. Feder, Phys. Rev. B **55**, 11476 (1997) [2] M. Paleschke et al., Phys. Rev. B **112**, 054411 (2025).

O 64.9 Wed 17:30 HSZ/0403

Triple-Q state in magnetic breathing kagome lattice — Hangyu Zhou[1,2], Manuel dos Santos Dias[3], Weisheng Zhao[1], and •Samir Lounis[4,2] — [1]Fert Beijing Institute, Beihang University, Beijing, China — [2]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, Jülich, Germany — [3]Scientific Computing Department, STFC Daresbury Laboratory, Warrington, United Kingdom — [4]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany

Magnetic frustration in two-dimensional triangular spin lattices produces a variety of exotic states, from multi-Q configurations to disordered spin glasses. The antiferromagnetic kagome lattice, built from corner-sharing triangles, is a paradigmatic frustrated system with macroscopic degeneracy. Building on the kagomerization mechanism we recently introduced [1], we examine the magnetic breathing kagome lattice formed by an Mn monolayer on a heavy-metal substrate capped with h-BN [2]. The Mn kagome geometry induces strong frustration, reflected in the nearly flat bands obtained from spin-spiral energy calculations. Including further-neighbor interactions yields a spin-spiral energy minimum along Γ-K and a triple-Q state with nonzero topological charge, potentially causing highly nonlinear Hall responses. The flat-band character can also stabilize more complex spin textures featuring multiple Q-pockets in the spin structure factor. These findings provide a fertile platform for studying multi-Q states and emergent topological phenomena. [1] Zhou et al., Nature Communications 15, 4854 (2025); [2] Zhou et al., npj Spintronics 3, 31 (2025)

O 65: Solid-liquid interfaces: Reactions and electrochemistry II

Time: Wednesday 15:00–18:00 Location: TRE/PHYS

O 65.1 Wed 15:00 TRE/PHYS

Effect of Organic Additives in Aqueous Dye-Sensitized Solar Cells with TEMPO$^{+/0}$ Radicals as Redox Mediator Studied by Perturbation Techniques — •Daniel Holzhacker and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Understanding the complex interactions among the electrolyte, dye, and semiconductor (TiO_2) in dye-sensitized solar cells (DSSCs) is crucial to uncover and optimize the individual roles of each component. Organic electrolyte additives, such as 1-methylbenzimidazole (1MBI), are commonly used to enhance cell performance. In aqueous TEMPO$^+$ solutions, a distinctive color change was observed upon addition of 1MBI. Cyclic voltammetry revealed that the redox potential of the electrolyte shifted systematically to higher potentials with increasing 1MBI concentration. Photoelectrochemical analysis of DSSCs demonstrated a clear effect of 1MBI on the conduction band edge, which shifted in parallel to the redox potential of the electrolyte. It was shown that reduced recombination losses, i.e., a shift of the electron Fermi level in the TiO_2 closer to the conduction band edge, were responsible for an increased open-circuit voltage. Additionally, the shifts of both the conduction band edge and the redox level of the electrolyte may facilitate electron injection from the dye into TiO_2 and/or the regeneration of the oxidized dye by the redox mediator, thereby explaining the higher photocurrents, also observed at increased 1MBI concentrations.

O 65.2 Wed 15:15 TRE/PHYS

Laser-treated activated carbon derived from date stone for energy storage and environmental remediation applications — •Ahmad Jabr[1], Iyad Sadeddin[1], Amer El Hamouz[1], Hyun Jungb[2], and JeongWon Parkb[2] — [1]An-Najah National university, Nablus, Palestine — [2]Dongguk University, Seoul-Campus, Korea

In this study, Activated Carbon (AC) was synthesized via traditional ZnCl* and KOH routes followed by surface modification process using pulsed Nd:YAG laser (1064 nm) under aqueous conditions to produce laser-modified activated carbon (LAC).

Structural and surface analyses revealed that laser introduced new surface functionalities, increased surface roughness, promoted additional micropores and mesopores formation, resulting in 17% enhancement in SSA. Nitrogen adsorption isotherms indicated higher monolayer adsorption and more developed pore volume distribution in LAC compared with AC. Also, LAC exhibited improved surface chemistry with newly developed OCFGs, attributed to laser bombardment effects.

Electrochemical characterizations showed that AC and LAC exhibit typical EDLC behavior, with LAC achieving 70% higher specific capacitance, enhanced energy and power densities, reduced ESR, and better stability after 10000 cycles compared to AC. Furthermore, adsorption studies showed that LAC overcame AC with 400% enhancement in maximum adsorption capacity and initial rate adsorption, signifying improved surface heterogeneity and multilayer adsorption features.

O 65.3 Wed 15:30 TRE/PHYS

rationalizing capacitance differences across metal/water interfaces within a unified quantum electric double layer model — •Lang Li, Nicolas Hörmann, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Electrochemical routes to hydrogen and synthetic fuels promise sustainable energy storage, yet their advancement is limited by an incomplete microscopic picture of the electric double layer (EDL) that governs electrode behavior. Using extensive density-functional theory-based *ab initio* molecular dynamics simulations, we examine a series of noble-metal surfaces and capture the experimental capacitance trend $Pt(111) > Cu(111) > Ag(111) \approx Au(111)$. Subsequent data analysis rationalizes this trend within a unified EDL picture that rests upon a universal four-state interfacial water structure and material-dependent electron spillover [1]. We probe the generality of this understanding by performing alloy- or strain-mimicking "cross-geometry" simulations at interchanged lattice constants, and obtain capacitance variations in full accordance with the model predictions. This suggests applicability of the model for the rational design of next-generation electrode materials.

[1] L. Li, T. Eggert, K. Reuter, N. Hörmann, *J. Am. Chem. Soc.*, **147**, 22778 (2025).

O 65.4 Wed 15:45 TRE/PHYS

Formic Acid Oxidation on Gold Electrodes — •Johannes M. Hermann[1], Areeg Abdelrahman[1], Heiko Müller[1], Ludwig A. Kibler[1], and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Adsorption processes are an integral part of electrocatalysis. The use of extensively studied and structurally well-defined Au(111) single crystal electrodes allows for a better understanding of such processes. Formally, the formic acid oxidation (FAOR) is a relatively simple reaction as only one proton and two electrons have to be released to obtain CO_2. However, the reaction exhibits a self-inhibition on Au(111) electrodes due to the blocking of active sites by strongly adsorbed formate indicated by a bell-shaped current density-potential curve [1]. Similarly, the addition of specifically adsorbing anions typically lowers the catalytic activity [2]. In contrast, certain adsorbates enhance the reaction by orders of magnitude. An intersting example is irreversibly adsorbed 4-mercaptopyridine forming a self-assembled monolayer (SAM) on Au(111) with the enhancement being related to the highly ordered SAM structure [3]. Several aspects of FAOR on gold single crystals will be discussed.

[1] L.A. Kibler, M. Al-Shakran, J. Phys. Chem. C 120 (2016) 16238*16245. [2] J.M. Hermann, A. Abdelrahman, T. Jacob, L.A. Kibler, Electrochim. Acta 385 (2021) 138279. [3] J.M. Hermann, H. Müller, L. Daccache, C. Adler, S. Keller, M. Metzler, T. Jacob, L.A. Kibler, Electrochim. Acta 388 (2021) 138547.

O 65.5 Wed 16:00 TRE/PHYS

Improving Carbon Dioxide Reduction Reactivity and Stability of Ultra-High Vacuum Prepared Cu(111) Surfaces by Crystalline Ultrathin Oxide Films — •Patrick Giesbrecht[1], Mauricio Prieto[1], Mikhail Belozertsev[1], Sergio Tosoni[2], Markus Heyde[1], Thomas Schmidt[1], Beatriz Roldan Cuenya[1], and Juan Navarro[1] — [1]Department of Interface Science, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, Italy

Electrocatalytic carbon dioxide reduction reactions (CO2RR) to hydrocarbons at copper cathodes is one promising but complex route towards carbon capture and reutilization, where ultra-high vacuum (UHV) prepared single crystal electrodes can provide precise precatalyst structures to inform reactivity trends.[1,2] This work develops ultrathin crystalline Cu oxide phases and silica on Cu(111) electrodes under UHV conditions that activate Cu(111) toward hydrocarbon production and alter corrosion pathways under CO2RR conditions.[3] Ex situ and quasi-in situ UHV surface characterization as well as DFT computational analyses are presented that relate this altered reactivity and surface reconstruction to the pre-catalyst oxide structure, highlighting how atomic scale modifications of the surface can lead to macroscopic changes in electrocatalyst reactivity.

[1] Nguyen, K.C., et al. ACS Energy Lett. 9, 644-652 (2024). [2] Cheng, D., et al. Nat. Commun. 16, 4064 (2025). [3] Navarro, J.J., et al. J. Phys. Chem. C 124, 20942-20949 (2020).

O 65.6 Wed 16:15 TRE/PHYS

Mechanistic insights into liquid phase photocatalysis by studying the photoconversion of tertiary alcohols on titania — •Lucia Mengel, Elena Dietz, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Titania loaded with a metal co-catalyst represents a well-studied model photocatalyst, e.g. for investigating hydrogen evolution. For the reaction of most alcohols, the use of a co-catalyst is vital to enable hydrogen evolution and thus a fully catalytic reaction. Tertiary alcohols, however, can be employed as probe for the intrinsic photoactivity of bare titania, as they are catalytically converted in a surface photoreaction discovered by us on single crystals in UHV. In this work, we focus on the applicability of these findings to a liquid phase environment by performing photoconversion of 2-methyl-2-butanol on titania nanopowder. We investigate the catalytic activity under water- and oxygen-free conditions and discuss the reaction behavior under consideration of the catalyst's properties.

O 65.7 Wed 16:30 TRE/PHYS

Simulation of catalytic and corrosive processes via Thermopotentiostat Molecular Dynamics — •Andreas Kretschmer[1], Samuel H. Mattoso[2], Jing Yang[2], Ahmed Abdelkawy[2], Mira Todorova[2], Jörg Neugebauer[2], and Markus Valtiner[1] — [1]Institute of Applied Physics, TU Wien, 1040 Wien, Austria — [2]Max-Planck-Insitute of Sustainable Materials GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Ab Initio Molecular Dynamics (MD) provides valuable insights in dynamic processes at solid liquid interfaces on the electronic level. However, electrified interfaces have been inaccessible due to the interaction of charged systems with the periodic images. The recently developed thermopotentiostat enables the use of electric fields across a solid/liquid interface by a computational electrode. This electrode consists of a fixed layer of Ne atoms, which confines the water, and provides a compensating charge to keep the cell charge-neutral. The thermopotentiostat updates the charge of the Ne atoms after every MD step to drive the potential difference towards a desired value on average. The electronic minimization then distributes the charge, leading to a corresponding counter charge on the electrode surface, allowing the study of dynamic processes under the influence of electric fields. We apply this method to 2 model systems, one is a single Pt atom supported on two layers of graphene to study catalytic processes with water, the second is a Zn surface to study corrosion processes under H evolution at the interface in anodic and cathodic conditions.

O 65.8 Wed 16:45 TRE/PHYS

First Steps Matter Most: Free Energy Barriers of the Volmer Step in Hydrogen Evolution at Pt(111) — •Barbara Sumić, Karsten Reuter, and Nicolas G. Hörmann — Fritz-Haber-Institut der MPG, Berlin

The Hydrogen Evolution Reaction (HER) plays a central role in hydrogen-based energy conversion. The initial Volmer step, involving proton adsorption at the electrode interface, is key to understanding reaction kinetics and the influence of pH. Conventional approaches to estimating barrier heights based on density-functional theory are limited by the need for reduced system sizes and short simulation times, which restrict statistical sampling and hinder fully converged free-energy calculations, particularly when solvent reorganisation is involved.

Here, we explore machine-learned interatomic potentials (MLIPs) combined with enhanced sampling techniques to gain more comprehensive insight into the reaction mechanism and barrier for the Volmer step at Pt(111) in dynamically described interfacial water. Using data-driven collective variables, we aim to capture dynamic environmental and solvent effects that are difficult to access with standard sampling. We also investigate the applicability of the RAZOR (Response Analysis in z-ORientation) framework [1] for barrier calculations at applied bias to probe potential-dependent behavior.

Together, these approaches provide a pathway toward more consistent and physically grounded modelling of HER across different pH conditions.

[1] N. Bergmann *et al.*, Phys. Rev. Lett. **135, 146201 (2025).**

O 65.9 Wed 17:00 TRE/PHYS

Modeling chemical trends of Hydrogen adsorption and reactivity on Pt (111) surface alloyed with transition metals — •Bingxin Li, Jing Yang, Mira Todorova, and Jörg Neugebauer — MPI for Sustainable Materials, Düsseldorf, Germany

Platinum's near-optimal hydrogen binding energy, as dictated by the Sabatier principle, makes it the benchmark electrocatalyst for the hydrogen evolution reaction (HER). Alloying Pt with transition metals (TMs) is known to enhance catalytic activity, though the underlying mechanisms vary substantially across alloying elements. Here, we employ ab initio molecular dynamics to investigate hydrogen adsorption on Pt (111) surfaces whose top layer is alloyed with different TMs at varying concentrations. By generating lateral free-energy maps of chemisorbed hydrogen and combining them with nudged-elastic-band calculations, we determine the Tafel-step barriers of HER. We find that Tafel-step kinetics improves as on-top-site hydrogen binding is weakened on alloyed Pt surfaces. Electronic-structure analyses, coupled with a machine-learning model, reveal that on-top-site hydrogen binding energy (key HER activity descriptor) can be quantitatively predicted from d-band centre characteristics. These results link compositional tuning of Pt-based alloys to predictable changes in HER-activity, offering a rational design route for next-generation hydrogen evolution catalysts.

O 65.10 Wed 17:15 TRE/PHYS

Atomic-scale insights into enhanced oxygen reduction on Au(100) in alkaline solutions from ab initio molecular dynamics simulations — •Alexander von Rueden[1,2], Mal-Soon Lee[1], Vassiliki-Alexandra Glezakou[3], Roger Rousseau[3], and Manos Mavrikakis[2] — [1]Pacific Northwest National Laboratory, Richland, WA, USA — [2]University of Wisconsin-Madison, Madison, WI, USA — [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA

The unusually high 4e^- oxygen reduction reaction (ORR) activity of the Au(100) surface in alkaline environments has motivated numerous experimental and theoretical studies. Even so, atomic-scale insights into the origin of its high activity remain elusive, with static density functional theory (DFT) calculations under vacuum typically proving insufficient. Here, we instead developed atomistic models of Au(100)-water interfaces featuring fully explicit neutral or alkaline solvent environments. Using these models, we performed DFT-based ab initio molecular dynamics (AIMD) simulations to probe the dynamic atomic structures of ORR intermediates adsorbed on Au(100) in different solvent environments. Additionally combining the Blue moon ensemble enhanced sampling technique with AIMD, we demonstrated a low free energy barrier for O_2 dissociation and hydrogenation by water molecules to yield OH* on Au(100), which is consistent with its high experimental activity. Further, our alkaline simulations revealed these OH* products can form complexes with near-surface Na^+ cations, possibly leading to a more downhill reaction free energy.

O 65.11 Wed 17:30 TRE/PHYS

When Charged Intermediates Escape the Surface: Mass Transport Effects on the Electrocatalytic Selectivity of NO_3 Reduction — •Hemanth S. Pillai, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Electrocatalytic selectivity is often discussed at the atomic level on the basis of the active site, while ignoring effects of mesoscopic mass transport. And yet, transport can critically shape selectivity through the exchange of surface-bound intermediates between the electrode and bulk electrolyte. We recently explored this mechanism, originally coined "desorption–re-adsorption–reaction" [1], by developing a simple model that couples the surface reaction kinetics with diffusion [2]. Here, we advance and extend our approach to describe charged intermediates such as nitrite (NO_2^-) during the electrochemical NO_3 reduction reaction. Ion transport augments a mean-field microkinetic model and is treated at varying levels of sophistication to capture different double layer characteristics. Our simulations show that both the applied potential and catalyst morphology uniquely shape NO_2^- selectivity within the desorption–re-adsorption–reaction mechanism. The emerging trends are in qualitative agreement with experiments, while distinctly different from those obtained for analogous charge-neutral intermediates during e.g. CO_2 reduction. This comparison shows how the double layer affects selectivity due to transport and allows to gauge the level of detail that is required in corresponding reaction models.

[1] H. Wang *et al.*, J. Phys. Chem. B **108**, 19413 (2004).

[2] H.H. Heenen *et al.*, Nature Catal. **7**, 847 (2024).

O 65.12 Wed 17:45 TRE/PHYS

Electroreduction of Acetone on PtRu Model Catalysts — •Robert Hübsch[1], Daniel Schauermann[1], Pankaj Kumar Samal[2], Jan Škvára[2], Frederike Jäschke[1], Lesia Piliai[2], Tomáš Skála[2], Nataliya Tsud[2], Josef Mysliveček[2], Olaf Brummel[1], Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Interface Research and Catalysis, ECRC, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, Prague, 18000, Czech Republic

The isopropanol/acetone system functions as an electrochemically active liquid organic hydrogen carrier (EC-LOHC). In this context, direct electrochemical charging is particularly attractive but requires highly active and selective catalysts. In this study, we investigated acetone reduction on well-defined PtRu model surface alloys. Our approach combined cyclic voltammetry (CV), ex-situ emersion synchrotron radiation photoelectron spectroscopy (SRPES), electrochemical infrared reflection absorption spectroscopy (EC-IRRAS), and differential electrochemical mass spectrometry (DEMS). The PtRu/Ru(0001) surface exhibits low intrinsic catalytic activity; but can be activated through a dealloying procedure. This treatment produces small Pt aggregates on a rough Ru support. In contrast, the PtRu/Ru(10 10) surface, characterized by a lower coordination number, does not require dealloying. Unlike Pt(110), which predominantly produces propane, the PtRu model catalysts selectively yield the target product isopropanol.

O 66: Ultrafast electron dynamics at surface and interfaces III

Time: Wednesday 15:00–17:45 Location: TRE/MATH

Invited Talk O 66.1 Wed 15:00 TRE/MATH

Ultrafast exciton dynamics in 2D semiconductors and electric field gated devices — •Jan Philipp Bange — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

Two-dimensional (2D) semiconductors and moiré materials, formed by stacking and twisting atomically thin layers, provide an exciting platform to discover and engineer new quantum states. Precise and reversible control of carrier density and many-body effects is readily achieved through in-situ electric field gating. In combination with angle-resolved photoemission spectroscopy this has been a powerful probe of the static electronic band structure. However, capturing the ultrafast dynamics of excited states in gated 2D materials, including hybrid excitons [1], interlayer excitons [2], and trions [3], remains a fundamental challenge due to the limited real-space resolution of ultrafast time- and momentum-resolved spectroscopy techniques. In this talk, I will present how time-resolved momentum microscopy provides direct access to both the energy landscape and femtosecond dynamics of bright and dark excitons at nanometer length scales. This methodology enables the disentanglement of electron and hole transfer pathways across twisted transition metal dichalcogenide interfaces and reveals the ultrafast formation of quasiparticles as a function of gate voltage.
[1] Bange *et al.*, Science Advances **10**, eadi1323 (2024).
[2] Schmitt *et al.*, Nature Photonics **19**, 187 (2025).
[3] Meneghini *et al.*, arXiv.2511.11448 (2025).

O 66.2 Wed 15:30 TRE/MATH

Ultrafast signatures of Dirac - flat-band hybrid states from time-resolved ARPES — •Maria-Elisabeth Federl[1], Johannes Gradl[1], Franziska Bergmeier[1], Zamin Mamiyev[2], Niclas Tilgner[2], Thomas Seyller[2], Christoph Tegenkamp[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Chemnitz University of Technology

Hybridization of highly itinerant Dirac electrons with localized flat-band states is predicted to yield emergent phenomena such as exotic heavy-fermion behaviour. Epitaxial graphene resting on a flat-band system at the graphene-SiC(0001) interface offers a promising platform, yet direct spectroscopic signatures - such as avoided crossings in equilibrium ARPES - have remained unresolved. We solved this problem using time-resolved ARPES where evidence of hybridization manifested in three key observations: (1) accelerated Dirac-carrier relaxation due to an increased scattering phase space, (2) transient charging of the Dirac cone enabled by direct optical excitation from the flat bands, and (3) ultrafast charge transfer back into the flat bands on timescales set by the interlayer coupling strength. Our results thus provide a clear dynamical fingerprint of hybridization in a system where equilibrium probes have proven inconclusive.

O 66.3 Wed 15:45 TRE/MATH

Probing topological Floquet states in graphene with ultrafast STM — •Nils Jacobsen[1,2], Melanie Müller[3], Michael Schüler[4,5], Martin Wolf[3], and Angel Rubio[2,6] — [1]University of Bremen — [2]MPSD Hamburg — [3]FHI Berlin — [4]PSI Villingen Switzerland — [5]University of Fribourg Switzerland — [6]CCQ The Flatiron Institute New York USA

The light-induced anomalous Hall effect in graphene driven by circularly polarized light is a hallmark example of Floquet band engineering [1]. It has been observed in ultrafast transport experiments [2] and Floquet Bloch bands in graphene have recently been resolved by time- and angle-resolved photoemission spectroscopy [3]. Here, we propose ultrafast scanning tunnelling microscopy (USTM) as a complementary probe of topological Floquet states in graphene [4]. In our simulations, dynamical band gaps and topological edge states are directly reflected in the local density of states and the ultrafast tunnelling currents. The chirality of the edge states is revealed by the suppression of backscattering at impurities, which could be probed by ultrafast STM. These results establish ultrafast STM as a promising tool to access light-induced topological states in quantum materials. [1] Oka PRB 79, 081406(R) (2009) [2] McIver Nat. Phys. 16, 38-41 (2020) [3] Merboldt, Schüler et al. Nat. Phys. 21 1093-1099 (2025), Choi, Mogi et al. Nat. Phys. 21 1100-1105 (2025) [4] Müller Prog. Surf Sci. 99, 100727 (2024)

O 66.4 Wed 16:00 TRE/MATH

Ultrafast Band-Gap Renormalization in Bilayer Graphene — •Eduard Moos[1], ZhiYuan Deng[1], Hauke Beyer[1], Arpit Jain[4], Chengye Dong[4], Joshua A. Robinson[4], Kai Rossnagel[1,2,3], and Michael Bauer[1,2] — [1]Kiel University, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Germany — [3]Electron Synchrotron DESY, Germany — [4]Pennsylvania State University, United States

We demonstrate, by femtosecond time- and angle-resolved photoemission spectroscopy, that photoinduced interlayer charge transfer in a heterostructure consisting of Bernal-stacked bilayer graphen and a single atomic layer of silver on 6H-SiC(0001) transiently modulates the intrinsic potential landscape across the silver-graphene interface. Acting as an ultrafast electronic gate, this drives momentum-dependent band renormalizations, resulting in a transient band-gap opening on femtosecond timescales. Simultaneously, the photogenerated hot-carrier population enhances electronic screening, leading to a subsequent closing of the band-gap beyond the thermal equilibrium value. These findings reveal two different mechanisms for a photoinduced, reversible control of the electronic band structure in bilayer graphen — interlayer charge transfer and hot-carrier enhanced screening — providing a general framework for the ultrafast control of electronic properties in graphene-based heterostructures. They further open novel pathways for the realization of ultrafast optoelectronic devices and the exploration of correlated quantum phases in bilayer graphene under nonequilibrium conditions.

O 66.5 Wed 16:15 TRE/MATH

Attosecond spin-orbit delays in solid-state photoemission — •Andreas Gebauer[1], Walter Enns[1], Sergej Neb[2], Tillmann Schabbehard[1], Luis Maschmann[1], J. Hugo Dil[3], Ulrich Heinzmann[1], Stephan Fritzsche[4,5,6], Nikolay M. Kabachnik[7,8], Eugene E. Krasovskii[8,9,10], and Walter Pfeiffer[1] — [1]Bielefeld University — [2]ETH Zurich — [3]EPFL, Lausanne — [4]Helmholtz Institute Jena — [5]GSI Helmholtzzentrum für Schwerionenforschung GmbH — [6]Friedrich-Schiller-University Jena — [7]European XFEL GmbH, Schenefeld — [8]DIPC, San Sebastián — [9]Universidad del País Vasco, San Sebastián — [10]IKERBASQUE, Bilbao

Attosecond time-resolved photoelectron spectroscopy allows observation of photoemission dynamics in solids on its natural time scale. Photoelectrons typically need tens to hundreds of attoseconds to be released into the vacuum while various competing effects determine the emission dynamics. We report the first observation of unexpectedly large spin-orbit delays, i.e. relative photoemission delays between spin-orbit split core levels in Bi_2Te_3 and Bi_2Se_3. The observed delays can neither be attributed to intra-atomic delays nor to ballistic photoelectron transport. Instead, calculations based on one-step photoemission theory reveal that strong variations of the final state wave function on the energy scale of the spin-orbit splitting are responsible for the experimental observation. These variations reflect the complex interplay of propagating and evanescent waves in the photoelectron emission, exhibiting qualitatively different emission dynamics.

O 66.6 Wed 16:30 TRE/MATH

Electron Correlations in Ultrafast Transmission Electron Microscopy — •Nico Stumpp[1], Andreas Wendeln[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Ultrafast transmission electron microscopy (UTEM) strives to combine an atomic spatial resolution with a femtosecond temporal resolution, yet its performance is inherently limited by Coulomb repulsion within electron pulses. Research in free-electron quantum optics suggests that, rather than avoiding these dynamic interactions, exploiting their induced inter-electron correlations offers a pathway toward quantum-limited imaging performance [1,2].

Utilizing an event-based electron detector with nanosecond temporal resolution, we observe pronounced energy anti-correlations in few-electron states emitted from a high-coherence, laser-driven cold field-emission electron source [3]. Crucially, we demonstrate the ability to actively modify the magnitude and visibility of the induced energy separation depending on angular post-selection. We complement our experimental results with numerical multi-particle simulations of electron pulse dynamics within the electrostatic gun environment, focussing on the interplay between strongly interacting correlated electron pairs and the surrounding electron ensemble of the emitted photoelectron bunch.

[1] R. Haindl et al., Nat. Phys. 19, 1410 (2023).
[2] S. Meier et. al., Nat. Phys. 19, 1402 (2023).
[3] A. Schröder et al., Ultramicroscopy 275, 114158 (2025).

O 66.7 Wed 16:45 TRE/MATH

Ultrafast Investigation of Competing CDW Orders in $LaTe_3$

— •Francesco Sammartino[1], Wibke Bronsch[2], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Università degli Studi di Trieste — [2]Elettra - Sinctrotrone Trieste

The RTe_3 family hosts a rich landscape of charge-density-wave (CDW) phases. All members display a unidirectional CDW aligned along the *c*-axis, while only the heavier rare-earth compounds develop an additional equilibrium CDW along the *a*-axis at lower temperature. Intriguingly, recent ultrafast experiments have shown that $LaTe_3$, whose equilibrium state features only the *c*-axis CDW, can transiently exhibit a rotated CDW component oriented along the *a*-axis.

Building on time-resolved optical studies that first revealed the emergence of this orthogonal order, we investigated $LaTe_3$ through time-resolved ARPES (TR-ARPES) to track, with momentum resolution, the ultrafast evolution of its electronic structure.

We monitored the melting of the equilibrium *c*-axis CDW gap and searched for transient modifications of the electronic dispersions along the *a*-axis that could be linked to the emergence of the rotated order. This study provides direct insight into the nonequilibrium CDW dynamics of $LaTe_3$ and may help clarify the microscopic pathways that enable the formation of the rotated CDW state.

O 66.8 Wed 17:00 TRE/MATH

Electron and exciton dynamics in large-angle twisted bilayer graphene

— •Gianmarco Gatti[1], Anders Mortensen[1], Gesa Siemann[1], Zhihao Jiang[1], Alfred Jones[1], Chakradhar Sahoo[1], Thomas Nielsen[1], Naina Kushwaha[2], Jennifer Ridgen[2], Søren Ulstrup[1], Bruce Weaver[2], Yu Zhang[2], Charlotte Sanders[2], Emma Springate[2], Vibha Reddy[3], Ulrich Starke[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Central Laser Facility, STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, UK — [3]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569, Stuttgart, Germany

Tunable moiré superlattices naturally form in artificially stacked monolayers through control of their rotational misalignment (twist angle). In large-angle twisted bilayer graphene (TBG), orbital hybridization between the monolayer-derived π/π^* bands leads to avoided crossings and the emergence of pairs of occupied and unoccupied van Hove singularities at fixed wave vectors k*. We investigate the out-of-equilibrium electron dynamics near these points in 10°-TBG using IR-pump XUV-probe time-resolved ARPES experiments. Our measurements resolve the hot electron dynamics in TBG and reveal an additional, unexpected spectral weight within the local electronic band gap at k*. This observation is consistent with the signature of a strongly bound exciton in TBG, whose formation has been attributed by recent theoretical models to a unique destructive coherence between two energy-degenerate subband resonant transitions.

O 66.9 Wed 17:15 TRE/MATH

Hybrid Frenkel-Wannier excitons facilitate ultrafast energy transfer at a 2D-organic interface

— •Wiebke Bennecke[1], Ignacio Gonzalez Oliva[2], Jan Philipp Bange[1], Paul Werner[1], David Schmitt[1], Marco Merboldt[1], Anna M. Seiler[1], Daniel Steil[1], R. Thomas Weitz[1], Peter Puschnig[3], Claudia Draxl[2], G. S. Matthijs Jansen[1], Marcel Reutzel[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Institute of Physics, NAWI Graz, University of Graz, 8010 Graz, Austria

The combination of two-dimensional transition metal dichalcogenides (TMDs) and organic semiconductors (OSCs) is a highly promising material platform for the realization of future optoelectronic devices. While the excitonic properties of their individual components have been intensively studied, much less is known about excitons at the hybrid interface. Here, we use ultrafast momentum microscopy and many-body perturbation theory to investigate the exciton landscape at the PTCDA/WSe_2 interface [1]. In particular, we find an exciton state formed via Förster resonant energy transfer, which is of hybrid nature: Concomitant intra- and interlayer electron-hole transitions within the OSC layer and across the TMD/OSC interface, respectively, give rise to an exciton wavefunction with mixed Frenkel-Wannier character.

[1] Bennecke *et al.*, Nat. Phys. (2025)

O 66.10 Wed 17:30 TRE/MATH

Electronic friction simulations of laser-driven hydrogen evolution from copper. Does surface coverage matter?

— •Alexander Spears[1], Wojciech G Stark[2], and Reinhard J. Maurer[1,3] — [1]University of Vienna, AT — [2]Imperial College London, UK — [3]University of Warwick, UK

Plasmonic catalysts such as metal nanoparticles harness the energy transfer between light, electrons and phonons at interfaces to drive chemical reactivity at interfaces. However, even on clean metal surfaces with a regular structure, it is unclear whether these dynamics are the result of mode-selective energy transfer or photothermal heating effects. Molecular dynamics simulations with electronic friction (MDEF) offer a quantum-classical description of electron-phonon coupling and have previously been used to model ultrafast dynamics on metal surfaces. Using machine learning surrogate models to accelerate MDEF simulations, we show that mode-selective energy transfer has a negligible influence on light-driven hydrogen evolution from copper surfaces. By comparing energy partitioning in desorbed molecules, we conclude the choice of electronic friction approximation only determines the rate of energy transfer, while the energy distributions of desorbing molecules are governed by the potential energy surface. This suggests that thermal and laser-driven desorption may yield similar outcomes at low coverage. However, we expect mode-selective energy transfer to play a stronger role at higher coverage, and show preliminary results for surface coverage dependence in laser-driven desorption.

O 67: Focus Session: Unoccupied States by Inverse Photoemission II

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Wednesday 15:00–18:00 Location: WILL/A317

Invited Talk O 67.1 Wed 15:00 WILL/A317

New frontiers of one step model of photoemission for quantum materials — •Jan Minar — New Technologies Research Center, University of West Bohemia in Pilsen, Pilsen, Czechia

Quantum materials feature intertwined electronic correlations, topology, and magnetism, requiring realistic treatments of spin-orbit coupling, interactions, and spin fluctuations. Spin- and time-resolved ARPES (STARPES) is a key probe of their electronic and spin structures, but its quantitative interpretation demands advanced theory. I will present a fully relativistic multiple-scattering Green function (KKR) [1] framework for spin-dependent photoemission that incorporates correlations via DMFT, spin fluctuations via the alloy-analogy model, and light-induced electronic excitations [2,3]. Applications include a one-step photoemission description of altermagnets such as RuO* and MnTe, where spin-ARPES reveals lifted Kramers degeneracy relevant for spintronics, and kagome magnets such as FeSn thin films, where persistent flat-band splitting and selective band renormalization expose strong correlation and topological effects. This framework provides a unified route to unravel spin dynamics in complex quantum materials [4,5,6].

References: [1] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011) [2] J. Minár et al., Phys. Rev. B 102, 035107 (2020). [3] J. Braun et al., Physics Reports 749, 1 (2018). [4] J. Krempaský et al., Nature 626, 517 (2024). [5] A.D. Din et al., arXiv:2511.01690 (2025) [6] Z. Ren et al., Nature Communications 15, 9376 (2024).

O 67.2 Wed 15:30 WILL/A317

Surface-orientation-dependent unoccupied electronic states of Fe_3O_4 — •Jan Bieling and Markus Donath — Universität Münster, Germany

Experimental studies of the occupied electronic states of magnetite (Fe_3O_4) have revealed that the observed properties, such as band dispersions, are strongly surface-orientation-dependent [1,2]. However, comparable systematic studies of the unoccupied electronic states of different Fe_3O_4 surfaces are still lacking.

We report on the unoccupied electronic states of a well-characterized Fe_3O_4(111) surface using angle-resolved inverse photoemission and compare the results with our previous study of Fe_3O_4(100) [3]. This direct comparison allows for (re)interpreting the spectral features observed for both surfaces.

Finally, we discuss our findings in the context of recent theoretical studies [4,5]. We report a very good agreement between our inverse photoemission spectra of Fe_3O_4(100) and the theoretical results obtained from DFT+U+V for this surface.

[1] Y. Dedkov *et al.*, Phys. Rev. B **70**, 073405 (2004)
[2] W. Wang *et al.*, Phys. Rev. B **87**, 085118 (2013)
[3] J. Bieling and M. Donath, Phys. Rev. B **111**, 075117 (2025)
[4] N. Naveas *et al.*, J. Chem. Theory Comput. **19**, 8610-8623 (2023)
[5] N. Naveas *et al.*, Results Phys. **70**, 108158 (2025)

O 67.3 Wed 15:45 WILL/A317

Beyond the surface: Probing electronic structure with IPES in Valparaíso-Chile — Patricia Martínez[1], Rolando. Esparza[1], Jonathan Correa-Puerta[1], Valeria del Campo[1], Ricardo Henríquez[1], •Patricio Häberle[1], Sanber Viscaya[1], Eric Suárez-Morell[1], Patricio Vargas[1], Jean F. Veyan[2], Marcos Flores[3], and Samuel Hevia[4] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA — [3]Physics Department, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile — [4]Instituto de Física and CIEN-UC, Pontificia Universidad Católica de Chile, Av. Vicuña Mackenna 1860, Macul, Chile

Over the past few years, we have employed angle-resolved inverse photoemission spectroscopy (IPES) at the Valparaíso facility, utilizing both the isochromat mode and photon energy-resolving capabilities. This technique has enabled us to investigate systems exhibiting electronic structures modified by various forms of quantum confinement. We have characterized metallic thin films, carbon nanotubes, self-assembled monolayers (SAMs), and two-dimensional semiconductors. Whenever feasible, we have mapped unoccupied energy bands; however, in many instances, we have relied on simulations and inventive averaging to extract meaningful information from these low-symmetry nanoscale systems. A comprehensive overview of our experimental findings and future directions will be presented.

O 67.4 Wed 16:00 WILL/A317

Inverse photoemission studies of unoccupied electronic states of various Si(111)-based surfaces and interfaces — Younal Ksari, Hela Mrezguia, and •Jean-Marc Themlin — CNRS, Aix-Marseille Univ. University of Toulon, Marseille, France

We operate in Marseille an angle-resolved inverse photoemission (ARIPES) setup working in the isochromat mode. To illustrate the potential of this highly surface-sensitive technique, we give a comparative overview of the unoccupied part of the electronic structure of several Si(111)-based interfaces as revealed by ARIPES, from the hydrogenated H:Si(111) to 2D silicene monolayers grown on passivated Si(111) substrates.

The H-saturated (1x1) termination of Si(111) solely reveals bulk conduction band states. Upon segregation (B) or adsorption (H, As, Au) of foreign atoms on Si(111), specific surface states appear, leading to insulating (H, As, B) or metallic (Au) interfaces.

According to LEED, the adsorption of 1 ML of Si on the $\sqrt{3}\times\sqrt{3})R30^\circ$ reconstructed Au- and B- substrates leads to the formation of a non-covalently bound Si bilayer, alias silicene, which adopts the symmetry of the passivated substrates. Specific unoccupied electronic states appear on each substrate, with dispersions profiles which do not exhibit a $\sqrt{3}\times\sqrt{3})R30^\circ$ symmetry, small overall bandwidths and large bandgaps (resp. > 2 eV and > 1 eV), suggesting important correlation effects.

O 67.5 Wed 16:15 WILL/A317

Layer-Dependent Electronic Signatures of Tl on Ag(111) Revealed by Inverse Photoemission — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster — [2]Department of Applied Physics, The University of Osaka

The Tl/Ag(111) system is characterised by pronounced changes in its spatial and electronic structure when transitioning from sub-monolayer coverage to the monolayer [1,2] and further to the bilayer [3], making an accurate determination of the layer thickness essential. While low-energy electron diffraction and Auger electron spectroscopy provide valuable information on domain orientations and Tl coverage trends, neither technique allows an unambiguous identification of the bilayer. In contrast, inverse photoemission (IPE) gives direct access to unoccupied electronic states, which are highly sensitive to the Tl film thickness. We show that Tl/Ag(111) exhibits distinct layer-dependent unoccupied states whose characteristic intensity evolution with increasing Tl coverage enables a clear identification of the bilayer. These results highlight the particular strength of IPE as a layer-specific probe for ultrathin metallic films.

[1] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[2] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)
[3] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)

O 67.6 Wed 16:30 WILL/A317

Modeling a transient Dirac-like surface state in Floquet-driven SnTe — •Aki Pulkkinen[1], Frédéric Chassot[2], Hugo Dil[3], Claude Monney[2], and Ján Minár[1] — [1]New Technologies-Research Centre, University of West Bohemia in Pilsen, Czechia — [2]Department of Physics and Fribourg Center for Nanomaterials, Université de Fribourg, Switzerland — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We present a theoretical analysis of the ultrafast transient cone-like dispersion observed in pump-probe photoemission experiments on SnTe[1]. A semi-infinite (111) surface Hamiltonian is constructed from a Wannier tight-binding model, and the surface Green's function is obtained using the recursive López-Sancho method[2] in extended Hilbert space. The effect of the pump pulse is introduced through a time-periodic Peierls substitution and a Jacobi-Anger expansion of the driven Hamiltonian into Floquet sectors. The Floquet-Green's-function calculations show that photoexcitation induces a transient hybridization between the Floquet replica of the valence band and the conduction band, producing a momentary band inversion at the surface. The inversion generates a short-lived Dirac-cone-like surface state, reproducing the main experimental feature. The results indicate that the transient cone originates from Floquet-induced reconstruction rather than structural or thermal effects, and demonstrate the role of strong periodic driving in reshaping surface electronic structure in SnTe. [1] F Chassot et al. 2025 arXiv:2502.11967 [2] M. P. Lopez Sancho et al. 1985 J. Phys. F: Met. Phys. 15 851

O 67.7 Wed 16:45 WILL/A317

Peak separation analysis for inverse photoelectron spectra: Comparing second derivative, curve fitting, and deconvolution — •ryotaro nakazawa[1,2], haruki sato[2], and hiroyuki yoshida[2] — [1]Institute for Molecular Science, Aichi, Japan — [2]Chiba University, Chiba, Japan

Inverse photoelectron spectroscopy (IPES) is a powerful technique for probing the unoccupied electronic states of materials. Recently developed low-energy inverse photoelectron spectroscopy (LEIPS) can significantly advance the study of unoccupied states, owing to minimal sample damage and suppressed dark counts compared to conventional IPES. However, the instrumental resolution remains at around 0.2 eV, which is one order of magnitude lower than that of photoelectron spectroscopy. Spectral broadening caused by the low instrumental resolution often results in overlapping peaks. Peak separation is therefore crucial in the analysis of LEIPS spectra. In this study, we compared three peak separation methods: second derivative, curve fitting, and deconvolution. These methods were applied to modeled and experimental LEIPS spectra of the lowest unoccupied molecular orbital-derived band of pentacene, which consists of two splitting peaks due to the two inequivalent molecules in the unit cell. We systematically and quantitatively evaluated the performance of each method in terms of analysis parameters and discussed its robustness to noise as well as its peak separation and detection capabilities. This work offers a practical framework for peak separation in LEIPS, with extensions to PES and a wide range of spectroscopies.

O 67.8 Wed 17:00 WILL/A317

The role of light polarization in inverse photoemission — •Marcel Holtmann, Pascal J. Grenz, and Markus Donath — Physikalisches Institut, Münster University, Germany

In inverse photoemission (IPE), electrons are directed onto a surface and the light emitted during radiative transitions into unoccupied states is detected. By detecting the emitted photons as a function of the kinetic energy of the electrons impinging at a defined angle of incidence, the dispersion of conduction-band states can be traced. We focus on the role of light polarization in IPE and how the simultaneous detection of photons with multiple detectors provides additional symmetry information.

In the spirit of "50 years of IPE", this talk aims to give an overview of this aspect of IPE analysis. Building on early work from the 1980s [1,2], we will present measurements of the AgTe/Ag(111) surface alloy. The polarization contrast allows us to identify the orbital character of spin-dependent unoccupied states. We will also discuss the recent improvement of our setup, in which a polarizing mirror was added to the photon detector [3], enabling us to select the detected light polarization.

[1] M. Donath *et al.,* Solid State Commun. **60**, 237 (1986)
[2] T. Fauster *et al.,* Phys. Rev. B **40**, 7981 (1989)
[3] P. J. Grenz *et al.,* Rev. Sci. Instrum. **96**, 033905 (2025)

O 67.9 Wed 17:15 WILL/A317

Sub-100 meV low-energy inverse photoelectron spectroscopy using an electrostatic monochromator — •Tomoko Onishi[1], Taichi Suruga[1], Daichi Honma[1], Masaya Kai[1], Issei Ishimori[1], François C. Bocquet[2], F. Stefan Tautz[2], Harald Ibach[2], and Hiroyuki Yoshida[1] — [1]Chiba University, Chiba, Japan — [2]Forschungszentrum Jülich, Jülich, Germany

Inverse photoelectron spectroscopy (IPES) is the optimal experimental method for probing unoccupied electronic states but its applicability has been limited by modest energy resolution. This resolution is determined by the convolution of the electron energy spread and photon-detector bandwidth. The best reported resolution to date is 165 meV, limited by the photon detector [1]. Low-energy IPES (LEIPS) [2], using an optical bandpass filter, achieves a photon-detection resolution of 38 meV. However, the total resolution remains limited to 250 meV due to electron-beam thermal broadening [3]. In this work, we report a LEIPS system with an electron source consisting of a LaB6 cathode, electrostatic monochromator, and deceleration lens system. This design is based on high resolution electron energy loss spectroscopy (HREELS). We modified it to deliver several hundred nA with a capability of energy scan for LEIPS [4]. An electron energy spread of 90 meV is obtained, resulting in a total LEIPS energy resolution of 98 meV. [1] M. Budke et al., Rev. Sci. Instrum. 78, 083903 (2007). [2] H. Yoshida, Chem. Phys. Lett. 539*540, 180 (2012). [3] H. Yoshida, J. Electron Spectrosc. Relat. Phenom. 204, 116 (2015). [4] H. Ibach et al., Rev. Sci. Instrum. 94, 043908 (2023).

O 67.10 Wed 17:30 WILL/A317

Towards high resolution IPES in the VUV range — Giacomo Merzoni[1], Samuele Comizzoli[1], Giacomo Panzera[1], Lucio Braicovich[1,2], and •Giacomo Ghiringhelli[1,3] — [1]Politecnico di Milano, Italy — [2]ESRF, Grenoble, France — [3]CNR/SPIN, Politecnico di Milano, Italy

Since its concept was introduced and its feasibility was demonstrated, the conceptual interest of angle-resolved inverse photoemission (ARIPES) has not declined. Unfortunately, for decades technical challenges have kept ARIPES in a niche. At the same time direct photoemission, ARPES, has become a popular and unmissable technique for the determination of the electronic structure of solids. ARPES spectra are commonly measured with energy resolution better than 30 meV, a figure still unachieved in ARIPES. Which explains the different popularity of the two complementary techniques.

Is it possible to design today an ARIPES instrument that better exploits the technological progress undergone over the years by detectors and optical elements for VUV radiation, and by monocromatized electron-beam sources?

We present some ideas guiding the realization of an ARIPES apparatus working in the 20-100 eV energy range. Aiming at a combined instrumental bandwidth smaller than 50 meV, it is based on a high-luminosity grating spectrometer and a 2D position sensitive semiconductor detector.

O 67.11 Wed 17:45 WILL/A317

2D IPES intensity maps of MoS_2 — •Patricia Martínez-Rojas, Sanber Vizcaya, Rolando Esparza, and Patricio Häberle — Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

Inverse photoemission spectroscopy (IPES) offers direct access to the unoccupied electronic structure of solids and is particularly well suited for investigating layered transition-metal dichalcogenides such as MoS_2. We present momentum-resolved IPES measurements on a bulk 2H-MoS_2 single crystal, performed with a normal-incidence grating spectrometer operated at a fixed electron kinetic energy of 25.6 eV. The sample was prepared by ex-situ exfoliation and subsequently annealed, in UHV, up to 400°C to remove surface contaminants. By recording the photon intensity as a function of emission energy and incidence angle, we constructed two-dimensional maps of the unoccupied states along the ΓK and ΓM directions of the Brillouin zone. The data reveal several dispersive features whose energy-momentum dependence closely matches density-functional theory (DFT) band-structure calculations. In particular, the conduction-band minimum is experimentally found away from high-symmetry points, consistent with theoretical predictions. These results highlight the capability of momentum-resolved IPES to characterize the unoccupied band structure of MoS_2 and provide a benchmark for future studies of two-dimensional materials.

O 68: Nanostructured surfaces and thin films – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 68.1 Wed 18:00 P2

Electrospray Ion-Beam Deposition of Organic Molecules — •Grigori Pasko, Florian Münster, Lukas Heuplick, Jan Herritsch, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The preparation of molecular adsorbates on surfaces is often constrained by limitations of conventional deposition methods. While small molecules can typically be thermally evaporated from a Knudsen cell, this approach becomes unsuitable for larger or non-volatile species. Electrospray ion-beam deposition (ESIBD) provides a powerful alternative, enabling the transfer of intact, non-volatile molecules from solution into ultrahigh vacuum. Although its use is increasing, ESIBD remains an emerging technique, and the chemical state of the molecules after deposition is often insufficiently understood. Determining the oxidation state and overall chemical composition of the deposited species therefore represents a central challenge. In this study, meso-tetraphenylporphyrin (TPP) serves as a model system for evaluating the chemical integrity of ESIBD-prepared films. By combining X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), and density functional theory (DFT) calculations, we demonstrate that the porphyrins preserve the protonation state acquired during the electrospray process and remain intact upon deposition.

O 68.2 Wed 18:00 P2

Nitrogen plasma induced surface modification of nickel electrodes for enhanced electrochemical performance — •Karla Siecker[1], Christina Meinert[1], Christian Marcks[2], Timo Wagner[1], Nicolas Wöhrl[1], and Axel Lorke[1] — [1]Faculty of Physics, University Duisburg-Essen — [2]Electrochemical Reaction Engineering, RWTH Aachen University

Nickel sheets are widely used as electrode materials for electrolyzers due to their low cost and ease of handling. Here, we report on the use of a microwave-induced remote nitrogen plasma to modify the sample surface, adjusting both the electrochemical and mechanical properties of the nickel electrode. The plasma treatment leads to the formation of coral-like nanostructures on the nickel surface and promotes measurable surface nitridation. As a result, the surface roughness and wettability increase, directly affecting the electrochemical activity. For this purpose, contact angle measurements, 3D optical profilometry and electrochemical measurements were conducted to evaluate the catalytic activity of the modified electrodes.

O 68.3 Wed 18:00 P2

Nanostructured TiO_2 surfaces by low-energy ion erosion — •Berk Yildirim and Jens Bauer — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Ripple nanostructures on titanium surfaces are explored as a means to enhance protein adsorption and potentially introduce directionality for implant applications. We aim to produce large areas of consistent nanostructuring on titanium surfaces. Firstly, titanium/titanium oxide thin films are deposited using argon ion beam sputtering (IBS), followed by low-energy oxygen ion etching at an angle to create the ripple structures. Four main parameters are used for control. 1) thin-film composition, adjusted by supplying a background oxygen during deposition to produce fully TiO_2 films, or by depositing without oxygen to obtain titanium films, 2) etching time, 3) etching ion beam energy, where we applied 1.4 kV and 800 V, and 4) etching ion beam incidence angle. The morphology was analysed using AFM, SEM, Thin-film Reflectometry and the composition using XPS, ToF-SIMS. At 80°, the shadowing effect dominates and produces ripples or nanoneedles aligned in the same direction as the beam, which we consistently observe across a 5 cm radius sample. Roughnesses of the unetched films were $Sq = 1\,\text{nm}$ (Ti) and $Sq = 4.8\,\text{nm}$ (TiOx). We obtain much rougher and larger structures on the titanium oxide thin films with $Sq \approx 15\,\text{nm}$, and smoother ripple structures on the titanium thin films with $Sq \approx 3\,\text{nm}$. Controlling etching time and beam voltage allows fine-tuning of roughness and topography.

O 68.4 Wed 18:00 P2

Anomalous morphologies in ion-beam induced surface nanopatterning — •Denise J. Erb and Stefan Facsko — Ion Beam Center, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Irradiating solid surfaces with broad beams of low-energy ions often results in nanaoscale patterning, emerging from a combination of erosive, ballistic and diffusive processes between ions and surface atoms. Typical pattern morphologies comprise ripples, dots, or pits and mounds. The patterning outcome was typically explained as being dominated by either adjustable properties of the ion beam such as incident angle or ion energy, or by inherent properties of the solid material such as elemental composition or crystal symmetry. However, under appropriate experimental conditions, unexpected pattern morphologies can be formed and their understanding requires considering a more complex interplay between ion beam and solid surface. We present such anomalous surface patternings as well as the current state of understanding and modeling these morphologies.

[1] D.J. Erb et al., Intermediate morphology in the patterning of the crystalline Ge(001) surface induced by ion irradiation, PRB 109 (2024) 045439

[2] D.J. Erb and S. Facsko, Tuning the Morphology of Self-Assembled Nanopatterns on MgO(001) Surfaces by Sequential Broad-Beam Ion Irradiation, Phys. Status Solidi RRL (2025) 2500117

O 68.5 Wed 18:00 P2

Fabrication of Self-Assembled Carbon Nanodot Patterns on Quartz Glass Surfaces by Means of Ion Beam Processing — •Jamal Ghaith and Jens Bauer — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Graphite Nanodot patterns can be used as a negative mask for subsequent etching of quartz glass surface to bring about anti-reflective properties required in high-power laser applications. This requires uniformity in size and distribution of the nanodots over large areas. Silicon wafers with a $\sim 200\,nm$ thick thermal oxide layer are used as silica test sample material. A carbon layer is initially deposited using Ion Beam Sputtering (IBS), followed by 800 eV Argon ion etching at an angle, with sample rotation. The parameters used to control the nanodot formation are incidence angle of the ion beam, etch time, and carbon layer thickness. We found that an incidence angle of 70 degrees produces the most uniform nanodot distribution. Interestingly, increasing etch time does not necessarily lead to larger (or higher amplitude) dots. Instead of an increased size coalescence of the dots is observed, at least as long as the carbon layer thickness is high enough. The morphology was analysed using AFM and SEM, and the composition using ToF-SIMS.

O 68.6 Wed 18:00 P2

Reversible and persistent changes in nanofilms of the ionic liquid BMP DCA after application of an electric current — •Mirco Wendt[1,2], Anton Schün[2], Regina Lange[2], Jens Berdermann[1], Ingo Barke[2], and Sylvia Speller[2] — [1]Deutsches Zentrum für Luft-und Raumfahrt, Institut für Solar-terrestrische Physik, Neustrlitz — [2]Universität Rostock, Institut für Physik

1-Butyl-1-methylpyrrolidinium dicyanamide (BMP DCA) layers with a thickness of 10 to 20 nm were shown to be effective as charge mitigation layer in the context of spacecraft charging [1]. While at moderate exposures to electrons in a scanning electron microscope (10^12 e/m^2), no changes were observed, intense electron exposure led to irreversible damage with reversible alterations occurring at intermediate conditions. To better understand the conductive mechanism and how these layers react to the presence of excess electrons, ionic liquid nanofilms on interdigitated electrodes were prepared and a voltage applied between them. The monitored currents indicated that charges were permanently transferred into the sample. Atomic force microscopy revealed changes to the film*s morphology as well as shifts in dynamic mode phase, indicating trapping of charges. These findings are compatible with theoretical studies, suggesting additional electrons in this particular ionic liquid do neither pair with cations nor form cation shells, but further reduce anions into a doubly negative charge state [2]. [1] Wendt et al., J. Space Weather Space Clim. 2024, 14, 18 [2] Xu et al., J. Phys. Chem. B 2015, 119, 2, 532-542

O 69: Nanostructures at surfaces:1D, 2D, networks – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 69.1 Wed 18:00 P2

Study of different structural phases of Ni-DCA networks on graphene/Ir(111) — •Ayesha Jabeen[1], Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Anna Kurowska[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic

2D metal-organic frameworks (MOFs) represent a promising class of two-dimensional nanomaterials with tunable electronic and magnetic properties, which could have potential applications in catalysis and spintronics. In this study, we investigate the structural phases and thermal stability of Ni-DCA (9,10-dicyanoanthracene) networks supported on graphene/Ir(111). Employing Low-Energy Electron Microscopy (LEEM), Scanning Tunnelling Microscopy (STM), and X-ray Photoemission Spectroscopy (XPS), we identified three distinct structural phases: two phases composed of isolated $Ni_1(DCA)_3$ coordination complexes coexisting with hydrogen-bonded DCA molecules, and one extended metal-organic framework with $Ni_2(DCA)_3$ stoichiometry. Despite their different long-range order, all three phases have the same local Ni coordination environment. Thermal annealing reveals that the $Ni_2(DCA)_3$ network is the least stable of the three, dissociating into the individual complex phases upon mild annealing around 80 °C. These findings elucidate the polymorphic nature and thermal limitations of Ni-DCA networks supported on graphene/Ir(111), contributing to the understanding of DCA-based MOFs.

O 69.2 Wed 18:00 P2

Examining the character of coordination bonding in two-dimensional MOFs by photoemission tomography — •Dominik Brandstetter[1], Simone Mearini[2], Andreas Windischbacher[1], Yan Yan Grisan Qiu[2], Daniel Baranowski[2,3], Vitaliy Feyer[2,4], Claus Micheal Schneider[2,4,5], and Peter Puschnig[1] — [1]University of Graz, Graz, Austria — [2]Jülich Research Centre, Jülich, Germany — [3]Present address: Pacific Northwest National Laboratory, Richland WA, USA — [4]University of Duisburg-Essen, Duisburg, Germany — [5]UC Davis, Davis CA, USA

We investigate the nature of the coordination bonds in 2D MOFs by examining a well-ordered nickel tetracyanoquinodimethane (Ni-TCNQ) monolayer on a Ag(100) substrate. Notably, photoemission data shows a splitting of the valence band into bonding and anti-bonding states, resulting from the interaction between the Ni d-states and the ligand orbitals. By making use of the energy-resolved photoemission momentum maps, we are able unambiguously reveal signatures of covalent bonding between the organic ligands and the transition metal d-states by identifying fingerprints of the involved orbitals in momentum space. These hybridized states are crucial in understanding the MOF's electronic structure, which is a determining factor for their electronic and magnetic properties. Our results are concrete evidence of the covalent character within 2D MOFs, offering a deeper understanding of their fundamental electronic properties.

O 69.3 Wed 18:00 P2

Superconducting quantum corrals — •Divya Jyoti[1] and Nicolás Lorente[2] — [1]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]Centro de Fisica de Materiales (CFM), Donostia - San Sebastian, Spain

Quantum corrals enable atomically precise control of electronic confinement on surfaces, and their extension to superconductors opens new possibilities for manipulating in-gap Bogoliubov quasiparticles. In this work, we develop a microscopic Bogoliubov-de-Gennes Green-function framework [1-2] for multiple δ-like impurities on 2D superconducting lattices. As a benchmark, the method reproduces the superconducting mirage associated with Yu-Shiba-Rusinov states in elliptical corrals. By tuning the corral geometry, and material parameters, the spatial structure and spectral evolution of in-gap quasiparticle states is determined. We further explore the effect of confinement on engineered topological phases by placing a Majorana-hosting ferromagnetic spin chain inside an elliptical corral and showing that geometric confinement strongly hybridizes its zero-energy modes, redistributing their spin texture and shifting spectral weight to finite energies. These confined in-gap states offer a new route to engineer topological features, linking atomically crafted quantum matter to emerging platforms for topological quantum computation. [1] Morr et al., Phys. Rev. Lett. 92, 107006 (2004) [2] Flatté et al., Phys. Rev. B 56, 11213 (1997)

O 69.4 Wed 18:00 P2

Cooperative Rotation and Spin Switching of Molecules in Artificial Arrays — •Niklas Ide, Arnab Banerjee, Richard Berndt, and Alexander Weismann — IEAP, Kiel, Germany

Artificial arrays of tin phthalocyanine (SnPc) molecules on Pb(100) substrate are investigated using a low-temperature scanning tunneling microscope. Switching the central SnPc molecule between its two out-of-plane configurations (SnPc↑ → SnPc↓) triggers a collective rotation of all surrounding molecules in the array. This correlated structural response is accompanied by a change of the molecular spin states. A model of the intermolecular and molecular substrate interactions reproduces the experimental observations.

O 69.5 Wed 18:00 P2

Nonalternant Carbon Nanoribbon with 4-5-6-8 Topology via Indenofluorene Polymer Fusion — •Dong Han[1], Tim Naumann[1], Faming Kang[1], Alexandr Oshchepkov[2], Mikhail

Kalinin[2], Ye Liu[1], Zilin Ruan[1], Konstantin Y. Amsharov[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Organische Chemie, 06120 Halle (Saale), Germany

Carbon nanoribbons (CNRs) with nonhexagonal rings constitute a fascinating class of low-dimensional carbon materials exhibiting tunable chemical and physical properties distinct from those of conventional graphene nanoribbons (GNRs). Here, we report the on-surface synthesis and characterization of a nonalternant 4-5-6-8 CNR. This nanoribbon is obtained via lateral fusion of cis-linked indeno[2,1-a]fluorene (IF) polymer chains, formed by sequential debrominative and dehydrogenative C-C coupling reactions of a halogenated arene. Bond-resolved scanning tunneling microscopy (BR-STM) confirms the atomic structure of the resulting CNR. Scanning tunneling spectroscopy (STS) and density functional theory (DFT) calculations reveal its distinct electronic properties arising from the nonhexagonal rings. Notably, the 4-5-6-8 CNR exhibits a bandgap of 1.13 eV, highlighting the critical role of ring topology in modulating quantum confinement. X-ray photoelectron spectroscopy (XPS) further elucidates reaction pathways and intermediate species. This study establishes a controlled on-surface synthetic route towards structurally complex CNRs.

O 69.6 Wed 18:00 P2

Tuning electronic properties in 2D Covalent Organic Frameworks via on-surface chemistry — •Mira Sophie Arndt[1], Christoph Wachter[2], Roman Pallach[3], Yan Yan Grisan Qiu[4], Simone Mearini[4], Vitaliy Feyer[4], Sebastian Henke[3], Oliver T. Hofmann[2], Mirko Cinchetti[1], and Giovanni Zamborlini[5] — [1]Departement of Physics, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Department of Chemistry, TU Dortmund, Otto-Hahn-Straße 6, 44227 Dortmund, Germany — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [5]Institute of Physics, NAWI Graz, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Two-dimensional covalent organic frameworks (2D COFs) arranging in a Kagome lattice exhibit intriguing electronic properties, like flat bands and Dirac cones. We investigate the carbonyl-bridged aza-triangulene (P^2TANGO), which assembles into a Kagome lattice on Au(111). Inspired by reports that deoxygenation of the precursor induces an open-shell triplet ground state, we explore hydrogen-assisted deoxygenation to tune the COF's electronic properties. Our angle-resolved photoemission measurements reveal changes in the electronic structure upon oxygen removal, including energy shifts of the dispersive valence band features. DFT confirms that the shift grows with the deoxygenation, and that, in case of a complete deoxygenation, the degeneracy between the flat bands and the Dirac-dispersing bands is lifted.

O 69.7 Wed 18:00 P2

On-surface Synthesis of Aza-Coronoids — •Tim Naumann[1], Zilin Ruan[1], Olaf A. Kleykamp[1], Linus Pohl[2], Anton Nizovtsev[2,3,4], Alix Kaczmarek[2], Eugen Sharikow[1], Jörg Sundermeyer[1], Doreen Mollenhauer[2,3,4], and J. Michael Gottfried[1] — [1]Marburg University, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [3]Helmholtz Institute for Polymers in Energy Applications Jena, Lessingstr. 12-14, 07743 Jena, Germany — [4]Institute for Technical and Environmental Chemistry, Friedrich-Schiller-Universität Jena, Philosophenweg 7a, 07743 Jena, Germany

Chemical reactivity and electronic properties of nanographenes are tailored by functionalization, edge topology and doping. A versatile subclass within the nanographenes are coronoids, defined as benzenoids featuring a cavity. π-extended coronoids possess low solubility and are challenging target molecules for in-solution chemistry. However, reliable access via on-surface synthesis was demonstrated. Here, we combined in-solution and on-surface techniques to gain access to various aza-coronoids. Besides planar armchair-edge and zigzag-edge terminated coronoids, a curved coronoid was synthesized. Nitrogen functionalization of the inner cavity allows for hosting a metal atom and yields coronoid-metal complexes. In contrast, nitrogen core-doping significantly alters the electronic properties. Low-temperature scanning tunneling microscopy/spectroscopy (STM/STS), non-contact atomic force microscopy (nc-AFM) and DFT calculations were performed.

O 69.8 Wed 18:00 P2

Bottom-up fabrication of molecular islands utilizing an SPM-based manipulation approach — •Mong-Wen Gu[1,2], Ruslan Temirov[1,2,3], F. Stefan Tautz[1,2,4], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [4]Institut für Experimentalphysik IV A, RWTH Aachen, Aachen, Germany

The scanning probe microscope (SPM) allows single molecules to be manipulated with very high precision. SPM-based manipulation provides an opportunity for the fabrication of nanostructures through bottom-up construction. One critical challenge is using molecules other than conventional CO molecules as building blocks. Here, we explore the parameter space of the manipulation process in which a single PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule bridges the SPM junction. We demonstrate the bottom-up construction of artificial PTCDA islands on Ag(111). These islands reproduce the native monolayer lattice structure, can be customized in size and shape and thus allow studying their electronic properties in a systematic way.

O 69.9 Wed 18:00 P2

Effect of the catalytic-substrate and graphene-films on the growth and physical properties of non-stoichiometric silicon-oxide nanoparticles — •Mehmet Selim Imamoglu, Cem Kincal, and Oguzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

It is well known that silicon-oxide particles form during the growth of graphene by chemical vapor deposition (CVD) in a quartz furnace. Our studies showed that the creation and structure of these particles is mostly governed by the hydrogen flow rate during growth. Moreover, we have proven that they can be covered by graphene films depending on their morphology; showing that graphene growth during CVD process can continue over a non-catalytic substrate. In this work we have further investigated the formation and physical properties of such nanoparticles. Our results indicated that CVD grown silicon-oxide nanoparticles have non-stoichiometric nature leading to photoluminescent behavior. In this presentation their structure and physical properties as a function of the growth substrate (Ni and Cu foils) and the existence or in-existence of graphene films will be discussed. We will also present the methodology to transfer these nanoparticles on to random substrates.

O 69.10 Wed 18:00 P2

Towards on-surface synthesis of helicene chains — •Jung-Ching Liu[1], Miguel Gavara[1], Kévin Martin[2], Narcis Avarvari[2], Karl-Heinz Ernst[3,4,5], and Johannes Barth[1] — [1]Department of Physics, Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany — [2]University of Angers, CNRS, MOLTECH-Anjou, SFR MATRIX, 49000 Angers, France — [3]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [4]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague 6, Czech Republic — [5]Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zürich, Switzerland

Helicenes are polycyclic aromatic helical compounds which have been investigated at surfaces regarding their spin selectivity due to their chirality and potential use in organic spintronics. To enhance chirality-induced spin selectivity, extended helicene chains are of interest. However, fabrication of such helicene chains has not yet been reported. Here, we present atomically precise dibromohexahelicene chain formations on Au(111). Investigated by STM and bond-resolving nc-AFM at 4K, we found self-assembled supramolecular clusters at low coverage. Coupling reactions occur as the annealing temperature reaches 330C. By further annealing to 380C, short segments of planar structures are found along with 3D chains. The findings indicate potential nanographenes formation, tentatively ascribed to a Diels-Alder pathway. Our study provides insights into extended on-surface synthesis using non-planar molecular precursors.

O 69.11 Wed 18:00 P2

Orthogonally oriented molecular motors assembled on the surface: from liquid-solid to ultrahigh vacuum — •Robby Reynaerts[1], Cosima Stähler[2], Steven De Feyter[3], Ben L. Feringa[2], and Leonhard Grill[1] — [1]Department of Chemistry, Division of Physical and Theoretical Chemistry, University of Graz, Heinrichstraße 28, 8010 Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, 9747 AG Groningen, The Netherlands — [3]Department of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

Molecular motors continue to attract wide interest, due to their capability to convert energy into uni-directional rotary motion at the nanoscale. Immobilization of molecular motors on a solid surface through molecular self-assembly could amplify their nanoscale motion. Applying specific molecular design such controlled assembly of molecular motors was achieved at the liquid-solid (LS) interface under ambient conditions and studied using scanning tunnelling microscopy (STM). However, the dynamics inherent to ambient conditions were inseparable from the response of the molecular motors to external stimuli. Bringing the system over to low temperature and ultra-high vacuum (LT-UHV) conditions would rid any inherent dynamics from those ambient conditions. In this contribution I will discuss the controlled self-assembly of molecular motors on a solid surface achieved through molecular design under ambient and LT-UHV conditions and the experimental transition between these conditions. References: Chem. Rev. 2005, 105, 1281; Chem. Eur. J. 2024, e202303994.

O 69.12 Wed 18:00 P2

Manipulation of Atomically Precise Nanostructures from Single Atoms and Molecules — •Nikita Osipov, Christophe Nacci, Grant J. Simpson, and Leonhard Grill — Physical Chemistry Department, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Quantum corrals are of particular interest in surface science as they can be used to investigate quantum phenomena, such as quantum mirage [1] or function as quantum simulators that mirror the electronic properties of real atoms or molecules [2]. Currently, investigating these prominent structures requires researchers to manually assemble the objects on a surface using atomic manipulation techniques, a process that is extremely time-consuming. Our work aims to solve this critical bottleneck and save valuable research time. A primary goal of our project is to create an instrument for automatic and autonomous atomic manipulation. We are developing this system using machine learning algorithms to enable the careful, precise positioning of atoms or molecules [3]. This novel instrument will facilitate the assembly of large-scale objects or complex compositions of multiple smaller ones with high precision, thereby enabling the collection of significantly more data. In this work, we present our current status of assembled quantum corrals on noble metal surfaces. First results of manually assembled nanostructures will be presented together with the computational algorithm in the automated construction. [1] Li, Q. et al., Nat. Commun. 11 (2020) 1400. [2] E. Sierda et al., Science 380 (2023) 1048-1052. [3] B. Ramsauer et al., J. Phys. Chem. A 127 (2023) 2041.

O 69.13 Wed 18:00 P2

Atomic-Scale Sequencing of Biomolecules with nc-AFM — •Benjamin Mallada[1], Alejandro Lynch-Gonzalez[1], Marko Grabarics[1], Pavel Jelinek[2], Bruno de la Torre[3], and Stephan Rauschenbach[1] — [1]Department of Chemistry, University of Oxford, Oxford, UK — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]Nanomaterials and Nanotechnology Research Center (CINN-CSIC) , Mieres, Spain

Glycans, peptides, and cyclodextrins present major challenges for structural analysis due to branching, heterogeneous modifications, and stereochemical diversity. Conventional tools such as MS and NMR often fail to resolve these features at the single-molecule level. Noncontact AFM, combined with STM and KPFM under cryogenic UHV conditions, has recently demonstrated chemical sensitivity sufficient to discriminate functional groups and stereochemical arrangements by probing electrostatic and non-covalent interactions. Applications include the direct visualization of glycans in protein and lipid conjugates [1], submolecular resolution of cyclodextrins [2], and progress toward sequencing of complex carbohydrates and peptides. These results underline the potential of nc-AFM to expand the scope of SPM from imaging and identification toward true atomic-scale sequencing of biomolecules.

O 70: 2D materials: Stacking and heterostructures – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 70.1 Wed 18:00 P2

Unexpected Ordered Interfaces in WSe_2-$MoSe_2$ Lateral Interfaces Observed by STEM — •Matvei Kislitsyn[1], Max Bergmann[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

Two-dimensional WSe_2-$MoSe_2$ lateral heterostructures offer a platform for engineering band alignment and excitonic behavior through atomic-scale control of composition, making this material attractive for use in 2D optoelectronic devices. In this contribution, we present a systematic scanning transmission electron microscopy (STEM) study of monolayer WSe_2-$MoSe_2$ heterostructures synthesized by chemical vapor deposition (CVD) directly on SiO_2 TEM grids. While some investigated 2D flakes show atomically sharp interfaces with minimal intermixing, we also observe a highly ordered and unexpected interface configuration consisting of alternating Mo and W atomic rows. By comparing experimental observations with STEM image simulations and theoretical predictions, we analyze the structural origins of both interface types and discuss the mechanisms that may give rise to this unusual ordering. These results provide insight into interface formation mechanisms in lateral transition-metal dichalcogenide heterostructures and their potential impact on material properties.

O 70.2 Wed 18:00 P2

Superdomains and Strain Localization in Twisted Two Dimensional Transition Metal Dichalcogenides — •Riya Patel[1], Daniel Wolf[1], Kristina Weinel[1,2], Silke Hampel[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, 01069 Dresden — [2]Faculty of Physics, Technical University Dresden, 01069 Dresden

Bilayers of 2D transition metal dichalcogenides (TMDCs) exhibit special structural and electronic phenomena when stacked with a low-twist-angle. Particularly, they undergo lattice reconstruction, forming large triangular stacking domains, separated by domain walls that concentrate strain (soliton regime), which was shown in simulations. However, direct experimental quantification of these strain features and their correlation with electronic properties remains limited. Here we investigate low-twist-angle TMDCs using high-resolution transmission electron microscopy to visualize the reconstructed super lattice and identify the resulting superdomains structure. We employ geometric phase analysis to quantitatively map the strain distribution at the domain walls with nanometer resolution, revealing spatial maps of different strain components. We use Electron Energy Loss Spectroscopy to further probe the electronic properties of the reconstructed system. The understanding of strain localization in superdomain structures and the related electronic properties in such systems facilitate strain-engineered electronic properties in twisted TMDCs.

O 70.3 Wed 18:00 P2

Pseudomonolayer TMDCs via organic intercalation — •Katharina Steinkirchner[1,2], Jakob Dilling[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Markus Scholz[4], and Kai Rossnagel[1,2,3,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are a versatile class of layered materials with tuneable electronic properties. One approach to tailoring these properties is to manipulate the material's effective dimensionality. Specifically, intercalating cationic organic molecules with different alkane carbon chain into the van der Waals gaps between the layers increases the interlayer distance of the TMDC host material. This transforms the crystal from a bulk state to a monolayer-like state, thereby altering the electronic structure [1]. Here, we present a comprehensive study of the geometric and electronic structures of intercalated and non-intercalated TMDCs, such as NbSe$_2$, using SEM, EDS, and 11eV laser-based ARPES.

[1] H. Zhang *et al.*, Nat. Phys. **18**, 1425 (2022).

O 70.4 Wed 18:00 P2

Preparation of quasi-freestanding few-layer samples of 2D materials — •Seyedeh Helya Alaei, Hanna Shirin Pulikkal Hamza, Mashood Tariq Mir, Lukas Nöding, Ahmed Hassanien, Arne Senftleben, Jochen Mikosch, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

Two-dimensional (2D) materials have garnered significant attention in the last two decades and have been analyzed using various methods in the fields of materials science and physics. To study the dynamic behavior of 2D materials upon irradiation with femtosecond laser pulses using ultrafast electron diffraction, it is necessary to isolate few-layer structures from bulk crystals and prepare them in a quasi-freestanding manner. Due to the weak van-der-Waals forces between the layers relative to the in-plane forces of the structure, mechanical exfoliation is a commonly used method. However, the transfer is challenging, due to the thinness of the flake and the adhesive force between the flake and the surface. Our preparation involves three major steps: (1) exfoliation using adhesive tape and viscoelastic gel, (2) isolation of 2D material nanosheets with thicknesses ranging from 3 to 50 nm, and (3) transfer onto a standard sample mesh of transmission electron microscopy with a high success rate. The transfer exploits liquid-solid phase transitions of a soluble wax-like material. In this ongoing study, the 2D ferromagnetic material Fe$_5$GeTe$_2$ has been of interest. We will discuss the different steps in detail and the challenges associated with the preparation of this material, including the fragility of the crystals due to oxidation and the partially covalent out-of-plane forces.

O 70.5 Wed 18:00 P2

Ordering Phenomena in MoS$_2$ Nanocrystals on Graphite — •Lukas Nöding[1], Ahmed Hassanien[1], Mashood Tariq Mir[1], Hanna Shirin Pulikkal Hamza[1], Seyedeh Helya Alaei[1], Thomas Baumert[1], Jochen Mikosch[1], Florian Grassme[2], Claudia Backes[2], and Arne Senftleben[1] — [1]University of Kassel, Institute of Physics, Kassel, Germany — [2]University of Kassel, Institute of Chemistry, Kassel, Germany

Two-dimensional transition-metal dichalcogenides (TMDCs) such as MoS$_2$ offer a platform for tailoring electronic and optical properties through controlled stacking and orientation. Achieving ordered assemblies of MoS$_2$ nanocrystals on crystalline substrates is, therefore, of considerable interest. In this work, we study the crystallographic alignment of MoS$_2$ nanocrystals on a graphite substrate. The samples were prepared using the Langmuir-Schäfer technique, enabling the reproducible deposition of nanocrystals with controlled density. To probe the crystallographic alignment of the deposited nanocrystals with respect to the graphite lattice, we performed wide field static electron diffraction measurements at an acceleration voltage of 35 kV, complemented by selected area electron diffraction at 200 kV.

Our preliminary analysis reveals a pronounced localized and short-range ordered crystallographic alignment of the MoS$_2$ nanocrystals, extending over at least a few micrometers. A quantitative evaluation of the global ordering behavior, as well as its dependence on crystal size and deposition parameters, is currently underway and will be discussed.

O 70.6 Wed 18:00 P2

Multiferroic Two-Dimensional Cu(CrX2)2 (X = S, Se, and Te) as Anode Materials for Lithium-Ion Batteries: A First-Principles Study — •Muhammad Fayaz[1] and Zijing Lin[2] — [1]Department of Physics, University of Science and Technology of China, Hefei 230026, China — [2]Department of Physics, University of Science and Technology of China, Hefei 230026, China

Identifying two-dimensional (2D) materials with the desired electrochemical performance for lithium-ion batteries is of great interest in developing next-generation energy devices. Motivated by the successful synthesis of multiferroic 2D materials, Cu(CrX2)2 (X = S, Se, and Te), which exhibit simultaneous ferroelectricity and ferromagnetism, we performed first-principles calculations to investigate their potential as anodes for lithium-ion batteries. We comprehensively investigate the electrochemical properties of the predicted systems and demonstrate that lithium exhibits sufficient mobility on their surface, with appreciable stability. For instance, the binding energy (Eb) of the lithium adatom on Cu(CrS2)2 is -4.034 eV, with a diffusion barrier as low as 0.212 eV. As a consequence, the maximum theoretical specific capacity for lithium adatoms reaches as high as 1089 and 666 mAhg-1, respectively, for Cu(CrS2)2 and Cu(CrSe2)2, which can be attributed to a much higher storage capacity of lithium adatoms compared to previously identified 2D anode materials. All of these remarkable properties, including high binding energy (Eb), low diffusion barrier, high specific capacity, and good electrical conductivity.

O 70.7 Wed 18:00 P2

Valence-Band Renormalization and Spin Splitting in a Monolayer WTe2/WSe2 Heterostructure — •Daiyu Geng, Natalie Lehmann, Jiabao Yang, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

Monolayer WTe2 (1L-WTe2) hosts a variety of broken-symmetry phases, including a quantum spin Hall insulator, a topological excitonic insulator, and several intriguing spin-ordered states. The dielectric environment and charge-carrier density play crucial roles in the competition among these electronic phases. In this work, we investigate the band structure of 1L-WTe2 interfaced with semiconducting WSe2 using laser- and synchrotron-based micro-ARPES. We observe strong valence-band renormalization accompanied by pronounced spin splitting in 1L-WTe2. Additionally, multiple replica pockets emerging in the Fermi surface indicate a substantial moiré effect in this heterostructure.

O 71: 2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 71.1 Wed 18:00 P2

Observation of many-body-localization in substituted 1T-TaS$_2$ — •Jesumony Jayabalan[1], Gael Reecht[1], Ricards Kristers Knipšis[2], Florian K Diekmann[3], Friedemann Queisser[2], Walter Schnelle[4], Ping Zhou[1], Kai Rossnagel[3], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Uni. of Duisburg-Essen, Fakultät für Physik and CENIDE — [2]HZ Dresden-Rossendorf, — [3]CAU of Kiel and DESY — [4]MPI for Chemical Physics of Solids, Dresden

Random modulations in the potential landscape are known to localize a single quantum particle, the Anderson localization leads, to stable non-thermalizing states. Adding interaction is expected to cause delocalization and a quick thermalization of such single particles, but in a strongly disordered system, the many-body quantum state itself becomes localized, known as the Many-Body Localization (MBL). Using time-resolved photoelectron spectroscopic measurements, we show that it is possible to realize MBL states in a Tungsten substituted 1T-TaS$_2$ material. Electrons are excited by using a 1.51 eV, 50 fs pulses and a 6 eV probe pulse was used to photoemit electrons. In contrast to ultrafast (<20 fs) decay of doublons in pristine 1T-TaS$_2$[1], we observe that some of the doublons decay in hundreds of femtosecond time scale, while the rest lasts for more than few microseconds. This observation is supported by scanning tunneling microscopic measurements and Fermi-Hubbard model calculations. Funding by DFG through QUAST-FOR5249 and SFB 1242 is acknowledged. [1] M. Ligges et al., Phys. Rev. Lett., 120, 166401 (2018).

O 71.2 Wed 18:00 P2

Exciton Transport in Monolayer TMDs — •Lifeng Ou, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV, University of Valencia, Valencia, Spain

Atomically thin transition metal dichalcogenides semiconductor emerges as promising candidates for novel optoelectronic application, displaying weak dielectric screening due to its truly two-dimension character. The optical properties are mostly related to inter-band transitions between valence and conduction bands, also called the strongly binding electron hole pair, exciton. Strain is expected to impact spatiotemporal distribution of excitons, e.g. spatially inhomogeneous strain acts as a driving force for exciton/carrier funneling, similarly to bias fields for charged particles. In this work we demonstrate the capability to manipulate exciton motion via spatially modulated strain fields, where excitonic energy especially its bandgap is largely tunable and the effective mass of electronic valleys is modified resulting in a qualitative change of the excitonic landscape and efficiency of exciton-phonon scattering channels. These transport properties are represented by the coupled two equations, continuity equation and drift-diffusion equation, which derive from zero-order and first-order moment of Boltzmann equation, respectively. In addition, the simulation diffusion coefficient and mobility in latter equation are evaluated by first-principle and experiment qualitatively, as the function of strain fields.

O 71.3 Wed 18:00 P2

trARPES investigation electron-phonon coupling in CrSBr — •Maurits Houmes, Karl Schiller, Lasse Sternemann, Jonah Nitschke, and Mirko Cinchetti — Departement of Physics, TU Dortmund University, 44227 Dortmund, Germany

CrSBr is a magnetic, semiconducting van der Waals material that has recently attracted significant interest. It hosts both localized Frenkel excitons and delocalized Wannier-Mott-like excitons, and its excitonic properties are strongly influenced by magnetic ordering and lattice distortions. [1,2,3] These features make CrSBr a compelling platform for exploring correlated phenomena in condensed matter systems.

To advance our understanding of the interplay between excitons, magnetism, and lattice dynamics in this material, a more complete characterization is essential. In this work, we present time- and angle-resolved photoemission spectroscopy (trARPES) measurements performed on CrSBr, with particular emphasis on quantifying the electron-phonon coupling. Aiming to provide a previously missing component needed to build a comprehensive picture of the interactions in CrSBr, offering a foundation for future studies and potential technological applications of this promising material.

1. Smiertka, M. et al. Preprint at ArXiv:2506.16426 (2025). 2. Lin, K. et al. ACS Nano 18, 2898-2905 (2024). 3. Bork, S. et al. Preprint at ArXiv:2511.20268v1 (2025).

O 71.4 Wed 18:00 P2

Probing defect-induced wave patterns and superconductivity in $2H$-NbS$_2$ — Werner M.J. van Weerdenburg, •Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) host a variety of electronic phases, including superconductivity and charge-density-wave (CDW) order. Recent reports on $2H$-NbS$_2$ have added a coexisting pair-density-wave (PDW) order to this set, inspiring new questions about the coexistence and driving mechanisms of these phases [1]. In contrast, the closely-related superconducting compound $2H$-NbS$_2$ lacks a CDW phase, but has been suggested to be close to a CDW instability and sensitive to the presence of defects [2,3].

Using low-temperature scanning tunneling microscopy and spectroscopy, we probe the electronic, phononic and superconducting properties of $2H$-NbS$_2$. We observe wave-like modulations around intrinsic defects in differential-conductance maps and compare them to band-structure calculations. To assess the nature of these modulations, we probe the modulated regions and characterize the superconductivity spatially. These observations add to the ongoing exploration of superconducting, CDW, and PDW phases in TMDC materials.

[1] Liu et al., Science 372,1447-1452 (2021); [2] Heil et al., PRL 119, 087003 (2017); [3] Wen et al., PRB 101:241404, 6 (2020)

O 71.5 Wed 18:00 P2

Theory of few- and many-body excitations in carbon nanotubes — •Maurice Beringuier[1,2] and Richard Schmidt[1,2] — [1]Institut für Theoretische Physik, Philosophenweg 16, 69120 Heidelberg — [2]Universität Heidelberg, Grabengasse 1, 69117 Heidelberg

Even decades after their discovery, some properties of Carbon Nanotubes (CNTs) are still not fully understood. One of the phenomena still lacking a satisfying explanation is the behaviour of the absorption spectrum of semiconducting CNTs under doping. A resonance in these spectra appears only in the presence of additional charge carriers.

This has in the past been described with phenomenological models or few body physics (using trions and excitons), but experimental data (e.g. time resolved measurements of the spectra) hint at potential signatures of many-body physics. Inspired by their abundance in 2D or 3D semiconductors and cold quantum gases, we investigate whether quasiparticles like Fermi polarons could be responsible for the observations in CNTs, which due to their interesting geometry exhibit aspects of both 1D and 2D materials.

We tackle these questions by modeling charge carriers and excitons on CNTs interacting using a combination of exact diagonalization and variational techniques to gain insight into the interplay of few- and many-body physics in these systems.

O 71.6 Wed 18:00 P2

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden

In recent years, the rising class of non-van der Waals 2D materials [1] has garnered substantial attention for their distinctive electronic and magnetic properties. In this contribution, we explore the impact of spin-orbit coupling (SOC) on the properties of these non-van der Waals 2D systems and its potential to induce topological properties. Given the presence of heavy elements like Bi and Tl in several 2D candidates, SOC effects notably influence the electronic structure. In our approach, we utilize AFLOW's standardized workflows [2] for initial screening. Subsequently, we extract metadata using AFLOW and tailor the parameters with an AiiDA-plugin [3] for precise electronic structure calculations employing the full-potential all-electron program FLEUR [4] within AiiDA. We analyze the influence of SOC on band structures and densities of states, with a particular focus on topologically protected 1D conduction edge channels.

[1] R. Friedrich *et. al.*, Nano Lett. **22**, 989 (2022).
[2] Divilov *et. al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.

O 71.7 Wed 18:00 P2

Strain Engineering Single Photon Emission in hBN and MoS2 Monolayers using First Principles — •Paulina Chodyra, Chengcheng Xiao, Johannes Lischner, and Arash Mostofi — Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K

Point defects in monolayer hexagonal boron nitride (hBN) and molybdenum disulphide (MoS$_2$) are promising single-photon emitters (SPEs) for quantum technologies due to their potential for room-temperature operation and high photon emission efficiency. In this work we use density-functional theory calculations to investigate the nitrogen antisite-vacancy complex ($\mathrm{N_BV_N}$) and boron vacancy ($\mathrm{V_B}$) in hBN, and the sulphur vacancy ($\mathrm{V_S}$) in MoS$_2$. We calculate the defect formation energy of different charge states of these defects as a function of biaxial strain and electronic chemical potential. For the charge states that are likely candidates for SPE, we find that their stability can be enhanced via application of biaxial strain. Furthermore, the range of electronic chemical potential over which these charge states are stable can also be increased. These findings can provide predictive design rules for strain-engineered SPEs with improved resilience against electrostatic fluctuations. It also establishes our first steps toward an accelerated discovery of stable SPEs across 2D materials, where DFT-derived stability criteria combined with optical absorption and emission spectra could enable a deeper understanding of SPE operation under realistic conditions.

O 71.8 Wed 18:00 P2

Beyond the Gamma point: Scanning tunneling spectroscopy on MoS$_2$/graphene/Ir(111) — Borna Pielić[1,2], Dino Novko[2], Nina Girotto Erhardt[2], Vito Despoja[2], Alice Bremerich[1], Sumanasa Begur Prakash[1], •Robin Ohmann[1], and Carsten Busse[1] — [1]Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany — [2]Institute of Physics, Bijenička cesta 46, 10000 Zagreb, Croatia

Scanning tunneling spectroscopy (STS) reveals information about the band structure of surfaces by measuring the local density of states, and it also allows detection of quasiparticles. For semiconducting transition-metal dichalcogenides the conduction- and valence-band edges have been readily explored with this method. However, STS studies at higher energies than the Γ-point are limited. Here, we investigate epitaxially grown monolayer islands of MoS$_2$ on graphene/Ir(111) using STS at low-temperature (T=10 K). Specifically, we employ the constant-current STS method, which enables easier access to spectroscopic features with higher energies, than the more commonly used constant-height STS. We find several peaks a few hundred meV above the Γ-point. We do not see them on graphene, allowing us to exclude substrate- or tip-related effects. When measured near the step edge of an island, these peaks bend closer to the Fermi level, similar to the peak at the Γ-point. Their appearance also varies depending on tip condition and intercalation. Our observations cannot be explained in a single-particle picture. Possible many-body models, such as phonon assisted inelastic tunneling or plasmarons are discussed.

O 71.9 Wed 18:00 P2

Band structure and Work Function in Ultrathin HfSe2 — •Young Jun Chang — University of Seoul, Seoul, Republic of Korea

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit significant modifications in their electronic structures when reduced from bulk to monolayer thickness. In this study, we investigated the thickness-dependent electronic properties of epitaxial 1T-HfSe2 thin films. The films were grown via molecular beam epitaxy (MBE) and monitored in situ by reflection high-energy electron diffraction (RHEED). Scanning tunneling microscopy (STM) revealed atomically flat surfaces with well-defined 1T hexagonal lattices, while scanning tunneling spectroscopy (STS) measured a bandgap of ~1.1 eV for the monolayer. Angle-resolved photoemission spectroscopy (ARPES) revealed thickness-induced band splitting in the valence band, while the valence band maximum (VBM) remained pinned regardless of thickness. In contrast, the work function increased monotonically with film thickness. Density functional theory (DFT) calculations reproduced the observed band structures and attributed the thickness-dependent work function to the screening effect of the underlying graphene substrate. These findings provide key insights into band alignment and interface engineering in 2D semiconductor-based electronic and optoelectronic devices. (RS-2023-00220471, RS-2023-00284081, RS-2024-00334854)

O 71.10 Wed 18:00 P2

Exciton and trion dynamics of 2D transition metal dichalcogenides — •Seawoo Moon[1], Alessandro De Vita[1], Lawson T. Lloyd[2], Tania Mukherjee[1], Anh T. Nguyen[3], Dong-Wook Kim[3], Martin Wolf[2], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1] — [1]Institute for Physics and Astronomy, TU Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Germany — [3]Department of Physics, Ewha Womans University, South Korea

Key functionalities of transition metal dichalcogenides (TMDs) are determined by excitons whose behaviour can be tweaked by interface–induced external perturbation such as proximity effects, charge transfer and local electromagnetic fields. Excitonic behaviors and band alignment of TMDs with interfacing materials are explored. We studied the band alignment of monolayer WS$_2$ on nanostructured Ag by Kelvin probe force microscope, a tool that can map electrical potential of sample surface. By this method, the exciton–to–trion conversion mechanisms in WS$_2$ could be explained, including the role of the localized surface plasmons. For a more direct approach, time and angle–resolved photoemission spectroscopy (TrARPES) with pump–probe technique is employed to directly map the equilibrium and non–equilibrium electronic structure of TMD–metal and TMD/TMD interfaces. In–situ and ex–situ techniques are required to achieve pristine TMD surfaces and interfaces, since TrARPES is a highly surface sensitive technique.

O 71.11 Wed 18:00 P2

Ultrafast Photocarrier-Induced Ionic Rearrangement in Monolayer ReS$_2$ Probed with Femtosecond Electron Diffraction — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Martin Wolf[1], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Rhenium disulphide (ReS$_2$) exhibits a distorted crystal structure compared to prototypical hexagonal transition metal dichalcogenides. This Peierls-like distortion results in quasi-1D chains of Re ions running in plane through each layer of ReS$_2$, which give rise to prominent anisotropic properties, such as polarization dependent optical absorption and anisotropic effective carrier masses.

We investigate the ultrafast lattice dynamics of monolayer ReS$_2$ with femtosecond electron diffraction (FED). Leveraging the strength of FED as a direct and quantitative measurement of the crystal lattice, we fit the intensities of many hundreds of Bragg peaks at each time delay to extract time resolved crystallographic information.

With this method, we not only resolve the increase in the incoherent phonon population (Debye-Waller), but also reveal a concerted atomic rearrangement within the lattice, with the ions rapidly (< 1 ps) moving away from their equilibrium atomic coordinates and returning on timescales of a few picoseconds. We associate this response with the aforementioned distortion, and discuss the physical origin.

O 71.12 Wed 18:00 P2

Exploring Zincblende (100) Semiconductor Surfaces as Platforms for Correlated Adatom Lattices — •Olga Kashirina, Niklas Enderlein, and Philipp Hansmann — Friedrich-Alexander-Universität Erlangen-Nürnberg

Adatom lattices on (111) surfaces of zincblende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting strong electronic correlations and associated emergent behavior near the Fermi energy (see [1] and references therein). Our recent study [2] reveals transition metals adatom lattices on 3C-SiC(111) surfaces to be intriguing candidates for strongly correlated material design. In the present contribution we continue this strategy by leaving the hexagonal/triangular lattices. Specifically, we explore the (100) surfaces of silicon, diamond, and 3C-SiC which in the infinite bulk exhibit a fourfold rotoinversion symmetry enabling square/rectangular adatom lattices. As the (100) surface is prone to dimerization, an additional complication arises from dimer-derived electronic states inside the bulk gap, which - depending on the chosen adatom and substrate combination - may or may not hybridize with the adatom states. In this context, the adatom coverage is another crucial parameter as it directly influences the nature of surface reconstructions and dimerizations. To assess the structural stability of our candidate systems, we employ phonon calculations based on density-functional perturbation theory as well as molecular-dynamics simulations. [1] X. Cao, et al., PRB 97, 155145 (2018). [2] H. Menke, N. Enderlein, et al., arXiv:2410.17165.

O 71.13 Wed 18:00 P2

Engineering correlated electrons in adatom lattices on semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project, we explore promising adatom lattices on semiconducting/insulating substrates such as SiC and cubic BN in order to realize one-, two-, and three-band Hubbard models at different fillings. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field. [1] H.Menke, N.Enderlein, *et al.*, arXiv:2410.17165.

O 71.14 Wed 18:00 P2

Investigation of the atomic and electronic structures of WSe2-xTex — •Ganbat Duvjir[1], Nguyen-Hoang Dang[2], Younghun Hwang[1], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Electricity and Electronics and Semiconductor Applications, Ulsan College, Ulsan 44610, Republic of Korea

Ternary transition metal dichalcogenides (TMDs) exhibit diverse crystal structures and electronic properties depending on their composition. In this study, we systematically investigate the atomic and electronic structure of ternary WSe2-xTex as a function of Te concentration using scanning tunneling microscopy/spectroscopy (STM/S). Notably, STM topography indicates that increasing the Te content induces structural deformation of the hexagonal lattice of WSe2-xTex. This deformation manifests as the stretching of 2H structure along the zigzag direction and compression along the armchair direction. STS measurements reveal a significant reduction in the band gap of WSe2-xTex with increasing Te concentration. While the valence band maximum shifts toward the Fermi level, the conduction band minimum remains relatively unchanged.

O 71.15 Wed 18:00 P2

STM study on tuning the Fermi level of transition metal dichalcogenides — •Nguyen-Hoang Dang[1], Mincheol Kim[2], Ganbat Duvjir[1], Young Jun Chang[2,3], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Department of Physics, University of Seoul, Seoul 02504, Republic of Korea — [3]Department of Smart Cities, University of Seoul, Seoul 02504, Republic of Korea

Controlling the Fermi level is essential for tailoring the electronic properties of semiconductors. Here, we investigate two routes of chemical doping and defect control using scanning tunneling microscopy and spectroscopy. For V-doped $MoSe_2$, we study how substitutional V atoms influence its electronic structure. Although STM primarily probes the top Se layer and the dopants are not directly imaged, the topography exhibits defect-like features whose contrast reverses with the bias polarity: dark at positive sample bias and bright at negative bias. This is characteristic of negatively charged acceptor states, consistent with V substituting Mo. STS spectra show a Fermi-level shift toward the valence band, indicating that V doping drives $MoSe_2$ from intrinsic n-type toward p-type. For $HfSe_2$, we study defect control via thermal annealing. STS measurements under different annealing conditions show Fermi level shifts toward the conduction band, suggesting that prolonged annealing enhances Se-vacancy formation, which acts as an electron donor. These results highlight how STM/STS links local defects with electronic properties, offering microscopic insight into Fermi level tuning through doping and defect engineering.

O 71.16 Wed 18:00 P2

Impact of Mo doping on the charge density wave in $1T$-TaS_2 studied by laser-ARPES and LEED — •Adina Timm[1,2], Finja Schillmöller[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Controlling charge density waves (CDWs) in quantum materials enables the fine-tuning of their electronic properties, paving the way for future electronic and optoelectronic devices. The layered compound $1T$-TaS_2 exhibits various temperature-dependent CDW phases that we aim to modify through doping. We introduced the dopant molybdenum during crystal growth via the chemical vapor transport method. Using 11-eV laser-based angle-resolved photoelectron spectroscopy (ARPES), we comparatively measured the electronic band structures of pristine and Mo-doped $1T$-TaS_2 crystals. Complementary low-energy electron diffraction (LEED) measurements revealed the structural rearrangements during the CDW transitions and partial CDW suppression at specific doping levels. Our results suggest that modest Mo doping allows for subtle adjustments to the CDW landscape of $1T$-TaS_2, yielding different transition temperatures while preserving the underlying electronic-structural order.

O 71.17 Wed 18:00 P2

Probing Electronic Structure Modulation in WSe_2 and $MoTe_2$ under Out-of-Plane Electric Fields via ARPES and XPS — •Sonja Reinheimer[1,2], Lukas Bruckmeier[1,2], Jakob Dilling[1,2], Jens Buck[1,2], Matthias Kalläne[1,2,3], Chithra Sharma[1,2,4], Markus Scholz[5], and Kai Rossnagel[1,2,3] — [1]IEAP, CAU Kiel, 24098 Kiel, Germany — [2]RHL, DESY, 22607 Hamburg, Germany — [3]KiNSIS, CAU Kiel, 24098 Kiel, Germany — [4]Universität Hamburg, 22761 Hamburg, Germany — [5]DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are quantum materials that exhibit a broad spectrum of emergent electronic phenomena, arising from layer-dependent band structures. Owing to their tunable (opto-)electronic properties, TMDCs are promising candidates for next-generation photovoltaic devices and highly integrated electronic components. A key challenge is to systematically control charge transport and band alignment in these layered systems. Here, we investigate vertically stacked $2H$-WSe_2/$2H$-$MoTe_2$ heterostructures using angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy. By performing in-operando ARPES on a sample with an applied out-of-plane electric field during the measurements, we can directly probe field-induced modifications to the electronic band structure and the density of states. This approach enables us to identify electric-field-driven changes in the electronic and lattice structure and contribute to a deeper understanding of electric control mechanisms in TMDC heterostructures.

O 71.18 Wed 18:00 P2

Many-body localisation in the Fermi-Hubbard model? — •Ričards Kristers Knipšis[1], Jesumony Jayabalan[2], Gael Reecht[2], Vivek Mondal[2], Florian Konstantin Diekmann[3], Friedemann Queisser[1], Ping Zhou[2], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[1,6], Manuel Gruber[2], and Uwe Bovensiepen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-University of Kiel, Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]Ruprecht-Haensel-Laboratory, DESY, Hamburg, Germany — [6]Institute of Theoretical Physics, Dresden University of Technology, Dresden, Germany

Motivated by recent experimental results, we study the 2D Fermi-Hubbard model in the Mott insulator state under the influence of a disorder potential. Special emphasis is placed on signatures of many-body localisation.

Using the hierarchy of correlations, we find that the disorder potential can localise the effective quasi-particle wavefunctions, resulting in their spatial separation. This, in turn, can be used to explain the drastic increase in the quasi-particle lifetimes observed in experiment.

Funding by the DFG through the SFB 1242 is gratefully acknowledged.

O 71.19 Wed 18:00 P2

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Robert Zierold[4], Tim Riedel[1,2], Adina Timm[1,2], Robert H. Blick[4], and Kai Rossnagel[1,2,3] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]RHL, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]CHyN, Universität Hamburg, 22761 Hamburg, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a quasi-two-dimensional hexagonal $2H$ structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping. This makes it a highly attractive candidate for spintronic applications. Density functional theory calculations and scanning transmission electron microscopy studies support this assumption, and RKKY interactions are predicted to be the driving mechanism. Pristine WSe_2 and vanadium-doped WSe_2 crystals were synthesized in separate in-house batches using the chemical vapor transport (CVT) method. The doped samples were grown with varying nominal concentrations of V intended to induce substitutional doping at the tungsten sites. The samples were investigated using a vibrating-sample magnetometer (VSM). The results provide insight into the magnetic characteristics of the doped material compared to the pristine reference crystal.

O 71.20 Wed 18:00 P2

Coexistence of a fully metallic antiphase boundary and the semiconducting charge density wave phase in 1T-TaS_2 — •Georg A. Traeger[1], Kai Rossnagel[2,3], and Martin Wenderoth[1] — [1]IV. Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Transition metal dichalcogenides are an ideal platform for studying the interplay between charge density waves (CDWs), electronic correlations, and defect states. Using scanning tunneling microscopy and spectroscopy, we investigate a new type of intrinsic antiphase boundary (APB) in the commensurate CDW phase of 1T-TaS_2. In contrast to previous studies, we find a metallic APB extending laterally across several nanometers. We observe evanescent states spilling out from the defect into the metallic region and find that the fingerprint of the semiconducting system gradually disappears within the APB, without signs of strong interactions, suggesting the orthogonality of the two systems wave functions. Our findings highlight the crucial role of domain boundaries in the interpretation of other, especially conductivity-based, measurements. Furthermore, we propose this new type of metallic APB as a model system to study interlayer coupling in correlated layered materials.

O 71.21 Wed 18:00 P2

Temperature-dependent VUV-ARPES of $1T$-$\mathrm{Mo}_x\mathrm{Ta}_{1-x}\mathrm{S}_2$ — •Torben Petersen[1,2], Matthias Kalläne[1,2,3], Adina Timm[1,2], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Examining the charge density wave (CDW) phase transitions of transition metal-substituted transition metal dichalcogenides (TMDCs) provides insight into tuning transition behavior by doping. To this end, we use the $1T$-$\mathrm{Mo}_x\mathrm{Ta}_{1-x}\mathrm{S}_2$ reference system, comparing the pristine sample with two doped samples (x = 0.5% and x = 1%) using 11 eV laser-based VUV-ARPES. We investigate work function changes alongside doping-induced band structure changes in the temperature range of 60 K to 370 K. This allows us to observe the high- and low-temperature CDW phase transitions known from the pristine material and determine how the CDW-induced band structure changes vary with doping.

O 71.22 Wed 18:00 P2

STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111) — •Alina Drechsler, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDs) exhibit thickness-dependent electronic properties and are highly sensitive to structural defects, which can strongly modify their density of states even at low concentrations. Defect engineering has therefore become an important route to tailor their electronic, magnetic, optical, and catalytic behaviour. While most of the current research focuses on naturally occurring defects in chemical vapour-deposited TMDs, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE) to improve control in defect engineering.

We present scanning tunneling microscopy and spectroscopy (STM/STS) studies of Fe-doped monolayer MoS_2 on Gr/Ir(111), achieved by co-evaporation Fe during MBE growth. By comparing to undoped MoS_2 grown under identical UHV conditions, we identify the Fe-related defects and measure their electronic signatures. STS reveals in-gap states associated with single-atom Fe inclusions, whose spatial distributions are resolved via differential conductance mapping. Additionally, resonant tunneling spectroscopy shows that Fe inclusions modify the image potential states by locally shifting their energetic positions. Our work demonstrates the potential of single-atom substitutions for tailoring the electronic properties of two-dimensional TMDs.

O 71.23 Wed 18:00 P2

Layer thickness dependent band gap of MBE grown single- to few-layer MoS_2 — •Maciej Bazarnik[1], Marta Przychodnia[1,2], Thorsten Deilmann[3], and Anika Schlenhoff[1] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Physics, Poznan University of Technology, Poland — [3]Institute of Solid State Theory, University of Münster, Germany

In light of the rise of transition metal dichalcogenides as 2D semiconductors for device applications, band engineering becomes very important from an application point of view. In many of these materials, such as the canonical example of MoS_2, the semiconductor band gap depends on the layer number. There is a transition from an indirect band gap semiconductor in bulk to a direct band gap for a monolayer. Interestingly, it was predicted and experimentally confirmed that, by thinning the material from bulk to a bilayer, the indirect transition blue-shifts.

Here, we present the results of scanning tunnelling spectroscopy measurements on MoS_2 that has been grown in situ via molecular beam epitaxy (MBE) on graphene on Ir(111) at thicknesses ranging from 1 to 6 layers. We observe a decrease in the band gap with increasing layer number. We also find a pinning of the conduction band, which vanishes for layer thicknesses beyond 4 layers. Comparing our experimental data with DFT and GW calculations indicates that a screening in addition to that of the substrate needs to be introduced to explain the experimentally obtained relation. We discuss possible sources of this additional screening in light of our findings.

O 72: 2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 72.1 Wed 18:00 P2

In-Situ CVD growth of vertical Heterostructures of Borophene and Hexagonal Boron Nitride — •Niels Ganser[1], Marko Kriegel[1], Smruti Ranjan Mohanty[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1,3], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Intrinsic segregation provides a promising and scalable route for the in situ fabrication of 2D heterostructures. Using UHV chemical vapor deposition (CVD) of a single borazine ($B_3N_3H_6$) precursor [1], we demonstrate the growth of an hBN/borophene heterostructure on Ir(111). At high temperatures and low precursor pressures, boron dissolves into the Ir subsurface region, creating a boron reservoir below the surface [2]. Largely increasing the precursor dosing pressure shifts the chemical potential toward the formation of a complete hBN layer. Upon cooldown, the decreasing boron solubility of the Ir substrate drives segregation to the surface, where a borophene layer forms underneath the hBN overlayer and thus completing the heterostructure. The resulting structure and its growth kinetics were investigated using a combined low energy electron diffraction (SPA-LEED) and microscopy (LEEM) approach.

[1] K. Omambac et al., ACS Nano 17 (2023) 17946

[2] K. Omambac et al., ACS Nano 15 (2021) 7421

O 72.2 Wed 18:00 P2

Growth of 2D molecular networks on graphene — •Haruto Shibahara and Toyo Kazu Yamada — Dept. Materials Science, Chiba Univ., Chiba, Japan

We demonstrate the engineering of qubits on solid surfaces using organic molecules and transition-metal magnetic atoms. Atomically flat and clean graphene (Gr) grown on an Ir(111) substrate was selected as the platform. Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) revealed the characteristic moiré pattern, while scanning tunneling spectroscopy (STS) and angle-resolved photoemission spectroscopy (ARPES) confirmed the presence of Dirac bands. Although single atoms can in principle serve as qubits, they tend to thermally diffuse on surfaces and their energy levels may remain degenerate. To overcome these issues, it is necessary to coordinate the atoms with organic ligands, whose ligand fields can lift the degeneracy. As a first approach, we attempted to employ 1,3,5-tris(4-bromophenyl)benzene (TBB) molecules to form a two-dimensional (2D) covalent organic framework. However, on the Gr surface we found that thermal activation desorbed the TBB molecules before they could undergo Ullmann coupling. As a second approach, we attempted to grow a 2D metal organic framework (MOF) on Gr. The details of this effort will be discussed.

O 72.3 Wed 18:00 P2

Probing the Electrostatic Potential of hBN by AFM with Oxygen-Terminated Copper Tips — •Jan ter Glane[1,2], Philipp Wiesener[1,2], Thorsten Deilmann[3], Milena Merkel[1,2], Maciej Bazarnik[2], Anika Schlenhoff[2], and Harry Mönig[1,2] — [1]Center for Nanotechnology, University of Münster, Germany — [2]Institute of Physics, University of Münster, Germany — [3]Institute of Solid State Theory, University of Münster, Germany

Monolayer hexagonal boron nitride (hBN) hosts point defects with promising optoelectronic properties, yet their atomic structure remains unclear [1]. Conventional scanning tunneling (STM) and atomic force microscopy (AFM) lack elemental contrast, making it difficult to reliably distinguish B and N sites. Non-contact AFM with oxygen-terminated copper tips (CuOx-tips) has previously enabled elemental discrimination and defect identification on metal oxides [2].

Using CuOx-tip AFM, we demonstrate elemental contrast on NaCl thin films, suggesting its broad applicability to polarized surfaces. Leveraging this capability, we investigate its application to monolayer hBN. DFT-optimized electrostatic potential calculations predict clear B-N contrast. To realize these measurements, we employ in-situ chemical vapor deposition growth procedures for high-quality hBN on single-crystalline substrates. We outline the benefits of CuOx-tip AFM and present initial results towards correlating STM/STS measurements, aiming to enable atom-specific defect identification in hBN.

[1] Grosso *et al.*, Nat. Commun. **8**, 705 (2017)
[2] Wiesener *et al.*, ACS Nano **18**, 21948 (2024)

O 72.4 Wed 18:00 P2

Pt-doped borane nanomembranes — •Martha Frey[1], Julian Picker[1], Christof Neuman[1], Jan Macháček[2], Tomáš Baše[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec Rez, 1001, Czech Republic

Boranes are clusters of boron and hydrogen atoms that form three-dimensional, cage-like molecules. We have recently employed them as convenient starting precursors for synthesising two-dimensional (2D) carbon-free nanomembranes. In this study, we present the preparation and characterisation of the self-assembled monolayers (SAMs) of two thiolated *syn*-$B_{18}H_{22}$ clusters on silver substrates. Subsequently, these SAMs were cross-linked laterally to form boron nanomembranes (BNMs) via low-energy electron irradiation under ultra-high vacuum (UHV) conditions. We investigated the structural and chemical properties of these 2D nanomembranes using surface-sensitive techniques such as X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). Both the starting SAMs and the resulting boron nanomembranes exhibited reactivity toward Pt-containing complexes. While such reactivity was expected for the SAMs, it was particularly noteworthy that the BNMs also enabled the insertion of Pt atoms. This Pt-doping positions borane-derived SAMs and BNMs as a promising 2D platform for nanoscale catalytic studies.

O 72.5 Wed 18:00 P2

Defects and Initial Approaches to TMDC Heterostructure Growth on Pt_xTe_y films — •Isabella Stollberg, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Transition-metal dichalcogenides (TMDCs) can generally be synthesised either by co-evaporating the metal and chalcogen onto a suitable substrate [1] or by depositing only the chalcogen onto the desired metal surface. Using STM, STS, and DFT, we investigate Pt_xTe_y films on Pt(111) prepared via the latter approach. With increasing Te content, different initial growth surface telluride structures are observed, followed by the formation of Pt_2Te_2 and $PtTe_2$ layers [2]. This contribution focuses on STM and spatially resolved STS analyses of point defects in $PtTe_2$, as well as domain boundaries within a $PtTe_2$ or Pt_2Te_2 layer. Furthermore, we evaluate the suitability of these telluride films as substrates for TMDC heterostructure growth. First results on attempting to grow $TiTe_2$ and $PdTe_2$ demonstrate considerable intermixing. While $TiTe_2$ islands can be identified by their apparent height and other lattice constants, $PdTe_2$ islands cannot be distinguished from $PtTe_2$ based on topography due to their similar vertical and lateral lattice parameters.

[1] K. Lasek et al., Nano Lett. **22**, 23 (2022)
[2] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)

O 72.6 Wed 18:00 P2

Boosting the Efficiency of Quantum Replica-Exchange Molecular Dynamics — •Jan-Niklas Mohr, Shubham Sharma, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Replica exchange molecular dynamics can be combined with path-integral techniques in order to incorporate quantum statistics in the sampled ensembles [1]. However, the efficiency in swapping replicas is decreased to a point that makes simulations extremely inefficient at lower temperatures.

We propose a new acceptance criterion for path-integral replica-exchange molecular dynamics (PI-REMD) that incorporates the path-integral spring term in the Hamiltonian and rescales it consistently. As a result, the acceptance probability is only sensitive to potential-energy differences, and the efficiency of the method is thus increased. Benchmarking on several test systems, including asymmetric double wells and glassy-like potentials, shows that our method outperforms standard PI-REMD in sampling efficiency and exchange frequency. We also show improvements for realistic materials, such as monolayer 1H-TaS_2 [2], where it is paramount to obtain an accurate description of the charge-density-wave phase transition. Our acceptance criterion therefore provides an efficient and reliable tool for studying quantum phase transitions and exploring thermodynamic ensembles under challenging conditions.

[1] Kapil *et al.*, Comput. Phys. Commun. 236, 214-223 (2019).
[2] Schobert *et al.*, SciPost Phys. 16, 046 (2024)

O 73: Graphene: Growth, structure and substrate interaction – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 73.1 Wed 18:00 P2

Towards enhanced spin-orbit coupling in epitaxial graphene via Pb intercalation — •Markus Gruschwitz[1], Sergii Sologub[1,2], Hoyeon Jeon[3], Saban Hus[3], An-Ping Li[3], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]Institute of Physics, NAS of Ukraine, Kyiv, Ukraine — [3]CNMS, ORNL, Oak Ridge, USA

The design of noval quantum phases by combining low dimensional materials poses the next evolution step of electronics. Intercalated epitaxial graphene on SiC embodys a van-der-Waals heterostack with well defined lattice arrangement. Stabilizing monolayers of heavy elements in proximity to graphene, potentially enhances the spin-orbit interaction (SOI) in graphene. Using Pb as intercalant, we reliably decouple and neutralize graphene by minimizing the substrate influence. At the interface coexisting striped and hexagonal superstructures emerge from local strain and density variations in the Pb monolayer. [1] Multi-probe transport measurements, assisted by finite element simulations, revealed a temperature dependent resistance. This emergent behavior was attributed to a gap opening in graphene in the order of 3-5 meV. [2] Tip–sample spacing dependent spectroscopy supports this finding by a clearly reduced density of states at the Dirac point. The desired enhanced intrinsic SOI competes with Rashba-SOI and modulations of the sublattice potential by the Pb superstructure. Although the nature of this gap was not revealed yet, it has potential to stabilize a quantum spin Hall state. [1] Adv. Mater. Interfaces 12, 21: e00617 (2025) [2] Phys. Rev. B 109, 245430 (2024)

O 73.2 Wed 18:00 P2

Graphene-Based Coatings on Titanium Alloy for Implants — •Franziska Gladitz[1], Christof Neumann[1], Guobin Jia[2], Jonathan Plentz[2], and Andrey Turchanin[1] — [1]Friedrich-Schiller-University Jena, Institute of Physical Chemistry, Jena, Germany — [2]Leibniz-Institut of Photonic Technology (Leibniz-IPHT), Jena, Germany

Titanium alloy implants are essential for bone replacement surgeries; however, they are susceptible to infection. To improve their antimicrobial properties, we develop graphene-based coatings on the implant substrates (alloy Ti6Al4V), taking advantage of the antibacterial and biocompatible properties of graphene (G) or graphene oxide (GO). For this purpose, the titanium alloy is coated with G or GO nanosheets using different coating techniques like double self-assembly procedure and electrochemical deposition. The coatings are characterized using complementary characterization techniques including scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, atomic force microscopy (AFM) and optical microscopy. The morphological and chemical properties of the obtained graphene coatings are analyzed in respect to their growth conditions to elucidate influences on the quality, uniformity, and possible biofunctional performance.

O 73.3 Wed 18:00 P2

Graphene on 4H-SiC and 6H-SiC: The Influence of the SiC-Polytype onto the Local Transport Properties of Graphene — •Simeon Bode[1], Benno Harling[1], Klaus Pierz[2], Teresa Tschirner[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

Studies of Graphene on silicon carbide have shown a strong dependence of the surface termination of the SiC substrate on the local transport properties. In this study, we investigate the influence of the polytype of the substrate SiC onto the local properties of Polymer Assisted Sublimation Growth (PASG) graphene. It is known that graphene on 6H-SiC displays two distinct surface terminations [1], while on 4H-SiC it is only one dominant surface termination. Here, local characterization is done by AFM and STM, while the local electronic properties are investigated by STS. Graphene on both polytypes present a similar characteristic in multibias topographies. To gain access to local transport properties, we utilized Scanning Tunneling Potentiometry (STP), which revealed two distinct sheet resistances attributed to the different surface terminations. Although PASG graphene on 4H-SiC shows only one surface termination, the spread of the sheet resistance is much larger than the difference of the two distinct sheet resistances on 6H-SiC. This work was financially supported by the DFG through the FOR5242. [1] Sinterhauf et al., Nat Commun 11, 555, 2020

O 73.4 Wed 18:00 P2

Sn intercalation of Zero-Layer Graphene — •Jan-Lucas Hornbostel, Benno Harling, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August Universität Göttingen

Graphene is a 2D material with a wide range of potential applications. Our research area is the intercalation of epitaxial graphene with tin, a system that has recently shown interesting phenomena such as Mott states [1]. To achieve such systems, zero-layer graphene (ZLG) as starting point is intercalated. Tin binds to the SiC substrate transforming the ZLG into quasi-freestanding monolayer graphene. ZLG graphene can be epitaxially grown on SiC using various methods. The intercalation of Sn on polymer assisted sublimation growth (PASG) samples has shown to be strongly influenced by substrate steps [2]. In this study, we grow ZLG samples using resistive heating under UHV conditions on 6H-SiC. Compared to PASG, AFM and KPFM reveal a weakness of UHV growth for producing high quality ZLG samples, namely a generally disorder structure and depressions within the terraces. This type of defects disappears at higher temperatures. After ZLG growth and verification, Sn is deposited. We focus specifically on the influence of sample temperature (120-1000 K) during deposition. These are analyzed using AFM and KPFM. [1] Ghosal et al, Phys. Rev. B 111, 235426, 2025 [2] Harling et al, Carbon 244, 120711, 2025

O 73.5 Wed 18:00 P2

Ca-intercalation of epitaxial monolayer graphene — Luqman Mahdi Syed[1,2], Niclas Tilgner[1,2], •Philip Schädlich[1,2], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Technische Universität Chemnitz

Realizing proximity-induced correlation effects, such as superconductivity, in graphene is a major challenge in the field of research on two-dimensional (2D) materials. Among the graphite intercalation compounds (GICs), the Ca-GICs exhibit the highest critical temperature with T_c=11.5 K, where the electron doping from the Ca atoms may be a crucial factor. Hence, expanding this superconducting phase into the 2D limit of epitaxial monolayer graphene (EMLG) on SiC(0001) requires precise control over the arrangement of the intercalated Ca atoms. However, several structural models have been proposed for Ca-intercalated EMLG, and in particular, the vertical position - i.e., the gallery - in which Ca resides remains unresolved (S. Ichinokura et al. 2016 ACS Nano 10 2761, J.C. Kotsakidis et al. 2020 Chem. Mater. 32 (15) 6464). Here, we investigate Ca-intercalation into EMLG grown by polymer-assisted sublimation growth. Using x-ray and angle-resolved photoemission spectroscopy, we monitor the intercalation process and quantify the doping level. Our results indicate the saturation of the SiC interface by Ca. We observe the low-energy bands of the resulting intercalated bilayer graphene, and more interstingly regarding the superconducting state, a highly doped graphene π-band, which may point towards the presence of calcium in the upper gallery.

O 73.6 Wed 18:00 P2

Porphyrin derivatives on Graphene/Cu(111) — •Asma Khizar, Christophe Nacci, and Leonhard Grill — Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Molecules as well as their assemblies and reactions have been widely investigated on single-crystal metal samples, which represent a highly defined flat support for efficient diffusion and high-resolution imaging by scanning probe microscopy (STM). However, the interaction between the metal and the molecule can alter the intrinsic properties of the molecules, making a decoupling layer essential to understand the pristine molecular properties. Graphene, with its two-dimensional structure and weak interaction with adsorbates, serves as an excellent decoupling layer for molecules. On epitaxial graphene, the reduced molecule-metal interaction allows molecules to retain their intrinsic electronic features while still sensing the underlying metal, which influences adsorption energy and selective interactions. In this study, we use Cu(111) as a substrate for graphene growth, due to its cleanliness and minimal lattice mismatch. Our focus is on chemical reactions of porphyrin derivatives on the graphene layer, thus at a distance from the copper catalyst. Various stimuli are used to controllably dissociate side groups from the molecules and induce covalent coupling to get better insight into the chemical reactions.

O 74: Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 74.1 Wed 18:00 P2

Strong-Field Bloch Electron Interferometry for Band-Structure Retrieval — •Tamara Pröbster, Tobias Weitz, Christian Heide, and Peter Hommelhoff — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Physik, Staudtstr. 1, 91058 Erlangen

Strong optical fields drive electrons in solids far from equilibrium, enabling access to ultrafast quantum dynamics that directly reflect the underlying band structure. When Bloch electrons in graphene are exposed to an intense few-cycle laser field, they undergo coherent intraband motion during which they accumulate a quantum phase determined by the local band curvature. If this laser-driven trajectory encounters an avoided crossing between the valence and conduction bands, the electron wave packet can coherently split via a Landau-Zener transition. In our work, we exploit pairs of such transitions to realize strong-field Bloch electron interferometry, forming an interferometric sequence fully embedded in the electronic band structure. The resulting interference encodes band information in the phase-dependent photocurrent. We retrieve the Fermi velocity of graphene near the K points as 1.07 ± 0.04 nm·fs^{-1}, in excellent agreement with theoretical expectations. Our results establish strong-field Bloch electron interferometry as a general and versatile approach for band-structure reconstruction under ambient conditions. Because the method relies solely on ultrafast optical driving and detection, it is naturally suited for tracking light-induced modifications of electronic structure with femtosecond temporal resolution.

O 74.2 Wed 18:00 P2

Folding the electronic band structure of graphene-Bi and graphene-Pb heterobilayers — •Johanna Schurr, Alexander Korn, Andres Unigarro, Sibylle Gemming, and Nebahat Bulut — Institute of Physics, TU Chemnitz, Germany

Translational and rotational degrees of freedom in 2D material stacks open up a wealth of tunable materials properties, such as electrical conductivity, magnetism, or optical properties, in particular if heavy intercalant atoms are present. In this study, the band structure of the two hexagonal hetero-bilayer systems bismuthene-graphene and plumbene-graphene were investigated, because experiment gives evidence for a large number of structural varieties especially for plumbene.

The aim was to identify and characterise the influence of bismuthene and plumbene layers on the band structure of graphene. For this purpose a code was generated to correlate the k-path of the band structures calculated for supercells and primitive cells within their respective Brillouin zones. Subsequent folding back of the bands into the first Brillouin zone of the supercell, while maintaining the information of the original k-path in the primitive cell, provided an overview of all existing bands and the origin of their Brillouin zone.

O 74.3 Wed 18:00 P2

A tool for folding and unfolding of electronic band structures applying it to graphene and the gold(111)-surface — •Alexander Korn, Nebahat Bulut, and Sibylle Gemming — Institute of Physics, TU Chemnitz, Germany

The electronic band structure is an important property of materials. For comparison with experiments and other studies, as well as for better readability, it is useful to display and analyse the band structure of the primitive cell rather than a supercell. Studying more complex materials with dopants or adatoms is only possible using a supercell instead. Therefore, one must unfold the band structure of the supercell into the primitive cell.

For this purpose, we offer a tool for abinit (www.abinit.org) that can be used to unfold all possible supercells. The unit vectors of the supercell can be stretched and also rotated relative to the unit vectors of the primitive cell. We also offer an additional qualitative tool for band folding that also tracks the origin of the Brillouin zone of each band at each k-point. We provide a practical example of folding and unfolding using the gold(111) surface with sulfur as an adatom.

O 74.4 Wed 18:00 P2

Enhanced Screening in Indium Intercalated Graphene Enabled by 2D Nearly Free Electron States — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Stefan Enzner[2,3], Martin Kamp[1,4], Timur Kim[5], Giorgio Sangiovanni[2,3], Jörg Schäfer[1,2], Simon Moser[6], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [4]Röntgen Center for Complex Material Systems, Würzburg, Germany — [5]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom — [6]Experimentalphysik IV - AG Oberflächen, Ruhr-Universität Bochum, Germany

Intercalation of epitaxial graphene on SiC has been intensively explored to modify graphene's electronic properties, but previous intercalants provide only weak screening, leading to pronounced electron-plasmon coupling and the appearance of plasmaron bands in ARPES [1]. Here, we demonstrate that intercalated bilayer indium exhibits strongly Rashba-split bands, which acquire nearly free-electron-like character at the Fermi level. This induces exceptionally strong screening in graphene, significantly reducing many-body renormalization effects in the graphene bands, which arise from plasmaron coupling. This approach opens new opportunities to explore and control many-body interactions in graphene-based heterostructures.
[1] Bostwick A et al., Nat. Phys. 3, 36-40 (2007)

O 74.5 Wed 18:00 P2

Terbium intercalation as a route to n-doping of graphene past the van Hove singularity — •Bharti Matta[1], Philipp Rosenzweig[1], Craig Polley[2], Kathrin Küster[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]MAX IV Laboratory, Lund, Sweden

Exotic ground states driven by many-body interactions, such as unconventional chiral superconductivity and spin-density waves, were theoretically predicted more than a decade ago for heavily n-doped graphene near the van Hove singularity (VHS). In recent years, achieving such high doping levels in epitaxial graphene on SiC via intercalation has attracted considerable interest. Intercalation of rare-earth elements such as Gd, Yb, and Er has already proven promising in reaching these regimes. Here, we demonstrate that intercalation of Tb atoms at the graphene/SiC interface provides access to extreme n-doping levels beyond the π^* VHS, without requiring any adsorbates on the graphene surface. The extended VHS is shifted by 0.07 eV below the Fermi level (E_F) as seen in angle-resolved photoemission spectroscopy. From the area enclosed by the giant hole pocket around Γ, we extract an electron density of $\approx 5 \times 10^{14}$ cm^{-2}. Strong renormalization of the graphene bands leads to a Dirac point about 1.55 eV below E_F, indicating that the doping cannot be described by a rigid single-particle band shift. Based on these experimental parameters, theoretical calculations predict the emergence of topological superconductivity with a critical temperature up to 600 mK (S. A. Herrera *et al.*, *ACS Nano 18* (51), 34842–34857 (2024)).

O 74.6 Wed 18:00 P2

Vanishing Fermi velocity in Periodically Strained Graphene — •Leo-Malik Benneka[1], Taher Rhouma[2], Guy Trambly de Laissardière[2], Clemens Winkelmann[1], Mark Zelsmann[3], and Vincent Renard[1] — [1]Université Grenoble Alpes, CEA-IRIG-PHELIQS, 38000 Grenoble, France — [2]CNRS-LPTM, CY Cergy Paris Université, 95302 Cergy-Pontoise, France — [3]CNRS-LTM, 38000 Grenoble, France

Intense research has been made in engineering flat bands in twisted bilayer graphene, leading to various correlated phases [1]. An alternative route to realizing similar flat bands involves a monolayer graphene strained by a periodic triangular superlattice induced by a corrugated substrate. The height modulation h and the superlattice periodicity L serve as tuning parameters for controlling band flattening and the Fermi velocity v_F near the Dirac cones [2, 3]. Tight-binding calculations were performed by explicitly accounting for relative rotations between the graphene lattice and the superlattice, as would occur in an experimental device. These calculations not only reproduce the known decrease of the Fermi velocity with increasing h [4], but also reveal a renormalization of v_F that depends on the specific ratio $\sqrt{a_C C\, L}/h$ and on the relative lattice orientation. Remarkably, this behavior is universal for any superlattice size L. These predictions may assist in the design of experimental devices aimed at engineering flat bands. [1] Cao et al., Nature, 556 (2018) 43-50 ; [2] Mao et al., Nature, 7820 (2020) 215-220 ; [3] Yuan et al., Phys. Rev. B, 24 (2024) 245408 ; [4] S. P. Milovanović et al., Phys. Rev. B, 24 (2020) 245427.

O 74.7 Wed 18:00 P2

Optimizing the excitation cross section for graphene phonons in inelastic electron tunnelling via intercalation. — Karl Rothe[1], •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

Platinum-intercalated graphene on a (111)-oriented iridium surface gives rise to a variety of rotational domains, which exhibit characteristic moiré patterns. Independent of the twist angle subtended by the graphene and substrate lattice, inelastic electron tunnelling spectroscopy reveals elevated graphene phonon excitation only on the intercalated phases. Combining spatially resolved spectroscopy of the electronic structure with non-equilibrium Green's function simulations highlights the relevance for effective phonon creation of the balance between elastic and inelastic electron transport. The intercalation-induced shift of electron density of states from the Brillouin zone centre to its boundary enhances the inelastic channel at the expense of the elastic channel and thereby increases the phonon excitation cross section. Financial support by the Deutsche Forschungsgemeinschaft through KR 2912/18-1 is acknowledged.

O 74.8 Wed 18:00 P2

Se-intercalation of graphene on SiC(0001) — •Susanne Wolff[1,2] and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Technische Universität Chemnitz

The epitaxial growth of graphene on SiC in an argon atmosphere is a well-established method to produce homogeneous, high quality carbon layers. The first-grown carbon layer exhibits a $\left(6\sqrt{3}\times 6\sqrt{3}\right)R30^\circ$ periodicity and is partially covalently bound to the SiC substrate. Therefore, this so-called buffer layer lacks the typical electronic properties of graphene. One pathway to decouple the buffer layer from the substrate and obtain graphene-like electronic properties is intercalation, which involves introducing a certain element at the buffer layer/SiC interface. Furthermore, the choice of intercalant influences the electronic properties of the decoupled graphene.

In this study, we investigated the intercalation of a buffer layer with selenium (Se). This process was carried out in a two-zone tube furnace, with the selenium precursor SnSe$_2$ and the buffer layer positioned in different temperature zones. The samples were characterized using X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). XPS revealed successful decoupling of the buffer layer with intercalated Se at the interface and not-intercalated Se on the surface. ARPES measurements in the vicinity of the Dirac point of graphene showed a p-type doping of the decoupled carbon layer.

O 74.9 Wed 18:00 P2

Mesoscopic Lateral Intercalation Dynamics of Indium Between the Epitaxial Zero-Layer of Graphene and SiC — •Benno Harling[1], Zamin Mamiyev[2], Narmina Balayeva[2], Dietrich R.T. Zahn[2], Christoph Tegenkamp[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077, Göttingen, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Str. 70, 09126, Chemnitz, Germany

Intercalation, the process of diffusing a material species in-between layered materials, can be utilized for both bulk and 2D systems to achieve tailored electronic properties. [1] For the 2D limit, this work investigates the lateral diffusion dynamics of indium intercalation into the epitaxial zero-layer of graphene on SiC using Kelvin Probe Force Microscopy (KPFM). For tin, material transfer across surface substrate steps is observed at local sites at the mesoscopic scale. [2] With the used experimental parameters, we find that this is not the case for indium intercalation. Instead, only terrace transport is observed. The KPFM measurements were complemented by micro-Raman spectroscopy, assessing the extent and uniformity of In intercalation. Remarkably, intercalation through the carbon layer seems to be dependent on the graphene or substrate properties that still need to be further resolved. This leads to a situation where just some of the terraces are observed to be intercalated. Financial support by the DFG within Research Unit FOR5242 is acknowledged. [1] Stark et al., Adv. Mater. 2019, 31, 1808213 [2] Harling et al., Carbon 244 (2025) 120711

O 75: Topical Talk Bibes (joint session O/TT)

Time: Thursday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 75.1 Thu 9:30 TRE/PHYS

Oxide interfaces as platforms for emergent quantum phenomena — •Manuel Bibes — Laboratoire Albert Fert, CNRS, Thales, U. Paris-Saclay, Palaiseau (France)

Oxide surfaces and heterointerfaces host electronic phases that emerge from the combined effects of broken inversion symmetry, orbital reconstruction, and electrostatic boundary conditions. In this overview, I will discuss how two-dimensional electron gases (2DEGs) formed at oxide surfaces and interfaces give rise to large and tunable spin-orbit interactions, interfacial magnetism, and ferroic control of transport properties.

The focus will be on Rashba-type spin-orbit coupling in oxide 2DEGs and its interplay with ferromagnetism and ferroelectricity, leading to effects such as electrically tunable Anomalous Hall effect, spin and orbital Edelstein effects, and spontaneous non-reciprocal charge transport. Angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy (XPS) play a central role in elucidating the electronic structure, orbital character, and electrostatic landscape underlying these phenomena, and in establishing clear links between interface chemistry, symmetry breaking, and transport behavior.

Finally, I will discuss how these engineering 2DEGs enables new routes toward low-power spin-orbitronic and ferroelectric device concepts compatible with silicon technology. The talk will highlight open challenges and opportunities at the interface between surface science, correlated electron physics, and oxide electronics.

O 76: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Thursday 10:30–12:15 Location: HSZ/0201

O 76.1 Thu 10:30 HSZ/0201

Angle-resolved photoemission spectroscopy study on AgTe/Ag/Au(111) heterostructures. — •Muthu P. T. Masilamani, Sophia Munne, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimental Physics VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

We report a comprehensive angle-resolved photoemission spectroscopy (ARPES) study on the electronic band structure of AgTe/Ag/Au(111) heterostructures. We systematically explore the interplay between Rashba-like spin-split surface states (SS) of AgTe [1] and quantum well states (QWS) of Ag/Au(111) [2] by epitaxially varying the Te coverage and the Ag spacer-layer thickness. This allows us to address the influence of epitaxial composition on the electronic structure. Our measurements reveal decoupling of the Rashba-like SS and QWS, with no observable hybridisation, attributed to their distinct orbital symmetries. Furthermore, we investigate the emergence of moiré reconstruction in the AgTe/Ag/Au(111) heterosystem.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020)

[2] Forster, F. et al. PRB. 84, 075412 (2011)

O 76.2 Thu 10:45 HSZ/0201

One-step investigation of the electronic tapestry of 2H-WSe2 — •Ridha Eddhib[1], Samuel Beaulieu[2], Aki Pulkkinen[1], and Jan Minar[1] — [1]New Technologies Research Centre, University of West Bohemia, 301 00 Pilsen, Czechia — [2]Université de Bordeaux-CNRS-CEA, CELIA, UMR5107, F33405 Talence, France.

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool for unraveling the electronic band structure of crystalline solids. However, the intricate and multifaceted electronic structures of complex materials often require complementary measurement strategies and careful experimental design. In our research, we employed the one-step model of photoemission, as implemented in the SPRKKR code[1], supported by experimental studies. We combined circular dichroism in photoelectron angular distributions (CDAD) with the layer-dependent symmetry properties of 2H-WSe2, which enables a time-reversal operation (TRCDAD)[2]. This approach quantifies the modulation of photoemission intensity across a wide energy range, providing detailed insight into the material's fine electronic structure while suppressing extrinsic contributions to the photoemission cross section to some extent. We present the monolayer, bilayer, and trilayer contributions to the photocurrent alongside the bulk response, while accounting for final-state effects using both time-reversed low-energy electron diffraction and a free-electron-gas final-state. [1]Ebert, H., Koedderitzsch, D., & Minar, J. (2011). Reports on Progress in Physics, 74(9), 096501. [2]Beaulieu, S., Schusser, ... & Ernstorfer, R. (2020). Physical Review Letters, 125(21), 216404.

O 76.3 Thu 11:00 HSZ/0201

Spin-orbital signatures and topological evolution in the $Mo_x W_{1-x} Te_2$ alloy — •Sarath Sasi[1], Aki Pulkkinen[1], Raphaël Salazar[1], Jakub Schusser[1], Laurent Nicolaï[1], Christine Ritcher[2,3], and Karol Hricovini[2,3] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

We examine how compositional disorder modifies the electronic structure of the transition-metal dichalcogenide alloy $Mo_x W_{1-x} Te_2$[1], with particular attention to the evolution of band topology and the persistence of Type-II Weyl features. Using high-resolution spin-polarized ARPES and circular-dichroism ARPES provides complementary insights into the spin and orbital character of the electronic states. These measurements give insight into its intrinsic spin-orbital properties compared to WTe_2[2], and for identifying how alloying is affecting its properties, like Berry curvature. Together with fully relativistic one-step photoemission calculations within the SPR-KKR[3] framework, we yield a detailed picture of how alloying tunes the electronic structure and topological responses in this family of quantum materials.

[1] Belopolski, I., Sanchez, D., Ishida, Y., et al. Nat. Commun. 7, 13643 (2016).

[2] Heider, T., Bihlmayer, G., Schusser, J., et al. Phys. Rev. Lett. 130, 146401 (2023).

[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 76.4 Thu 11:15 HSZ/0201

electronic properties observation of kagome lattice Nb3X8 by angle-resolved photoemission spectroscopy

— •Xiaojing Liu[1], Antonija Grubisic-cabo[1], Joost aretz Aretz[2], Sergii Grytsiuk[2], Marco Bianchi[3], Malte Rosner[2,4], Mazhar Ali[5], Philip Hofmann[3], Zhiying Dan[1], Giovanna Feraco[1], Chrystalla Knekna[1,6], Muhammad Waseem[1], and Mikhail Katsnelson[2,7] — [1]University of Groningen, Groningen, The Netherlands — [2]Radboud University, Nijmegen, The Netherlands — [3]Aarhus University, Aarhus, Denmark — [4]Bielefeld University, Bielefeld, Germany — [5]Delft University of Technology, Delft, the Netherlands — [6]University of Amsterdam, Amsterdam, The Netherlands — [7]Constructor University, Bremen, Germany

The Nb3X8 family (X=Cl, Br, I) is a novel group of breathing kagome materials. Despite interest in these materials, their electronic properties are still unclear and are likely to differ among the family members. For instance, they could exhibit characteristics of either a strongly correlated Mott insulator or a weakly correlated obstructed atomic insulator. Moreover, the kagome lattice can naturally host flat bands, which give rise to exotic properties such as spin-liquids and high-temperature superconductivity. Here, I will present our recent experimental investigation of the band structure in bulk Nb3X8 kagome materials by means of angle-resolved photoemission spectroscopy (ARPES). With ARPES we directly image the flat bands in the Nb3X8 systems, and are able to verify their strong correlation character with the support of theoretical calculations.

O 76.5 Thu 11:30 HSZ/0201

Studying the polar surfaces of MAX and MAB phases using μ-ARPES

— •Gesa Siemann[1], Gianmarco Gatti[1], Amalie Svaneborg[5], Wu Bing[4], Anders S. Mortensen[1], Charlotte Sanders[2], Naina Kushwaha[2,6], Jenny Rigden[2], Yu Zhang[2], Matthew D. Watson[3], Kristian Thygesen[5], Zdeněk Sofer[4], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]Diamond Light Source, UK — [4]University of Chemistry and Technology Prague, CZE — [5]Department of Physics, Technical University of Denmark, Lyngby, DK — [6]School of Physics and Astronomy, St Andrews University, UK

Natural heterostructures with interlayer charge transfer in the bulk can exhibit distinctive surface effects when this transfer is interrupted, such as Rashba splitting and itinerant ferromagnetism, both absent in the bulk. These layered systems therefore provide a platform to study how charge redistribution and symmetry breaking shape the emerging surface electronic structure. Here, we introduce MAX and MAB phases as a promising material family to host similar effects due to their alternating MX and A layers. After cleaving the samples, we used photoemission experiments with a micrometer-scale light spot (μ-ARPES), allowing us to reliably distinguish different surface terminations and their electronic structures. This work furthermore explores how covalency and metallicity govern charge transfer, and thus the surface electronic properties, in layered compounds.

O 76.6 Thu 11:45 HSZ/0201

Spin-resolved momentum microscopy of BiX_2 surface alloys on Cu(111) and Ag(111) using a 2D imaging spin-filter

— •Fabian Göhler, Stefanie Suzanne Brinkman, Xin Liang Tan, Anders Christian Mathisen, Chul-Hee Min, and Hendrik Bentmann — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Despite the rapid development of angle-resolved photoelectron spectroscopy (ARPES), measurements of the electron spin over wide regions in momentum space remain challenging with single-channel spin detectors. In this contribution, we present spin-resolved ARPES measurements from a momentum microscope, which gives the photoelectron momentum distribution over the full half-sphere above the sample surface. When combined with a 2D imaging spin filter [1], this allows parallel measurement of the in-plane spin polarization for full constant energy cuts $E(k_x, k_y)$. We acquired data on BiX_2/X(111) surface alloys - formed by 1/3 monolayer of Bi atoms arranged in a $(\sqrt{3} \times \sqrt{3})R30^\circ$ periodicity on Cu(111) or Ag(111) - which are well established model systems for spin-orbit effects and (spin-dependent) photoemission from surfaces [2-4]. Using linearly polarized ($h\nu = 6.0\,\mathrm{eV}$) and unpolarized ($h\nu = 21.2\,\mathrm{eV}$) light sources, we probe the spin polarization in these systems for varying experimental conditions.

[1] C. Tusche et al., Ultramicroscopy 159, 520 (2015)

[2] R. Noguchi et al., Phys. Rev. B 95, 041111 (2017)

[3] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017)

[4] A. Winkelmann et al., New J. Phys. 14, 083027 (2012)

O 76.7 Thu 12:00 HSZ/0201

Distinguishing bulk vs surface states from designed cleaving planes in ruthenium dioxide with ARPES

— •Maria Visscher[1,2], Lea Richter[1], Sebastian Buchberger[2], Shu Mo[2], Bruno Saika[2], Mats Leandersson[3], Craig Polley[3], Andrew Mackenzie[1,2], and Phil King[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St Andrews, St Andrews, UK — [3]Max IV, Lund, Sweden

Ruthenium dioxide has a rich band structure, giving rise to phenomena like superconductivity under strain and hosting a Dirac nodal line network. Recent studies also found that the material hosts flat band surface states and unusual spin-polarisations. These phenomena motivate the need for more detailed studies into its electronic structure. ARPES would be an ideal probe for this, and there have been several pioneering studies to date. However, the material's strongly three-dimensional structure makes these experiments challenging because of difficulties both in preparing the required atomically flat and clean surfaces, and in disentangling bulk from surface states in the electronic structure. Here, we exploit a fabrication method based on Focused Ion Beam (FIB) structuring to stimulate cleaving along desired crystallographic planes. With this method, we obtained high quality surfaces in two distinct orientations, allowing high-resolution ARPES experiments. From this, and supporting density-functional calculations, we identify a rich hierarchy of bulk and surface states in this system and uncover a strong influence of structural relaxations and surface stoichiometry on the electronic states that form.

O 77: Nanostructures at surfaces:1D, 2D, networks II

Time: Thursday 10:30–12:15 Location: HSZ/0204

O 77.1 Thu 10:30 HSZ/0204

Interplay of flexibility, coverage, and host-guest interaction in the self-assembly of Tris(4-carboxyphenyl)amine (TCA) on Au(111) — Vishakya Jayalatharachchi[1], •Paul Philip Schmidt[1], Roberto Robles[2], Nicolas Lorente[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]University of Applied Sciences of the Grisons, Switzerland

Triphenylamine derivatives are attractive building blocks for molecular architectures owing to their strong electron-donating properties, structural versatility, and ability to form highly ordered structures. Here, we explore how the non-planar and conformationally flexible arms of the unbridged threefold-symmetric TCA influence its self-assembly on Au(111), with particular emphasis on the formation and stability of porous networks. Using a combination of STM, LEED, and DFT, we show that RT deposition of TCA on Au(111) produces a coexistence of hexagonal porous domains and close-packed structures. Upon subsequent annealing, well-ordered porous networks emerge, stabilized by the dimeric carboxylic acid bonding motif. At higher coverage, this motif persists but instead directs the formation of close-packed assemblies. These findings provide insights into the interplay between molecular flexibility, intermolecular interactions, and coverage in directing supramolecular architectures of unbridged triphenylamines on metal surfaces. In addition, we show on the example of molecular rotors the hosting properties of the porous TCA network.

O 77.2 Thu 10:45 HSZ/0204

Revealing and manipulating correlated protons in one-dimensional hydrogen-bonded chains at the atomic scale — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Hydrogen-bonded systems such as water and ice exemplify highly cooperative proton dynamics, where covalent bonds are broken and formed in a concerted fashion. Yet directly probing and controlling many-body proton configurations at the atomic scale remains challenging. Here, using bond-resolved atomic force microscopy and spectroscopy, we reveal multistate proton ordering in self-assembled one-dimensional chains of an imidazole derivative on a noble metal surface. In as-grown chains of varying length, we consistently identify an interior species bonded to an extra proton, forming a localized imidazolium cation (state 1). Selective removal of a single proton from either chain end triggers a collective rearrangement of protons, yielding unidirectional hydrogen-bonding along the entire chain (states 2 or 3). Further deprotonation creates a proton vacancy, enabling reversible switching of hydrogen-bonding directionality (states 4 and 5) via collective proton hopping above a threshold bias voltage. In conjunction with density functional theory calculations, we elucidate the microscopic origin of complex proton ordering in hydrogen-bonded chains and the correlated motion of multiple protons.

O 77.3 Thu 11:00 HSZ/0204

On-Surface Synthesis of a Janus Polyazaacene — •Faming Kang, Tim Naumann, Zilin Ruan, Ye Liu, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Str. 4, 35032 Marburg, Germany

Acenes are a fascinating class of polycyclic aromatic hydrocarbons that have gained considerable research interest due to their potential application in organic electronics as well as their role in advancing fundamental knowledge about conjugated aromatic systems. Isosteric exchange of CH units of the acenes by nitrogen atoms formally gives azaacenes. The nitrogen substitution pattern, i.e., the number, position, and type of nitrogen atoms enables topological design of azaacenes, which facilitates precise tuning of frontier orbital energy level alignment and radical characters. Guided by topological considerations, introducing distinct edge structures on either side further creates Janus azaacenes. Here, we successfully synthesized a Janus polyazaacene on the Au(111) surface, in which one edge was decorated by nitrogen atoms while the other edge keeping unchanged. The length of such a polymer chain can reach up to 50 rings. Using scanning tunneling microscopy, we characterized its geometric structure and electronic property on Au(111), as well as its stability in air.

O 77.4 Thu 11:15 HSZ/0204

Modeling the Registry of Molecular Adsorbates on Solid Surfaces — •David Ari Hofmeister[1], Christian Erik Selzer[2], Laura zur Horst[1], Simon Christian Rickert[1], Julia Kohn[2], Andreas Hansen[2], Stefan-Sven Jester[1], and Sigurd Höger[1] — [1]Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn (Germany) — [2]Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn (Germany)

Rationalizing the adsorption behavior of large organic molecules on crystalline substrates is crucial for the design of functional surfaces in supramolecular chemistry, catalysis, and electronics. Conventional quantum-chemical approaches often fail for large π-conjugated systems due to their size and conformational flexibility. Here, we present a physically intuitive and generalizable method that overcomes these limitations by optimizing the molecular registry through a geometry-based strategy: maximizing the overlap between surface-oriented hydrogen atoms ("spikes") and the periodic "pockets" defined by the hexagon centers of HOPG. Inspired by the Groszek alkane-on-graphite model, our approach extends to structurally complex architectures and assigns adsorption geometries with high resolution without costly computations. Combining registry scoring with STM data allows the determination of absolute atropisomer conformations, demonstrating that geometric registry is a broadly applicable metric for predicting the surface arrangements of large molecules.

O 77.5 Thu 11:30 HSZ/0204

Low Dimensional Assemblies of Endohedral Fullerenes on Surfaces — •Lukas Emanuel Spree[1,2], Caroline Hommel[1,2], Pierre Josse[1,2], Justyna Piwowar[1,2], Robert Ranecki[1,2], and Andreas Heinrich[1,3] — [1]IBS Center for Quantum Nanoscience, Seoul, South Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul, Republic of Korea

Scanning probe microscopy techniques like STM and AFM facilitate the characterization of atoms and molecules on flat substrates with nearly unrivaled spatial resolution. Utilizing the strengths of these techniques, our team is looking to build custom molecular structures in a bottom-up manner and characterize their physical properties.

The main focus of this work is on endohedral fullerenes, a class of compounds that facilitate the stabilization of exotic configurations of few-atom structures within a carbon cage. Among them are some of the best single molecule magnets discovered to date, as well as promising candidates for spin-qubits. These desirable traits are combined with very high chemical stability. Utilizing the physical properties of these fascinating compounds is limited by two main issues: synthetic yield and, to a lesser degree, crystalline order. Both can be addressed elegantly by focusing on their properties in low dimensional arrangements, like monolayers or single molecules on ultraflat surfaces.

In this presentation we will detail our ongoing efforts of utilizing a broad range of deposition techniques, molecule manipulation on the surface, and chemical self-assembly approaches.

O 77.6 Thu 11:45 HSZ/0204

Electronic Modulation by the Sc3N Cluster in Endohedral Fullerene Sc3N@C80 — •Seong-Hyun Hong[1,4], Dmitriy Borodin[1,2], Lukas Spree[1,2], Andrés Pinar Solé[1,2], Caroline Hommel[1,2], Merve Ercelik[1,2], Shinjae Nam[1,2], Robert Ranecki[1,2], Fabio Donati[1,3], Se-Jong Kahng[4], and Andreas Heinrich[1,3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS) — [2]Ewha Womans University — [3]Department of Physics, Ewha Womans University — [4]Department of Physics, Korea University

Endohedral fullerenes such as Sc3N@C80 present a unique platform to study confined molecular systems, where the behavior of an enclosed cluster can strongly influence the properties of the surrounding cage. Understanding how the Sc3N cluster interacts with the carbon framework at the submolecular level is essential, but direct observation of these interactions remains challenging due to existence of carbon cage.

Here, we combine low-temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with a CO-functionalized tip to investigate Sc3N@C80. Using scanning tunneling spectroscopy

(STS) and Kelvin probe force microscopy (KPFM), we map the charge distribution across the fullerene with submolecular resolution, revealing how the Sc3N cluster modulates the electronic structure of the cage. This approach provides significant insight into the interplay between core position and molecular charge distribution, uncovering details of the inner cluster that were previously unclear.

O 77.7 Thu 12:00 HSZ/0204

Ferroelectric vortices in elemental Bismuth square islands — •Shasha Xue and Hao Zheng — Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China

Ferroelectric vortices, with their unique topological polarization patterns, show great potential for next-generation electronics. Although they have been observed in compounds, their realization in single-element materials has remained elusive. Here, we experimentally prepare three-bilayer Bi(110) square-shaped islands on high-T_C superconductor ($Bi_2Sr_2CaCu_2O_{8+\delta}$) substrates by molecular beam epitaxy. Scanning tunneling microscopy/spectroscopy combined with first-principal calculations verify in-plane polarization and a ferroelectric vortex state in our islands, as well as reveals exceptional vortex stability against electric-field-driven switching. This work pioneers single-element ferroelectric vortices, advances topological ferroelectrics design and expands the understanding in related fundamental physics.

O 78: Vacuum Science & Technology: Theory and Applications I

Time: Thursday 10:30–12:15 Location: HSZ/0401

Invited Talk O 78.1 Thu 10:30 HSZ/0401

The Wendelstein 7-X plasma vessel vacuum system from a scientific perspective — •Georg Schlisio[1], Torsten Bräuer[1], Stylianos Varoutis[1], Paul McNeely[1], Dirk Hartmann[1], Chandra Prakash Dhard[1], Dirk Naujoks[1], Victoria Hak[1], and the W7-X team[2] — [1]Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald — [2]See author list of O. Grulke et al. Nuclear Fusion, 64(11), 112002 (2024)

Wendelstein 7-X (W7-X) is the world's most advanced stellarator, a long-overlooked concept for magnetic confinement fusion. Fusion devices require excellent vacuum conditions to minimize impurity influx and charge-exchange losses during high-temperature plasma operation. The W7-X plasma vessel vacuum system comprises the main vessel, 254 vacuum ports, and several auxiliary diagnostic vacuum systems, the largest of which is the Neutral Beam Injection (NBI) system.

We describe the W7-X plasma vessel vacuum system and its instrumentation for total and partial pressure measurements. A key parameter for valve and gauge calibration, as well as for exhaust quantification, is the effective plasma-vessel volume; we outline an approach for determining this volume with sufficient precision. We also report experimentally derived pumping speeds of the turbomolecular pumps (TMPs) and cryo vacuum pumps (CVPs), which are essential inputs for modelling and exhaust analysis.

As an application of these capabilities, a recent study of gas-species transport in the sub-divertor region is shown, comparing experimental measurements with modelling results.

O 78.2 Thu 11:00 HSZ/0401

Pulsed Molecular Beam Reactive Scattering for Investigation of Surface Chemical Reactions — •Oleksandr Arsatiants, Tobias Hinke, Kevin Bertrang, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Molecular beam reactive scattering (MBRS) is a powerful technique for investigating surface reactions on defined surfaces in UHV, providing complementary results to single-cycle experiments like thermal desorption spectroscopy (TDS) [1]. Pulsed MBRS is especially promising, as it can be used to investigate surface reaction kinetics under quasi steady-state conditions [2-5]. For molecules with complex MS fragmentation patterns, however, the short time scales present a challenge due to mass switching delays. Ongoing work on automation of p-MBRS measurements for rapid mass switching will be presented.

[1] F. Zaera, Surf. Sci. Rep. 72 (2), 59-104 (2017).

[2] P. N. Brier, J. N. Fletcher and P. A. Gorry, Surf. Sci. 365 (2), 525-534 (1996).

[3] P. Bond, P. N. Brier, J. Fletcher, P. A. Gorry and M. E. Pemble, Chem. Phys. Lett. 208 (3-4), 269-275 (1993).

[4] P. Bond, P. N. Brier, J. Fletcher, W. J. Jia, H. Price and P. A. Gorry, Surf. Sci. 418 (1), 181-209 (1998).

[5] M. D. Rötzer, M. Krause, T. Hinke, K. Bertrang, F. F. Schweinberger, A. S. Crampton and U. Heiz, Phys. Chem. Chem. Phys. 26 (18), 13740-13750 (2024).

O 78.3 Thu 11:15 HSZ/0401

Advancing Ultra-Clean Deposition of Fragile Molecular Building Blocks via Electrospray-Based Controlled Ion Beam Deposition — •Andreas Walz[1,2], Annette Huettig[1,2], Michael Walz[1,2], Hartmut Schlichtung[1,2], Patrick Lawes[2], and Johannes V. Barth[2] — [1]pureions GmbH, Gilching, Germany — [2]Technical University of Munich, Physics E20, Garching, Germany

The fabrication of functional nanostructures from organic, inorganic, or bio-relevant molecular building blocks regularly requires clean and gentle deposition in vacuum. Conventional approaches such as thermal evaporation (MBE, OMBE) are restricted to volatile species, while solution-based deposition techniques offer versatility but frequently suffer from impurities.

Controlled Ion Beam Deposition (CIBD) in UHV, equipped with an electrospray ionization (ESI) source overcomes these limitations by granting access to a broad class of large, reactive, and fragile species including functionalized organic molecules, graphene nanoribbons, proteins, and DNA. Efficient ion transfer and mass selection is ensured through fully digitally driven ion guides and a digital quadrupole mass filter (dQMF) with ”virtually unlimited” mass range. Control over kinetic energy and dose allow for soft-landing or, when desired, reactive landing of the building blocks.

We present advances in ES-CIBD instrumentation and exemplary STM/AFM characterization of depositions. The technology provides a high degree of control during depositions, clean layers of mass selected molecules and access to otherwise low processability material.

O 78.4 Thu 11:30 HSZ/0401

Temperature-Programmed Spectroscopy: A Novel Tool for Kinetic and Mechanistic Studies for Processes on Surfaces — •Robert Bavisotto and Wilfred Tysoe — Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, Milwaukee, WI 53211, USA

Advances in computational chemistry have facilitated the integration of theoretical calculations to complement experimental findings. However, since computational methods depend on many approximations and variables, they require careful validation, which in the case of experimental validation can be challenging or unfeasible. For example, activation barriers are often predicted using climbing nudged elastic band calculations, whose benchmarking has traditionally relied on temperature-programmed desorption, a technique inherently sensitive only to processes that produce gas-phase products. To establish a surface-selective experimental approach capable of probing kinetic processes directly on surfaces without requiring gas-phase products, a suite of innovative spectroscopic techniques is introduced. These methods, collectively referred to as temperature-programmed spectroscopy (TPS), rely on precise control of sample conditions, enabling surface spectroscopic data to be collected quasi-continuously. These novel analytical tools can be easily combined with existing spectroscopic methods, such as IR or XPS, without the need for new capital equipment. This capability enables the detection of subtle changes over short time intervals, thereby facilitating kinetic measurements of surface-based processes that were previously unverifiable.

O 78.5 Thu 11:45 HSZ/0401

Traceable outgassing rate measurements of sticky gases — •Matthias Bernien[1], Annas bin Ali[1], Janez Šetina[2], and Karl Jousten[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Inštitut za kovinske materiale in tehnologije (IMT), Ljubljana, Slovenia

In the semiconductor industry, the outgassing of components in vacuum must be well controlled. These contaminants are monitored using quadrupole mass spectrometry. However, quantitative measurements of the amount of contamination are challenging as quadrupole mass spectrometers (QMSs) inherently lack stability of their sensitivity. To provide comparability and traceability of outgassing rate measurements, processes and transfer standards must be established. PTB together with IMT and industrial partners have developed and characterized outgassing reference samples for dodecane and water. These reference samples consist of a reservoir sealed with an elastomer through which the liquids permeate into vacuum. The reference samples provide well-defined outgassing rates that are used to calibrate QMSs in situ for water and hydrocarbon contaminants. When using sticky gases like water and dodecane, a significant amount of gas molecules adsorbs on the inner surfaces of the vacuum chamber. A numerical model is utilized to simulate the dynamics of the adsorbed phase and the gas phase.

O 78.6 Thu 12:00 HSZ/0401

A dynamic analysis of the static friction in microscopic Hertzian contacts: Size effects and 2D-material assisted superlubricity — •Ahmed Uluca[1,2], Pierce Sinnott[1,2], and Graham Cross[1,2] — [1]School of Physics, Trinity College Dublin, Dublin, Ireland — [2]CRANN, Trinity College Dublin, Dublin, Ireland

Friction governs how objects start to move, yet our understanding still relies on empirical laws that vary across materials and length scales. To build a more fundamental picture, we focus on the interfacial shear strength (ISS)-a concept adapted from fracture mechanics that describes friction in terms of shear stress over the contact area.

We developed a mesoscale dynamic analysis method capable of probing contact radii from tens of nanometers to micrometers with subnanometer displacement and 10-nanonewton force resolution. Starting from static contact, we gradually increase lateral oscillation amplitude while tracking contact radius and laterally stuck zone radius. This enables us to monitor the transition from sticking to sliding in real time while simultaneously measuring contact radius.

Using diamond-fused silica pairs, we map ISS across pressures from tens of MPa to several GPa and compare the results with theoretical models spanning from the Peierls (lattice) stress to the upper bound of a perfectly commensurate interface. Our findings reveal a pressure and scale dependent shear strength that is consistent with the dislocation emission models, extended to include the effects of deformation mode, nanoroughness, junction growth and interfacial modification by graphene layers.

O 79: Plasmonics and nanooptics: Light-matter interaction, spectroscopy III

Time: Thursday 10:30–12:15 Location: HSZ/0403

O 79.1 Thu 10:30 HSZ/0403

Cavity control of multiferroic order in the single-layer NiI_2 — •Chongxiao Fan[1,2], Emil Viñas Boström[1], Xinle Cheng[1], Lukas Grunwald[1], Dante Kennes[2], and Angel Rubio[1,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter — [2]Institute for Theory of Statistical Physics, RWTH Aachen University — [3]Initiative for Computational Catalysis, Flatiron Institute

Controlling materials in thermal equilibrium, through their interactions with quantum fluctuations of the electromagnetic field, is a promising new frontier in material engineering. Although recent experiments have demonstrated cavity effects in charge density wave, quantum Hall systems and superconducting systems, a smoking gun experiment is lacking for magnetic systems. To a large extent this comes from the focus on discontinuous phase transitions (e.g. from antiferro- to ferromagnetic), where a large light-matter coupling is required for cavity modifications to be observable. Here, we instead propose spiral magnets as a promising platform to explore cavity effects, where even a small cavity-mediated change in magnetic interactions is directly reflected in a change of the spiral wavelength. For concreteness we focus on the single-layer multiferroics NiI_2 and $NiBr_2$, with the surface phonon polaritons of the paraelectric substrate $SrTiO_3$ acting as the cavity. We show that the surface cavity suppresses the ratio J_3/J_1 of the third nearest and next nearest neighbor exchange interactions, leading to a increase of the spiral wavelength and the eventual transition into a ferromagnetic state. Our work proposes a realistic platform to observe cavity renormalization effects in magnetic systems.

O 79.2 Thu 10:45 HSZ/0403

Compressing few-cycle optical near fields in the tip-sample junction of a scanning probe microscope — •Sam S. Nochowitz, Tom Jehle, Juanmei Duan, and Christoph Lienau — Institute of Physics, University of Oldenburg, 26129 Germany

Plasmonic nanogaps confine light to dimensions in the nanometer or even sub-nanometer range while simultaneously enhancing the local electromagnetic field strength. This spatial confinement of light led to dramatic advances in nanosensing (1) and tip-enhanced Raman Spectroscopy. So far, the time dynamics of the fields emitted from such nanocavities have achieved little attention. Here, we introduce a broadband interferometric scattering-type SNOM technique to reconstruct amplitude and phase of light scattered from a sharp gold taper acting as a near-field probe. We isolate the near-field that is scattered from the apex and quantitatively measure its time structure (2). The apex field decays within 6 fs, a decay time mainly given by the radiative damping of the apex mode. Upon approaching the tip to a gold surface, the coupling of the apex field to its image dipole results in 2-fold reduction in the decay time to less than 2.7 fs, caused by phase shifts in the apex response, predicted in FDTD simulations (3). Our results pave the way towards linear and nonlinear ultrafast oscilloscopy with nm/fs resolution. (1) R. J. Chikkardy et al., Nature 535, 127 (2016); (2) T. Jehle, submitted (2025). (3) S. Thomas et al. New J. Phys. 17 (2015).

O 79.3 Thu 11:00 HSZ/0403

Symmetry Guidelines of Vacuum Cavity Material Engineering — •Jingkai Quan[1], Chongxiao Fan[1], Benshu Fan[1], I-Te Lu[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761, Hamburg, Germany — [2]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, New York City, New York, 10010, USA

Cavity material engineering, which manipulates material properties by exploiting vacuum-fluctuating photon modes in dark cavities, is a rapidly advancing field. Despite significant progress, most studies focus on isolated combinations of materials and cavity modes. In this study, based on a comprehensive group theory analysis, we develop a general framework for cavity material engineering with linearly polarized vacuum photon modes. We analyze the symmetry of the effective photon-free Hamiltonian inside dark cavities and establish a complete symmetry-breaking characterization induced by cavity photon modes across all 32 crystalline point groups. Building on this analysis, we predict phenomena such as the degeneracy lifting and emergence of new infrared and Raman spectral features induced by cavity modes. More intriguingly, we reveal a previously overlooked effect: cavity-induced polarization in non-polar crystals, and derive the corresponding tensor forms. These predictions are validated through advanced quantum-electrodynamical density-functional theory (QEDFT) calculations. Our work uncovers the fundamental symmetry principles governing light-matter interactions in the dark cavity and provides a systematic roadmap for future researches in cavity material engineering.

O 79.4 Thu 11:15 HSZ/0403

Low temperature near-field fingerprint spectroscopy of 2D electron systems in oxide heterostructures and beyond — Julian Barnett[1], Konstantin Wirth[1], Richard Hentrich[2], Yasin C. Durmaz[2], Felix Gunkel[3], Marc-Andre Rose[3], and •Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Attocube Systems AG, Munich — [3]PGI-7, Forschungszentrum Jülich

Scattering-type scanning near-field optical microscopy (s-SNOM) is a useful tool for the non-destructive investigation of buried confined electron systems with nanoscale resolution, however, a clear separation of carrier concentration and mobility was often not possible. Here, we predict a characteristic fingerprint response of the LaAlO3/SrTiO3 2DEG in the mid-infrared spectral range, which was not experimentally accessible in the past, and verify this using a state-of-the-art tunable narrow-band laser in cryo-s-SNOM at 8 K [1]. Our modeling allows us to separate the influence of carrier concentration and mobility on fingerprint spectra and to characterize 2DEG inhomogeneities on the nanoscale. We show that our fingerprint spectra are a universal feature and generally applicable to confined electron systems, like topological insulators or stacked van-der-Waals materials.

[1] J. Barnett et al., Nat. Comm. 16, 4417 (2025).

O 79.5 Thu 11:30 HSZ/0403

Tunable skyrmion, meron, and skyrmion bag topologies in surface phonon polariton lattices — •Julian Schwab[1], Florian Mangold[1], Bettina Frank[1], Timothy J. Davis[1,2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany — [2]School of Physics, University of Melbourne; Parkville Victoria 3010, Australia

Surface phonon polaritons (SPhPs) enable nanoscale manipulation of mid-infrared light via deeply subwavelength topological vector textures, such as skyrmions. Achieving dynamic, real-time control over these topological features remains challenging. Here, we theoretically propose and numerically demonstrate an actively tunable platform on a silicon carbide membrane that creates diverse topological lattices, including skyrmions, merons, and skyrmion bags. By exploiting the sublinear SPhP dispersion, we dynamically adjust the excitation wavelength to tune the topological character of the lattices. This allows for the tunability between bubble-type and Néel-type configurations in the electric field and the spin angular momentum. Furthermore, we identify a novel singularity-type meron arising from the interplay of electric and magnetic spin components. This texture exhibits topological charge conservation in moiré superlattices and a spatially confined spin reversal with tunable lateral sizes as low as $\lambda_{\text{SPhP}}/29$. These findings provide a versatile framework for on-chip, reconfigurable topological photonic devices with potential applications in high-resolution imaging and precision metrology.

O 79.6 Thu 11:45 HSZ/0403

Raman Studies of Proximity Effects in Epitaxial Graphene: Emphasis on Strong Light-Matter Coupling — •Zamin Mamiyev, Narmina O.Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Proximity engineering provides a route to tailor the electronic and vibrational properties of epitaxial graphene without introducing structural disorder. Because phonons and electronic states in graphene are strongly coupled, Raman spectroscopy provides a reliable approach to studying the quasiparticle dynamics and their modification in graphene.

In this work, we investigate how Sn and In intercalation, their nanoscale distributions, and the resulting interfacial reconstructions modify the phonon dynamics of quasi-free monolayer graphene on SiC(0001), particularly focusing on the plasmonically enhanced light-matter interaction regimes, such as in surface- (SERS) and tip- (TERS) enhanced Raman spectroscopies. Using resonance μ-Raman and TERS, we map the charge doping, electron-phonon coupling, and anharmonicities with high spectral and spatial resolution. Combined with electron diffraction, scanning tunneling microscopy (STM), and atomic force microscopy (AFM), our measurements allow us to study the optical fingerprints of strain, charge transfer, and symmetry-breaking that originate from distinct metal-intercalated interfaces and confined 2D metallic layers [1-2]. [1] Z. Mamiyev et.al., Adv. Optical. Mat. e00979 (2025); [2] Z. Mamiyev et.al., Carbon 234, 120002 (2025)

O 79.7 Thu 12:00 HSZ/0403

Inelastic electron-light interaction probed by holographic scanning transmission electron microscopy — •Tim Dauwe[1,2], Nora Bach[1,2], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Ultrafast Transmission Electron Microscopy (UTEM) is a unique tool to study inelastic electron-light scattering (IELS). Photon-Induced Near-Field Electron Microscopy (PINEM) can now routinely image optical fields at laser-excited nanostructures in magnitude. Phase-resolved imaging is enabled by sequential interactions [1,2]. However, this requires an elaborate geometry with multiple optical interaction stages and offers only limited variability in tailoring the interaction. In this work, we combine IELS with a STEM holography approach, using two spatially separated, coherent electron probes [3]. By recording the interference pattern in the far field behind an electron spectrometer, we get simultaneous access to the energy of the electrons and the phase imprinted during the inelastic interaction. Our results from two interfering quantum walks reveal exotic electron states governed by interaction strengths and relative phase differences. Our approach further enhances the UTEM near field imaging capabilites and enables tailoring of electron states by multiple parallel electron-light interactions.

[1] D. Nabben et al., Nature 619 (2023)

[2] J.H. Gaida et al., Nat. Photon. 18 (2024)

[3] F.S. Yasin et al., J. Phys. D: Appl. Phys. 51 205104 (2018)

O 80: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: TRE/PHYS

O 80.1 Thu 10:30 TRE/PHYS

Surface chemistry of silicate minerals at the atomic scale — Luca Lezuo[1], Andrea Conti[1], Alexander Hoheneder[1], Elena Vaníčková[2], Domitilla Aloi[1], Rainer Abart[3], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], and •Giada Franceschi[1] — [1]Inst. Appl. Phys., TU Wien, Austria — [2]CEITEC, Brno, Czechia — [3]Dept. Lithospheric Res., Uni Wien, Austria

Silicate minerals underpin key processes in geochemistry, atmospheric science, and materials technology, yet their atomic-scale surface chemistry remains insufficiently understood. Their intrinsic heterogeneity and electrical insulation have limited experimental characterization, leaving most mechanistic insight to simulations. Here, we extend the capabilities of noncontact atomic force microscopy (ncAFM) in ultrahigh vacuum to achieve atomic and chemical resolution on natural silicates such as muscovite mica,[1,2] feldspar microcline[3] and wollastonite.[4] Our measurements provide direct evidence for processes central to mineral reactivity, such as ion hydration, ice nucleation, and carbonation reactions. They demonstrate that ncAFM affords fundamental insights previously restricted to theory and offer benchmark data to guide and challenge emerging computational models of mineral-gas interactions.

[1]G.F. *et al.*, *Nat. Commun.* **14**, 208 (2023); [2]G.F. *et al.*, *Faraday Discuss.* **249**, 84 (2024); [3]G.F. *et al.*, *JPCL* **15**, 15 (2023); [4]Conti *et al.*, *submitted* (2025).

O 80.2 Thu 11:00 TRE/PHYS

First Principles Investigations of Energy Dissipation Processes during Atom-Surface Collisions — •Nils Hertl[1,2] and Reinhard J. Maurer[1,2,3] — [1]Department of Chemistry, University of Warwick, Coventry, UK — [2]Department of Physics, University of Warwick, Coventry, UK — [3]Department of Physics, University of Vienna, Vienna, Austria

H atom scattering experiments have emerged as a powerful tool for selectively probing the energy transfer mechanisms between adsorbate and surface, which are relevant for adsorption—the first elementary step in heterogeneous catalysis. This typically includes both phonon and electron excitation in the substrate. Yet, the latter is challenging to model with molecular dynamics because it requires simulation techniques that go beyond the Born-Oppenheimer approximation. In this talk, I will demonstrate how combining electronic structure theory, machine learning, and non-adiabatic molecular dynamics enables a quantitative study of energy transfer between H atoms and surfaces across diverse material classes. I will show that the computed energy loss spectra agree well with experimental findings, enabling detailed characterisation of individual energy transfer channels as well as processes that are experimentally inaccessible, such as adsorption. Based on these findings, I will present a conceptual framework that links adsorbate and surface electronic structure to the probability for non-adiabatic effects to occur in gas-surface collisions.

O 80.3 Thu 11:30 TRE/PHYS

Exchange-driven magnetoelastic coupling in a correlated itinerant ferromagnet — •Carolina A. Marques[1], Luke

C. Rhodes[1], Weronika Osmolska[1], Harry Lane[1], Izidor Benedičič[1], Masahiro Naritsuka[1], Siri A. Berge[1], Rosalba Fittipaldi[2], Mariateresa Lettieri[2], Antonio Vecchione[2], and Peter Wahl[1,3] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, UK — [2]CNR-SPIN, c/o Università di Salerno, Italy — [3]Physikalisches Institut, Universität Bonn, Germany

The electronic properties of materials are the result of the complex relationship between lattice and electronic degrees of freedom. In magnetic materials, exchange interactions leads to magnetoelastic coupling, whose effect can be enhanced by the presence of electronic correlations. In the itinerant ferromagnet $Sr_4Ru_3O_{10}$, its magnetic and electronic properties are strongly influenced by electron correlations driven by Van Hove singularities close to the Fermi level. Here, we detect changes to the electronic structure, magnetic ground state and lattice in $Sr_4Ru_3O_{10}$ using scanning tunneling microscopy and spectroscopy (STM/STS). By switching between ferromagnetic and antiferromagnetic alignment of the magnetization of the surface and subsurface layers, we study the impact of exchange interaction on the electronic structure and detect jumps in the interlayer spacing, revealing giant exchange magnetostriction in $Sr_4Ru_3O_{10}$. Our measurements reveal a direct link between exchange interaction, electronic and crystal structures, providing a platform to test theoretical descriptions of strongly correlated electron materials.

O 80.4 Thu 12:00 TRE/PHYS

Effect of atomic-scale defects on light-matter interaction in transition-metal dichalcogenides — •Vibhuti N. Rai, Junyoung Sim, Florian Faaber, Sergey Trishin, Nils Bogdanoff, Paul Wiechers, Caroline Firschke, Tom S. Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

Defects crucially affect the physical properties of (quasi-) two-dimensional materials, such as transition metal dichalcogenides (TMDCs). Here, by using THz scanning tunneling microscopy [1], we excite and detect long-range coherent in-plane shear and out-of-plane breathing modes on the surface of 2H-$MoTe_2$. We find that atomic-scale intrinsic defects influence their relative excitation efficiency. We attribute this response to local tip-induced band bending [2].

In the monolayer limit, where quantum confinement enhances defect sensitivity, we further show ultrafast charge modulation in defect sites of quasi-freestanding nanopatches of a monolayer MoS_2 on Au(111) driven by THz pulses. These insights into defect-mediated phonon excitation and charge transfer provide a pathway toward future ultrafast electronics.

[1] Cocker et al., Nature Photonics 7, 620-625 (2013)

[2] Rai et al. arXiv:2506.08219v2 (2025)

O 80.5 Thu 12:30 TRE/PHYS

Topological Dirac Quasiparticles Tailored by Moiré Engineering — •Maximilian Ünzelmann, Romana Ganser, Muthu Masilamani, Begmuhammet Geldiyev, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

Moiré heterostructures have become a promising platform for tailoring electronic states in a highly controllable manner. The emergent superlattice potential gives rise to band gaps in the folded moiré band structure, which lead to a quenching of kinetic energy and thus increase of electron-electron interactions. Emergent flat bands have been observed in nano-focused angle-resolved photoemission spectroscopy (ARPES) experiments and demonstrated to trigger correlation-driven phenomena. Here, we go beyond the mere creation of flat bands and demonstrate that surface moiré engineering allows transforming a 'simple' epitaxial monolayer-substrate heterostructure into topological Dirac matter. In particular, using ARPES experiments, we will (i) prove the existence of one-dimensional Dirac fermions in the moiré-driven band structure, (ii) show that those are robustly protected by the emergent superlattice symmetry, and (iii) demonstrate how the entire mini-band structure can be controlled by epitaxial manners and sample temperature. Overall, this expands the potential of moiré materials by shifting the focus from almost exclusively flat bands to the creation of new, highly controllable Dirac quasiparticles.

O 81: Catalysis and surface reactions II

Time: Thursday 10:30–12:15 Location: TRE/MATH

O 81.1 Thu 10:30 TRE/MATH

Pd/Cu single atom alloys for selective alcohol dehydrogenation: from single crystalline to nanostructured model catalysts — •Philipp Alexander Fredersdorff[1], Jan Smyczek[1], Carsten Schroeder[1], Paul Froehlich[1], Paul Kohlmorgen[1], Stephan Appelfeller[2], Konstantin Neyman[3], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, University Kiel, 24118 Kiel, Germany — [2]MAX IV Laboratory, Lund University, 22100 Lund, Sweden — [3]Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, Barcelona 08028, Spain

Single-atom alloy (SAA) catalysts offer atomic-level control of selectivity, yet structure reactivity relationships in realistic systems remain insufficiently understood. Here, we report the first preparation of well-defined Pd/Cu single-atom alloy nanoparticles under UHV on Al2O3/NiAl(110) and investigate their properties using IRAS CO titration, STM, and TPD. Temperature-dependent Pd de-aggregation shows the same behaviour as on Pd/Cu(111), with optimal incorporation at 550 K. Both de-aggregated materials catalyze the non-oxidative dehydrogenation of butanol, but only the nanostructured Pd/Cu-NP SAA achieves 100 percent selectivity, completely suppressing CO formation. A Pd-coverage-dependent analysis reveals that cluster formation rapidly decreases aldehyde selectivity on single-crystal Pd/Cu(111), whereas the newly developed nanostructured SAA catalysts maintain full selectivity across a wide Pd range.

O 81.2 Thu 10:45 TRE/MATH

Acetylene Cyclotrimerization to Aromatic Products on Coinage Metal Surfaces — Nipun T. S. K. Dewage[1], •Dennis Meier[1], Santu Biswas[2], Matthew M. Montemore[2], and E. Charles H. Sykes[1] — [1]Department of Chemistry, Tufts University, Medford, Massachusetts 02155, USA. — [2]Department of Chemical and Biomolecular Engineering, Tulane University, New Orleans, Louisiana 70118, USA.

Benzene and toluene are indispensable chemical feedstocks used in products ranging from pharmaceuticals to building materials. They are primarily produced through petroleum cracking and reforming, which require high energy input, severe operating conditions, and lack 100% selectivity. As the chemical industry transitions from oil to shale gas as its primary hydrocarbon feedstock, interest is growing in alternative routes to synthesize aromatics. One promising approach is the cyclotrimerization of acetylene, which uniquely yields benzene with 100% selectivity on Ag(111) in ultra-high vacuum. However, this reaction requires more than a monolayer of acetylene to initiate benzene formation, necessitating high pressures that may limit industrial viability. In this work, we investigate strategies to enhance the activity of this reaction on coinage metal surfaces.

O 81.3 Thu 11:00 TRE/MATH

Automated Workflow for Kinetic Modeling in Heterogeneous Catalysis: A Case Study of the Ammonia Oxidation Reaction — •Emanuel Colombi Manzi, Hyunwook Jung, Hendrik H. Heenen, Vanessa J. Bukas, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Developing reliable kinetic models in computational catalysis is a big challenge, especially when involving large reaction networks with complex intermediates. Atomistic models built upon first-principles energetics, typically density-functional theory (DFT), are widely used today for elucidating catalytic mechanisms and trends. The cost of DFT calculations, however, makes these models far too expensive to thoroughly sample the many structural configurations that are possible for all relevant surface-bound intermediates. As a result, assumptions on the preferred geometry or surface binding site are commonly adopted based on chemical intuition. Here, we present a fully automated workflow that derives an entire microkinetic model without any *a priori* knowledge or heuristics about the preferred binding configurations.

The approach is demonstrated on the kinetics of NH_3 oxidation over selected metal surfaces and alloys. Enabled by an efficient DFT-trained machine learned interatomic potential, an ensemble of low-energy adsorbate structures is identified through global optimization and all process barriers between them are systematically computed. Our simulations provide chemical insight beyond the limitations of standard DFT models and open the road for large-scale screening studies without the need of simplifying assumptions like scaling relations.

O 81.4 Thu 11:15 TRE/MATH

Adsorption of CO and CO_2 on MgO(100) single-crystal surfaces investigated by polarization-resolved IRRAS — •Wangtao Li, Zairan Yu, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institue of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

MgO, a low-cost alkaline metal oxide material, is widely used in heterogeneous catalysis. Comprehensive understanding of MgO-based catalysts requires reliable reference data from surface science studies on MgO model systems. Here, we present polarization-resolved reflection absorption spectroscopy (IRRAS) data obtained for CO and CO_2 adsorption on MgO(100) single-crystal surfaces using a sophisticated UHV apparatus (THEO). The low-temperature (67 K) and temperature-dependent IRRAS results provide deep insights into the interaction of CO and CO_2 with MgO(100). The p- and s-polarized IRRAS data enable detailed analysis of vibrational frequencies, adsorption configurations, and binding energies of different species bound to distinct surface sites including defects. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 426888090 - SFB 1441.

O 81.5 Thu 11:30 TRE/MATH

Experimental Modelling of Ti-based (Photo-)Catalysts for the Activation of Greenhouse Gasses — •Lars Mohrhusen — Carl von Ossietzky Universität Oldenburg, Germany

Sustainable catalysts are key materials for future energy technologies and the activation of greenhouse gasses via thermal and photocatalysis. To replace critical raw materials such as (noble) metals in (photo-)catalysts, we combine low-dimensional (semi-)metallic structures such as point defects or 2D materials with oxides to hybrid materials. Combined insights from spectroscopy, microscopy and reactivity studies on well-defined model systems under UHV or so-called operando conditions gains a comprehensive atomistic picture.[1−3]

Selected examples for such Ti-based materials relevant for solar photocatalysis will be presented. Therein, the activation of greenhouse gas molecules (esp. N_2O and CO_2) on Ti^{3+} and Ti^{2+} defects will be illuminated.[3,4] While such gases interact weakly with defective rutile TiO_2 in UHV, higher pressures of CO_2 combined with the presence of water as an H donor were found to enable a rich reduction chemistry along multiple parallel pathways in operando-XPS.[4] In addition to oxides, nanostructured 2D titanium disulphide (TiS_2) as well as conjugated organic polymers on metal and oxide surfaces represent potential candidates for photocatalytic applications.[5]

[1] L. Mohrhusen et al., J. Phys. Chem. C 2022, 126, 48, 20332. [2] L. Mohrhusen et al., Small 2024, 2405715. [3] L. Mohrhusen K. Al-Shamery, Catal. Lett. 2023, 153, 2, 321. [4] J. Klimek, et al. under review [5] N. Kruse et al. Small 2025, 38, e06023.

O 81.6 Thu 11:45 TRE/MATH

Studying low surface area photocatalysts at ambient pressure in a microreactor — •Paula Neumann[1], Clara Aletsee[2], Martin Tschurl[1], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]SurfCat Section for Surface Physics and Catalysis, Department of Physics, Technical University of Denmark, 2800 Kgs Lyngby, Denmark

While driving reactions with solar light is an ambitiously pursued goal, current approaches often suffer from low efficiencies due to missing knowledge about reaction dynamics on the catalysts surface. Here, the application of highly defined photocatalysts may allow deeper mechanistic insight but their low surface area imposes high demands on detection sensitivity for studying reactions at ambient conditions. Our gas-phase microreactor enables time-resolved investigation of planar photocatalysts by mass spectrometry in a well-defined reaction environment. Using the photo-oxidation of alcohols on a titania photocatalyst as a model system we show how reaction mechanisms first established in the ultra-high vacuum transfer to conditions of 1000 mbar. Disentangling the mechanistics of alcohol photochemistry might be a crucial step towards improving hydrogen formation as an important energy carrier as well as opening up pathways for the production of higher-value chemicals.

O 81.7 Thu 12:00 TRE/MATH

Model-Free Reconstruction of Local Kinetic Information on Catalytic Surfaces from Operando Profile Measurements — •Jinyi Zhou[1], Mishai Avila[2], Daniel Runge[3], Lukas Thum[4], Heinz Junkes[1], Michael Geske[2], Christian Merdon[3], Frank Rosowski[2,5], Karsten Reuter[1], Christoph Scheurer[1], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]BasCat - UniCat BASF JointLab, TU Berlin — [3]Weierstraß-Institut, Berlin — [4]Helmholtz-Zentrum Berlin — [5]BASF SE, Catalysis Research, Ludwigshafen, Germany

Operando characterization experiments are typically strongly affected by transport effects, which can cause strong local variations of reactivity and concentration on the catalytic surface. We present a framework that allows one to obtain this local kinetic information from a measured concentration profile away from the active surface, without assuming any specific kinetic model. Utilizing Green's functions of the transport operator and a function space formulation of the inverse problem, the approach allows robust reconstruction from finite, noisy data. We apply this approach to a compact profile reactor, where concentration is measured along the axis of a channel flow with catalyst deposited on the channel walls. Using synthetic data, we demonstrate that the approach has the potential to resolve sub-millimeter variations in surface reactivity with modest computational and experimental footprints. Additional challenges that need to be overcome in order to fully exploit this potential for high accuracy when using experimental data will be discussed.

O 82: Focus Session: Unoccupied States by Inverse Photoemission III

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Thursday 10:30–12:30 Location: WILL/A317

Invited Talk O 82.1 Thu 10:30 WILL/A317

Low-energy inverse photoelectron spectroscopy (LEIPS): probing unoccupied states and conduction band structure in functional materials — •Hiroyuki Yoshida — Chiba University, Chiba, Japan

We developed low-energy inverse photoelectron spectroscopy (LEIPS) in 2012 [1] to enable damage-free probing of functional materials such as organic semiconductors, polymers and hybrid perovskites. By reducing the incident electron energy below the damage threshold (about 5 eV), LEIPS allows damage-free measurements while simplifying operation and improving energy resolution. By incorporating an electron energy analyzer [2], we achieved an energy resolution of 98 meV. LEIPS enables determination of electron affinity with an uncertainty of 0.1 eV. These precise values provide access to key parameters including band gaps, exciton binding energies, polarization energies, and electron injection barriers. The technique has been commercialized, and more than 100 systems are now in operation worldwide. We further developed angle-resolved LEIPS (AR-LEIPS) [3], enabling for the first time direct observation of conduction band structure in organic semiconductors [4]. The measured band structures yield insight into electron-phonon coupling and polaron formation relevant to carrier transport. [1] Chem. Phys. Lett. 539-540, 180 (2012). [2] Rev. Sci. Instrum. 94, 043908 (2023). [3] Rev. Sci. Instrum. 94, 063903 (2023). [4] Nat. Mater. 21, 910 (2022).

Invited Talk O 82.2 Thu 11:00 WILL/A317

Enhanced Sensitivity in Low-Energy Inverse Photoemission Spectroscopy with an Off-Axis Parabolic Mirror for Efficient Light Collection — •Yongsup Park[1,2], Jong-Am Hong[1], Kyu-Myung Lee[1], and Min-Jae Maeng[1] — [1]Dept. of Physics, Kyung Hee University, Seoul, Republic of Korea — [2]Dept. of Information Display, Kyung Hee University, Seoul, Republic of Korea

Inverse photoemission spectroscopy (IPES) is a powerful tool for studying unoccupied electronic states but suffers from low sensitivity due to the low photon emission probability during free electron transitions. To improve sensitivity via better photon collection, an off-axis parabolic (OAP) mirror was designed and built for low-energy IPES (LEIPS). Optical simulations showed the OAP mirror raised photon collection efficiency from 3.06% to 63.3%, confirmed experimentally through LUMO spectra of C60 thin films. The OAP mirror-LEIPS system was applied to study energy level alignment (ELA) of pentacene films on substrates with different work functions (WF). By measuring HOMO and LUMO levels, the changes in transport gaps and the ELA with respect to the Fermi level were analyzed. Pentacene showed n-type behavior on low WF substrate (Cs2CO3) and p-type on high WF substrate (ITO). This OAP mirror-enhanced LEIPS system significantly shortened experiment times, enabling efficient and reliable measurements.

O 82.3 Thu 11:30 WILL/A317

Development of angle resolved low energy inverse photoelectron spectroscopy for conduction band structure measurements of functional materials — •yuki kashimoto[1], satoshi ideta[1], haruki sato[1], keita kawamura[1], hibiki orio[1], and hiroyuki yoshida[1,2] — [1]chiba university, chiba, japan — [2]chiba university MCRC, chiba, japan

Understanding the energy band structure is essential for clarifying charge-transport behavior in solids. Although angle-resolved inverse photoelectron spectroscopy (ARIPES) can measure conduction bands, it is unsuitable for emerging materials such as organic semiconductors due to their narrow bandwidths and electron irradiation damage. Low-energy inverse photoelectron spectroscopy (LEIPS)[1] overcame these issues by reducing the electron kinetic energy. In this study, we advanced LEIPS and enabled band-structure measurements by introducing angle-resolved detection. Stray electric and magnetic fields were suppressed, and a dedicated low angular spread, energy-scannable electron source was implemented. This enabled angle-resolved LEIPS (AR-LEIPS) with 0.23 eV energy resolution and 0.94 nm^{-1} momentum resolution[2]. Using AR-LEIPS, we determined the conduction band structure of pentacene, the first such measurement for an organic semiconductor[3] and revealed the conduction-band dispersion of the photovoltaic perovskite $CH_3NH_3PbI_3$. [1] H.Yoshida, Chem. Phys. Lett. 539-540, 180 (2012). [2]Y.Kashimoto, H.Yoshida et al, Rev. Sci. Instrum. 94, 063903 (2023) [3] H. Sato, H. Yoshida et al, Nature Mat. 21,910 (2022).

O 82.4 Thu 11:45 WILL/A317

Observation of conduction band structure of conductive polymer PBTTT — •Taichi Suruga[1], Shunichiro Ito[2], Taishi Takenobu[2], and Hiroyuki Yoshida[1,3] — [1]Chiba University, Chiba, Japan — [2]Nagoya University, Nagoya, Japan — [3]Chiba University MCRC, Chiba, Japan

The most fundamental information regarding the electron transport mechanism of these polymers is the conduction-band structure. However, until now, we did not have the appropriate methods to measure it. In 2020, we developed angle-resolved low-energy inverse photoelectron spectroscopy (ARLEIPS) [1] and successfully measured the conduction band structure of small-molecule organic semiconductors for the first time [2]. In this study, we applied ARLEIPS to a conductive polymer. Fabricating crystalline thin films with well-aligned molecular orientation is essential for the ARLEIPS measurement. We fabricated thin films using the blade-coating method [3]. Using ARLEIPS, we observed the conduction-band structure of a conductive polymer, PBTTT-C14 [4,5], in oriented films. As predicted by the DFT calculations, the bands split into two and exhibited large dispersion along the Γ-Z direction. These results demonstrate the first observation of conduction-band in a conductive polymer. [1] Y. Kashimoto, H. Yoshida et al., Rev. Sci. Instrum, 94, 043908 (2023) [2] H. Sato, H. Ishii, H. Yoshida et al., Nat. Mater. 21, 910 (2022). [3] D. Delongchamp et al., ACS Nano. 3, 780 (2009). [4] H. Tanaka, K. Kanahashi, T. Takenobu et al., Sci. Adv., 6, eaay8065 (2020) [5] S. Ito, H. Tanaka, T. Takenobu et al., Appl. Phys. Express 18, 021002 (2025)

O 82.5 Thu 12:00 WILL/A317

Effects of Crystallization on the Electronic Structure of Discrete Oligomers — •Alexander Ehm[1], Rukiya Matsidik[2], Michael Sommer[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics and Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Chemnitz, Germany — [2]Polymer Chemistry, TU Chemnitz, Chemnitz, Germany

Recently, organic photovoltaic cell efficiency surpassed the 20 % landmark, thanks to the development and improved crystallinity of non-fullerene acceptor (NFA) molecules and suitable polymer donors [1]. Low exciton binding energies (EBE), measured by the difference of the transport gap and the optical bandgap, were attributed as key factors in such improvements [2].

Photoemission and low-energy inverse photoemission spectroscopy (PES and LEIPES) in combination directly measure the transport gap. However, challenges are posed by their surface sensitivity in conjunction with the solution processing, low conductivity and radiation sensitivity of thin films of large organic molecules.

Here, we address strategies to avoid surface contamination and charging effects, while investigating the interfacial electronic structure of conjugated discrete oligomer films [3] spin-coated on Ag substrates. Their thermal crystallization reduced their bulk EBE to < 0.1 eV.

[1] F. Furlan, N. Gasparini, Nat. Mater. 24, 336 (2025)
[2] A. Sugie *et al.*, J. Phys. Chem. Lett. 14, 11412 (2023)
[3] R. Matsidik *et al.*, J. Am. Chem. Soc. 145, 8430 (2023)

O 82.6 Thu 12:15 WILL/A317

Development of near-ambient-pressure low-energy inverse photoelectron spectroscopy enabling measurement under the water vapor pressure — •Mihiro Kubo[1], Gaku Yokogawa[1], Hitoshi Tomizuka[2], and Hiroyuki Yoshida[1] — [1]Chiba University, Chiba, Japan — [2]TOYAMA Co., Ltd., Kanagawa, Japan

Inverse photoemission spectroscopy has evolved over fifty years, providing essential insight into the unoccupied electronic structure. In 2012, Dr. Yoshida developed low-energy inverse photoelectron spectroscopy (LEIPS[1]). This technique enables the measurement of organic materials without damaging the sample by reducing the kinetic energy below 5 eV, their typical damage threshold. To further extend the applicability of LEIPS, we are developing near-ambient-pressure LEIPS (NAP-LEIPS) capable of measurement under the vapor pressure of water (10^3 Pa). NAP-LEIPS will allow measurements of volatile samples, biomaterials, and catalysis with the introduction of reactive gases. To realize NAP-LEIPS, we use an electron gun with a yttria-coated disc cathode and an electrostatic energy analyzer. Because the electron source operates at pressures better than 10^{-5} Pa, a differential pumping system is installed between the electron source chamber and the main chamber (10^3 Pa). Electrons travel about 300 mm through the differential pumping section using an electrostatic transfer lens. Photons emitted from the sample are focused by a mirror, passed through a band-pass optical filter, and detected with a photomultiplier tube. The apparatus has been constructed and is currently in the start-up phase. [1] H. Yoshida, Chem. Phys. Lett. 539-540, 180 (2012).

O 83: Organic molecules on inorganic substrates: electronic, optical and other properties III

Time: Thursday 15:00–17:30 Location: HSZ/0201

O 83.1 Thu 15:00 HSZ/0201

Spin-Crossover and Structural Correlation in Surface Confined Indigo-Based Fe-Coordination Polymers — •Mohammad Salehi[1], Aliki Soufla[2], Hongxiang Xu[1,5], Fulden Eratam[3], David A. Duncan[3,4], Tien-Lin Lee[3], Joachim Reichert[1], Johannes V. Barth[1], and Anthoula C. Papageorgiou[2] — [1]Technical University of Munich, DE — [2]National and Kapodistrian University of Athens, GR — [3]Diamond Light Source, UK — [4]University of Nottingham, UK — [5]Peking University, CN

Surface confined coordination polymers (CPs) exhibiting spin-crossover (SCO) behavior hold promise for molecular spintronics. By harnessing the natural dye indigo as a molecular building block, we investigated [Fe-indigo]$_n$ CPs on Ag(111). Sub-molecular resolution scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) confirmed well-defined CPs. We employed Fe L-edge X-ray absorption near-edge spectroscopy and high-resolution Fe $2p$ soft X-ray photoelectron spectroscopy to probe the spin states of Fe-indigo CPs at different temperatures. The data analysis supports thermally activated spin-crossover behavior, as predicted by density functional theory calculations. Normal incidence X-ray standing wave analysis yielded varying adsorption heights of Fe centers. We correlate the spin state with structural variations, revealing the interplay between ligand fields and magnetic properties.

O 83.2 Thu 15:15 HSZ/0201

Probing pi-conjugation in functionalized pentacene via photoemission orbital tomography — Felix Otto[1], Andrei Matestskii[2], Maximilian Schaal[1], Elise Fürch[1], Jonas Brandhoff[1], Roman Forker[1], François C. Bocquet[2], Michael G. Ramsey[3], Serguei Soubatch[2], •Peter Puschnig[3], Frank Stefan Tautz[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]PGI-3, FZ Jülich & RWTH Aachen University, Germany — [3]Institute of Phyics, University of Graz, Austria

Tuning the electronic structure of polycyclic aromatic hydrocarbons is an effective route to control their physical and chemical properties. Here, we present an experimental approach that enables direct assessment of how chemical functionalization modifies the conjugation length of adsorbed molecules. We demonstrate the method using pentacenequinone (P2O), a functionalized pentacene derivative that forms a self-assembled monolayer on Ag(110), as confirmed by low-energy electron diffraction and scanning tunneling microscopy. Employing photoemission orbital tomography, we combine experimental photoelectron momentum maps with density-functional-theory simulations to elucidate the character of the frontier molecular orbitals. Our results provide direct experimental evidence that the functional group in P2O disrupts the conjugation of the parent pentacene backbone, causing the electronic structure of P2O to resemble two electronically decoupled naphthalene units. This interpretation is further supported by the observed increase in the band gap upon functionalization.

O 83.3 Thu 15:30 HSZ/0201

Stochastic spin-state transitions in an Fe(II) spin-crossover complex on Cu(111) — •Jasmeen Jasmeen[1], Sujoy Karan[1], Karl Ridier[2], Reecht Gaël[1], and Manuel Gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]2LCC, CNRS and Université de Toulouse, UPS, INP, 31077 Toulouse, France

Spin-crossover molecules can be switched between a low- ($S = 0$) and a high-spin ($S = 1$) state using external stimuli. Although the switching properties of crystalline powder were shown to strongly depend on the molecules environment, a full microscopic description is lacking. The switching of individual molecules in contact with a surface, evidenced in recent years, open new routes to further understand the impact of the local environment in the switching properties.

Using scanning tunneling microscopy at 4.5 K, we investigated the [Fe(HB(1,2,4-triazolyl)3)2] complex in direct contact with Cu(111) surface, focusing on the dynamics of its spin-state switching and the factors controlling switching behavior. The switching is triggered by injecting current at voltages above 0.5 V and monitored by the induced change in conductance.

We observe a drastic change of the switching yield with the local molecular environment, showing a clear dependence on both the number and the spin-state of neighboring molecules. These observations suggest that intermolecular interactions influence the switching efficiency.

Funding from the CRC 1242 is gratefully acknowledged.

O 83.4 Thu 15:45 HSZ/0201

Coordination and Molecular Band Dispersion of a 2D Metal-Organic Network — •Martin Anstett[1], Lu Lyu[2], Jannis Lessmeister[1], Alexander Schmid[2], Ralf Hemm[1], Vitaliy Feyer[3], Yan Yan Grisan Qiu[3], Simone Mearini[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany

Two-dimensional metal-organic porous networks (2D-MOPNs) provide a versatile platform exploring emergent electronic and magnetic phenomena at designed surface nanoarchitectures. Here, we prepare a cobalt-coordinated hexaaza-triphenylene-hexacarbonitrile (HATCN) network on Ag(111) to fingerprint the role of metal centers in mediating electronic behaviour. Scanning tunnelling microscopy (STM) reveals an ordered network structure. Photoelectron momentum microscopy identifies a distinct hybrid interface state arising from the Co-mediated coupling with the molecules. These results reveal the microscopic mechanism underlying the role of metal centers in tailoring the electronic structures of 2D-MOPN systems.

O 83.5 Thu 16:00 HSZ/0201

Phthalocyanine-based bipartite lattices: Towards a molecular Lieb lattice — •Tzu-Chao Hung[1], Luis M. Mateo[2], Leo Gross[3], Diego Peña[2], and Jascha Repp[1] — [1]University of Regensburg, Germany. — [2]Universidade de Santiago de Compostela, Spain. — [3]IBM Research Europe - Zurich, Switzerland.

The Lieb lattice is a text-book example of topology governing material properties: Its sublattice imbalance gives rise to extended degenerate states resulting in a flat band. Here, we realize several different covalently bonded phthalocyanine (Pc)-based Lieb-lattice prototypical structures by means of on-surface synthesis. Bond-resolved atomic force microscopy images reveal planar structures with extended π-conjugation. Differential conductance maps, combined with density-functional theory calculations and tight-binding models, confirm strong inter-site electronic coupling and quantum states with symmetry-enforced nodes and symmetry-protected degeneracy. Structures of increasing complexity allow exploring the evolu-tion of these symmetry-derived features.

O 83.6 Thu 16:15 HSZ/0201

Correlation-driven d-band modifications promote chemical bonding at 3d-ferromagnetic surfaces — •David Janas[1], Andreas Windischbacher[2], Alessandro Sala[3], Manuel Gruber[4], Mehdi Bouatou[4], Vitaliy Feyer[5], Iulia Cojocariu[5], Andrea Droghetti[6], Peter Puschnig[1,2], Giovanni Zamborlini[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Karl-Franzens-University Graz — [3]CNR-Istituto Officina dei Materiali (IOM), Trieste — [4]University of Duisburg-Essen — [5]Elettra Sincrotrone Trieste — [6]Ca' Foscari University of Venice

Many-body effects at adsorbate-metal interfaces play a crucial but often overlooked role in designing spintronic and electrocatalytic materials. We recently showed that a chemisorbed oxygen layer on ferromagnetic (FM) Fe enhances electron correlation, causing narrowing of the Fe d-bands near the Fermi level, and a reduced exchange splitting, with direct implications for surface reactivity [1]. Here, we study a pentacene monolayer on oxygen-passivated Fe using momentum-resolved photoemission, scanning tunneling microscopy/spectroscopy, and Hubbard-corrected density functional theory (DFT+U) guided by dynamical mean-field theory (DMFT). Non-standard U values reproduce unexpectedly strong molecule-substrate interactions on a nominally passivated surface, highlighting the decisive role of electron correlation at organic/FM interfaces [2].

[1] Janas, D.M., et al. Adv. Mater., 35, 2205698 (2023).
[2] Janas, D.M., et al. accepted in Small.

O 83.7 Thu 16:30 HSZ/0201

A quantum dot-functionalized scanning tunnelling microscope tip: Sensing through electron-vibron coupling — •Stefan Schulte[1,2,3], Emilio Scontrino[1,4], Taner Esat[1,3], F. Stefan Tautz[1,3,4], and Ruslan Temirov[1,2,3] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]Fundamentals of Future Information Technology, Jülich Aachen Research Alliance (JARA), Germany — [4]RWTH Aachen University, Germany

Scanning tunnelling microscope (STM) tips functionalized with a single-molecule quantum dot (QD) have been used for quantitative measurements of electrostatic surface potentials through a technique known as scanning quantum dot microscopy (SQDM) [1]. The functionalization of STM tips with large organic molecules has further enabled measurements of electrostatic and magnetic fields at the atomic scale [2, 3]. Here, we attach a naphthalene tetracarboxylic dianhydride (NTCDA) molecule, acting as a QD, to the tip of an STM and investigate charge transport through the resulting junction. In the resonant regime, the transport through the NTCDA QD exhibits signatures of electron-vibron coupling. We propose that this electron-vibron coupling can be leveraged to map surface polarizability with sub-nanometre resolution.

[1] C. Wagner *et al.*, Phys. Rev. Lett. **115**, 026101 (2015).
[2] B. Verlhac *et al.*, Science **366**, 623 (2019).
[3] T. Esat *et al.*, Nat. Nanotechnol. **19**, 1466 (2024).

O 83.8 Thu 16:45 HSZ/0201

Spatial Mapping of Vibronic Excitations in a Single Organometallic Complex — Xiangzhi Meng[1], Kai Uwe Clausen[2], Marie-Laure Bocquet[3], •Alexander Weismann[1], Niklas Ide[1], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [3]Laboratoire de Physique de l'École normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris Cité, 75005 Paris, France

Vibronic excitations in single molecules at nanoscale interfaces are central to molecular electronics and are usually modeled with a double-barrier tunneling junction that assumes a homogeneous electric field and ignores atomic details of the contacts. Using STM measurements of a nonplanar organometallic complex on Ag(111), we obtain spatially resolved vibronic maps that reveal shifts in excitation energies caused by reordering of occupied molecular orbitals under the rapidly decaying tip potential. These shifts vary strongly with tip position. Combined with modeling, our results show that tip-induced, atomically varying electric fields can actively control molecular orbitals and must be considered in studies of nonplanar molecules.

O 83.9 Thu 17:00 HSZ/0201

Exciton Dynamics and Charge Transfer at Prototype Organic/Organic Interfaces Studied with LEEM and 2P-PEEM — Franz Niklas Knoop, •Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

Organic semiconductor (OSC) films deposited on weakly interacting substrates, such as natively oxidized silicon, often suffer from poor structural order. Using low-energy electron microscopy (LEEM), we show that para-sexiphenyl (*p*-6P) molecules on SiO_2 serve as a wetting layer, promoting the growth of microcrystalline phthalocyanine (Pc) thin films, which renders Pc/*p*-6P/SiO_2 a structurally well-defined model for an organic heterojunction. Using two-photon photoemission (2PPE), we study the exciton dynamics in both CuPc and F_{16}CuPc films on *p*-6P/SiO_2. For F_{16}CuPc/SiO_2, i.e., in absence of *p*-6P, the S_1 exciton is observed with a lifetime of 50 ps, indicating negligible influence of the substrate on the exciton dynamics. In contrast, for F_{16}CuPc/*p*-6P/SiO_2, the S_1 exciton is quenched. Moreover, laser-induced changes in electron reflectivity reveal a surface potential shift for F_{16}CuPc/*p*-6P/SiO_2, which points to the formation of surface dipoles upon optical excitation of F_{16}CuPc. Accordingly, we attribute the S_1 exciton quenching to formation of charge transfer (CT) excitons, which is compatible with the type II energy level alignment at the F_{16}CuPc / *p*-6P interface. In contrast, at the CuPc/*p*-6P type I heterojunction no charge transfer takes place. Accordingly, neither exciton quenching nor significant surface potential shifts are observed.

O 83.10 Thu 17:15 HSZ/0201

Magnetic Excitations in on-surface metallacrown complexes — •Robert Ranecki[1,2], Stefan Lach[2], Anne Lüpke[3], Angeliki Athanasopoulou[3], Eva Rentschler[3], and Christiane Ziegler[2] — [1]QNS, Seoul, Korea — [2]RPTU Kaiserslautern-Landau and OPTIMAS, Kaiserslautern, Germany — [3]Inst. of Inorganic and Analytical Chemistry, JGU Mainz

The implementation of quantum information processing demands achieving electrical control over spin-qubits that can be integrated into scalable architectures. Addressing this challenge, multi-spin-carrying molecules on surfaces offer a route to surface-integrable qubits: chemically diverse with tunable spin properties. However, the interaction with the supporting substrate can dramatically modify the electronic and magnetic properties of such complexes. Here, we present spin-flip inelastic tunneling spectroscopy studies of pentanuclear metallacrown complexes, CuCu4 and CuFe4, under adsorption onto Au(111) surface. By comparing the experimental results with perturbative electron transport model simulations[1], we extract quantitative values of the exchange coupling constants and determine the ground spin states of the metallacrown complexes[2]. These findings advance our understanding of the spin interactions in complex molecular systems adsorbed on surfaces, paving the way towards future quantum technologies.

[1] Ternes, M. New J. Phys. 17, 063016 [2] Ranecki, R. et al., J. Phys. Chem. C 127, 13186; Ranecki, R. et al., J. Phys. Chem. C 126, 15907

O 84: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)

Time: Thursday 15:00–17:45 Location: HSZ/0204

O 84.1 Thu 15:00 HSZ/0204

Linearized augmented plane waves for low-dimensional materials — •Andris Gulans, Ernests Jansons, and Janis Uzulis — University of Latvia, Riga, Latvia

We address the challenge of efficient yet highly precise density-functional theory calculations of low-dimensional materials and present a set of tools and algorithms specific to linearized augmented plane waves (LAPW) that is implemented in the electronic-structure code `exciting`. First, we discuss our iterative eigensolver compatible with local and hybrid functionals. It is an extension of Davidson*s algorithm and does not require explicit Hamiltonian construction while overcoming difficulties associated with high condition numbers. The second important ingredient is the adaptively compressed exchange that represents the non-local (screened) Fock exchange via a low-rank approximation. This approach enables computational complexity as low as $O(N^3 \log N)$ floating-point operations (FLOPs) with N being the number of atoms. It is a novel feature in hybrid functional calculations using LAPW as the standard approaches require $O(N^4)$ FLOPs. Finally, we introduce a cylindrical cutoff for the Coulomb interaction for handling the $q = 0$ singularity.

O 84.2 Thu 15:15 HSZ/0204

Graphene-Enabled Mott–Metal Transition in Silicon Dangling Bonds — •Niclas Tilgner[1], Siheon Ryee[2], Zamin Mamiyev[1], Philip Schädlich[1], Christoph Tegenkamp[1], Tim O. Wehling[2], and Thomas Seyller[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]I. Institute of Theoretical Physics, University of Hamburg, Germany

Controlling emergent electronic phases in materials with strong Coulomb interactions remains a central challenge in condensed matter physics. Adatom lattices on semiconducting surfaces provide prototypical platforms for exploring such correlated phenomena. Recent advances have facilitated the synthesis of 2D Mott insulators in proximity to graphene (N. Tilgner et al 2025 2D Mater. 12 045022). Here, we demonstrate that alkali adsorption on a graphene/Si/SiC(0001) heterostructure – where the Si layer hosts correlated dangling bonds – enables controlled charge transfer to the Mott insulator. Beyond a critical carrier concentration, we observe a sudden collapse of the Mott gap, indicating a transition to a correlated metallic phase. Our results point to a finite proximity coupling between the Mott layer and graphene, as recently suggested by a theoretical study (N. Witt et al 2025 arXiv:2503.03700), which gives rise to nonlocal dynamical screening beyond simple electrostatics and provides a natural pathway for the observed phase transition.

O 84.3 Thu 15:30 HSZ/0204

From self-consistent DFT+DMFT to the two-particle level: Magnetic phase diagram of X:SiC(111) — •Lukas Bongardt[1,2], Niklas Enderlein[3], Giorgio Sangiovanni[4], Philipp Hansmann[3,5], and Henri Menke[1] — [1]Max Planck Computing and Data Facility — [2]Technical University of Munich — [3]FAU Erlangen — [4]Universität Würzburg — [5]University of Iceland, Reykjavík

Recently we have proposed a novel and versatile platform to realize a two-band Hubbard model with massless Dirac fermions and flat bands hosting strong correlations by depositing three different species of transition-metal adatoms on semiconductor surfaces (arXiv:2410.17165). Using state-of-the-art DFT+DMFT calculations we investigated the spectral properties of X:3C-SiC(111) (X = Ti, V, Cr). Due to the presence of well-defined Dirac cones and flat bands, indicating the potential for realizing topological and correlated phases, we identify transition-metal adatoms on SiC as a possible platform for exploring the interplay of correlations, topology, and magnetism in two-dimensional materials.

In this work, we explore the magnetic phase diagram of these systems within DMFT by calculating the generalized two-particle vertex and using it to solve the Bethe-Salpeter equation for the generalized susceptibility. This gives us a fully orbital-, spin-, and most importantly momentum-dependent susceptibility which carries the information about the ordering wave vector and is experimentally accessible through various techniques.

O 84.4 Thu 15:45 HSZ/0204

Cr $3d$ Orbital Hybridization and Electronic Structure in the Layered Magnetic Semiconductor CrPS$_4$ — •Lasse Sternemann[1], David Maximilian Janas[1], Richard Leven[1], Eshan Banerjee[2], Jonah Elias Nitschke[1], Marco Marino[1], Leon Becker[3], Ahmet Can Ademoglu[1], Frithjof Anders[1], Stefan Tappertzhofen[3], and Mirko Cinchetti[1] — [1]TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — [2]Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom — [3]TU Dortmund University, Department of Electrical Engineering and Information Technology, 44227 Dortmund, Germany

Despite its promising spintronic and magneto-optical characteristics, the electronic band structure of the van der Waals magnetic semiconductor CrPS$_4$ is still unknown. Here, we report angle-resolved photoemission spectroscopy measurements of its band structure in the para- and antiferromagnetic phase, complemented by DFT+U calculations. Theoretical results reveal dominating Cr $3d$ and S $3p$ contributions to the valence band and a ligand-to-metal charge-transfer band gap. Crystal field split Cr $3d$ orbitals display distinct hybridization regimes with S $3p$ orbitals: t_{2g} orbitals are only weakly affected by hybridization, while e_g states experience a 4 eV anti-bonding/bonding splitting with S-mixing relaxing dipole selection rules, otherwise darkening optical d-d transitions. These findings establish the ground state electronic and orbital structure of CrPS$_4$ and provide essential benchmarks for understanding its optical and magnetic responses.

O 84.5 Thu 16:00 HSZ/0204

Spectroscopic Investigation of the Ni Valence States in NiTe$_2$ — •Tassaphon Tirasutt[1], Sheng-Huai Chen[1], Alexander C. Komarek[1], Chun-Fu Chang[1], Yu-Chieh Ku[2], Po-Yu Cho[3], Chun Sum Brian Pang[4], Mizuki Furo[5], Naoki Ito[5], Ulrich Burkhardt[1], Simone G. Altendorf[1], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]The University of British Columbia, Vancouver, Canada — [5]Osaka Metropolitan University, Osaka, Japan

Nickel-based transition metal compounds exhibit a wide range of properties arising from the strongly correlated d electrons. In this study, we investigate NiTe$_2$, a layered transition-metal dichalcogenide with reported type-II Dirac semimetallic properties. While its topological nature has been the focus of interest, the fundamental question of the properties of the Ni ions in NiTe$_2$ has rarely been discussed. We address this issue using soft X-ray core-level and valence-band photoelectron spectroscopy, as well as Ni-$L_{2,3}$ absorption spectroscopy, combined with a theoretical approach using LDA+DMFT. Our findings provide insights into the Ni $3d$ occupation and degree of correlation of the Ni in a metallic ligand bath of the NiTe$_2$ system.

O 84.6 Thu 16:15 HSZ/0204

TMDC surfaces as scattering targets in spin-polarization detectors: A case study of MoS$_2$ — •Christoph Angrick[1], Annika Henriksen[1], Nicole Edossa[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

Spin-polarization detectors are employed in photoemission experiments to reveal the spin texture of electronic states. One well-proven approach is based on the VLEED process, where the spin-dependent electron reflection from targets influenced by exchange and/or spin-orbit interaction is used. The suitability of a target must be investigated beforehand [1,2]. In this talk, a first impression of TMDC-based detectors is given [3]. The spin-dependent electron reflectivity of spin-orbit-influenced MoS$_2$ is measured over a wide range of incident energies and angles for the following samples: a single layer of MoS$_2$ on Au(111) and cleaved MoS$_2$ single-crystal surfaces. On the basis of the resulting maps for the electron reflectivity, Sherman function, and figure of merit, promising features of MoS$_2$ for use in spin-polarization detection are discussed.

[1] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).

[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[3] Angrick *et al.*, Phys. Rev. B, accepted for publication (2025).

O 84.7 Thu 16:30 HSZ/0204

Efficient GW calculations for metals from an accurate ab initio polarizability: the case of doped MoS2 monolayer — •Giacomo Sesti[1], Pino D'Amico[1], Alberto Guandalini[2], Claudia Cardoso[1], Andrea Ferretti[1], and Daniele Varsano[1] — [1]CNR-NANO, Modena, Italy — [2]Università di Roma La Sapienza, Roma, Italy

Many-body perturbation theory in the GW approximation has proved very successful for the calculation of quasiparticle (QP) band structures of semiconductors. QP corrections are less significant in metals and are typically disregarded for the computational cost involved. Also, GW calculations of metals suffer of specific methodological challenges to properly treat the screening. This is typically solved under the addiction of a Drude term, that however is inadequate at low dimensionalities[1]. Furtherly, even for metals, QP corrections become more relevant at lower dimensionalites.

Here, we present GW calculations of QPs for doped MoS$_2$ monolayer showing excellent agreement with experimental ARPES measurements[2]. Such an unprecedented agreement has been possible thanks to the W-av method, which combines a Monte Carlo integration with interpolation approaches. This technique originally developed for 2D semiconductors[3] is here extended to the metallic case.

1) Champagne et al. NanoLett. 23.10 (2023)
2) Liu et al. PRL. 122 (2019)
3) Guandalini et al., npj Computational Materials, 9 (2023)

O 84.8 Thu 16:45 HSZ/0204

Ultrafast Momentum Dependent Relaxation Dynamics in TbTe$_3$ — •Florian Denizer[1], Noah Meyer[2,3], Anisha Singh[3], Ian R. Fisher[3], Uwe Bovensiepen[1], Zhi-Xun Shen[2,3], and Patrick S. Kirchmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University — [3]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University

Rare-earth tritellurides (RTe$_3$) form charge density waves (CDW) due to electronic instabilities at the Fermi-surface, because of an anisotropy of the crystal lattice between the two major in-plane crystal axes a and c. Unoccupied electronic states can be populated by ultrafast laser excitation. Electronic relaxation and coherent vibrational modes including the amplitude mode have been investigated by time and angle resolved photoelectron spectroscopy (*tr*-ARPES). Among the manifold of laser-driven processes, the one that is responsible for the electronic instability has not yet been identified. With this objective in mind we perform a *tr*-ARPES experiment on TbTe$_3$ and investigate the momentum transfer along the a- and the c-axis as a function of excitation strength. At sufficiently low pump fluence below $F = 0.3$ mJ/cm^2 we identify (quasi-)elastic scattering in the vicinity of the Fermi surface. In the talk we will discuss isotropic defect-induced elastic scattering and directed quasi-elastic scattering determined by the nesting vector. Funding through the DFG within SFB 1242 and through the DOE is gratefully acknowledged.

O 84.9 Thu 17:00 HSZ/0204

Unconventional Topological Superconductivity in CrCl3/NbSe2 heterostructures — •Souvik Das[1], Benjamin Zhou[2,3], Anshuman Padhi[1], Jing-Rong Ji[1], Niclas Heinsdorf[2,3], Prajwal Rigvedi[1], Tianzhe Chen[1], Weibin Li[4], Pierluigi Gargiani[4], Manuel Valvidares[4], Marcel Franz[2,3], Banabir Pal[1], and Stuart S.P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [4]ALBA Synchrotron Light Source, Barcelona, Spain

Topological p-wave superconductors can host non-Abelian particles useful for fault-tolerant quantum computing. Here we report experimental evidence of unconventional topological superconductivity in a heterostructure of monolayer, in-plane ferromagnetic CrCl3 islands on superconducting NbSe2. STM measurements show that, despite CrCl3 being ferromagnetic, the interfacial superconducting gap is more robust against out-of-plane magnetic fields than the s-wave gap of NbSe2, indicating unconventional pairing. We also find enhanced zero-energy states along CrCl3 island edges, consistent with the presence of edge modes. Theory suggests these features arise from an intrinsic helical p-wave state stabilized by interfacial Rashba spin-orbit coupling. This demonstrates a new route to create topological superconductivity via interface engineering.

O 84.10 Thu 17:15 HSZ/0204

Structural and Electronic Properties of CrSBr Nanoribbons: Insights from First-Principles Calculations — •Daniil Kruklinskii, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Experiments show that exfoliated CrSBr flakes naturally form nanoribbons along a specific crystallographic direction, and similar structures can be fabricated using an electron beam in the TEM as a cutting tool. Here, we employ density functional theory calculations to systematically investigate the stability as well as electronic and magnetic properties of CrSBr nanoribbons. Our results indicate that nanoribbons oriented along one of the two major crystallographic directions are the most stable under typical growth and exfoliation conditions and remain semiconducting, exhibiting pronounced electron-hole separation between the VBM and CBM. In contrast, nanoribbons in the perpendicular direction display a substantially reduced band gap due to strongly localized edge states. Both orientations retain strongly spin-polarized band-edge states near the Fermi level and show only a weak dependence of the band gap on ribbon width. Using *ab initio* molecular dynamics simulations, we further demonstrate that electron-beam irradiation with energies of at least 200 keV can facilitate the fabrication of nanoribbons directly from pristine monolayer CrSBr, favouring the formation of diagonal nanoribbons. These diagonal ribbons are metallic, in contrast to the monolayer, and host a high density of majority-spin edge states, giving rise to pseudo-half-metallic transport.

O 84.11 Thu 17:30 HSZ/0204

Band-selective coherent phonon-driven band renormalization in 1T-MoTe$_2$ — •Carl Jensen[1], Christopher Emeis[2], Stephan Jauernik[1], Petra Hein[1], Fabio Caruso[2], and Michael Bauer[1,3] — [1]nstitute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Understanding the coupling between coherent phonons and the electronic system is crucial for controlling nonequilibrium properties in solids. Here, we investigate mode- and band-selective electron-phonon coupling in centrosymmetric 1T-MoTe$_2$ using time- and angle-resolved photoemission spectroscopy combined with frequency-domain analysis (FDARPES). Femtosecond near-infrared pulses excite coherent Ag-symmetric phonon modes at 2.34 THz, 3.34 THz, and 3.86 THz, which manifest as oscillatory modulations in photoemission intensity and binding energy across the valence bands. Pixel-wise Fourier analysis, based on a recently developed methodology [1], reveals pronounced band selectivity with distinct coupling strengths for different electronic states and phonon modes, enabling the evaluation of band-renormalization amplitudes in the few-meV range. Ab initio calculations using DFT/DFPT qualitatively reproduce the experimentally observed coupling patterns and relative trends, demonstrating the capability of combined experimental and theoretical approaches to resolve ultrafast electron-phonon interactions in quantum materials.

[1] N. Gauthier, H. Soifer, J.A. Sobota, H. Pfau, E. J. Sie, A. M. Lindenberg, Z.-X. Shen, P. S. Kirchmann, Rev. Sci. Instrum. 96 (2025)

O 85: Vacuum Science & Technology: Theory and Applications II

Time: Thursday 15:00–17:00 Location: HSZ/0401

Invited Talk O 85.1 Thu 15:00 HSZ/0401
From light to pressure: Laser-based quantum technologies for the realization of high-precision pressure and vaccum standards — •Tom Rubin — Physikalisch-Technische Bundesanstalt (PTB), Berlin

The new realization of the pascal in the range between 1 Pa and 100 kPa is achieved by means of photonic pressure measurement. This not only enables significantly lower measurement uncertainties, but also more robust and faster-operating systems that can cover the entire pressure range continuously and for different gases. Gas-density-based methods open up new perspectives: from precise calibrations at the highest metrological level to non-invasive applications in vacuum technology and the development of innovative pressure sensors for the mass market.

This presentation is about key findings and highlights from the EU projects *QuantumPascal* and *MQB-Pascal*. These include overcoming major challenges, such as the need for sub-mK-level gas temperature knowledge, the advantages of the GAMOR (Gas Modulation Refractometry) method, and the latest results from validation and comparison measurements.

O 85.2 Thu 15:30 HSZ/0401
Near Ambient Pressure ARPES for Operando Surface Studies at Synchrotron SOLEIL — •L. Dudy[1], E. Auffray[1,2], J.-J. Gallet[1,3], F. Bournel[1,3], M. Bouaziz[3], B. S. Mun[4], S. Jang[4], Y. Tsujikawa[5], H. Kondoh[5], S. Moser[6], V. Jovic[10], V. Mischke[7], P. Kessler[8], and S. Maehl[9] — [1]Synchrotron SOLEIL, France — [2]U Paris-Saclay, France — [3]Sorbonne U, France — [4]GIST, South Korea — [5]Keio U, Japan — [6]U Bochum, Germany — [7]TU Dortmund, Germany — [8]U Würzburg, Germany — [9]SPECS, Germany — [10]GNS Science, New Zealand

We present a near-ambient pressure angle-resolved photoemission spectroscopy (NAP-ARPES) setup for operando studies of electronic structure under gas exposure at Synchrotron SOLEIL. This development bridges the gap between conventional UHV ARPES and realistic surface environments, enabling momentum-resolved measurements during catalytic and energy-related processes at pressures up to several millibars. The approach is demonstrated using model systems, showing that band structure evolution can be tracked in real-time during adsorption and reaction. These results highlight the potential of NAP-ARPES for investigating dynamic surface phenomena. By extending ARPES into near-ambient conditions, this method opens new opportunities for studying functional materials under realistic environments for operando electronic structure analysis in surface science.

O 85.3 Thu 15:45 HSZ/0401
A new framework for analysing transport ARPES applied to the current induced insulator to metal transition in Ca_2RuO_4. — •Anders Sandermann Mortensen, Hippolyte Raymond Bourel, Katarina Ogliara Praest, Davide Curcio, and Philip Hofmann — Institute of Physics and Astronomy, Aarhus University

The advent of μm-resolution spatially resolved ARPES-measurements allows for in-operando measurements of modifications to the electronic band structure of electrical devices (transport-ARPES). However, this technique poses a new set of challenges, as local biasing of the samples results in systematic shifts of the measured energy, hindering direct comparison of ARPES spectra.

Here, we propose a novel solution to this problem: Realigning the spectra by minimizing the L1-norm between them. Combined with k-means clustering, this provides an effective framework for real-time analysis and characterisation of transport-ARPES measurements.

As a proof of concept, we apply our analysis scheme to transport-ARPES measurements of the current-induced insulator to metal transition in Ca_2RuO_4, and thus provide new, high statistics measurements of the changes to the electronic band structure during the current-induced insulator to metal transition.

O 85.4 Thu 16:00 HSZ/0401
Cross-correlation measurements of a Two-Color Infrared Free-Electron Laser — •Akash Chandra Behera, América Yareth Torres Boy, Sandy Gewinner, Marco De Pas, Gert von Helden, Martin Wolf, Wieland Schöllkopf, Gerard Meijer, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Infrared-Free Electron Lasers (IR-FEL) uniquely provide high-power narrowband radiation for spectroscopic measurements, that is continuously tunable from the mid-IR to the terahertz spectral range.

The IR-FEL at the Fritz Haber Institute recently commissioned a two-color upgrade, enabling simultaneous lasing at two independently tunable wavelengths. This is realized by employing a high-frequency kicker cavity to feed alternating electron bunches into the two separate undulators. Within this scheme, a high intrinsic temporal synchronization between both FEL outputs is expected.

In our contribution, we present two-color optical cross correlation measurements proving this synchronization. By leveraging the independently tunable pulse durations in each FEL, we further explore the achievable time-resolution that can be expected when the two-color FEL is employed for future IR-IR pump-probe experiments

O 85.5 Thu 16:15 HSZ/0401
K-Means Clustering of Time-Resolved Diffraction: Dynamics of Laser-Excited Si(111)-(7x7) — •Jonas D. Fortmann[1,2], Alexander Neuhaus[1], Pascal Dreher[1,3], Birk Finke[1], Christian Brand[1], and Michael Horn-von Hoegen[1] — [1]Uni Duisburg-Essen, Duisburg, Germany — [2]MAX IV, Lund, Sweden — [3]Uni Würzburg, Würzburg, Germany

We present an unsupervised analysis workflow that leverages k-means clustering to extract characteristic dynamics from time-resolved diffraction data, using ultrafast reflective high energy electron diffraction (URHEED) measurements of laser-excited Si(111)-(7x7) as a case study. Delay-dependent intensity profiles of diffraction features are clustered by trajectory shape to reveal characteristic dynamics without prior model assumptions. When combined with a simple population model, relative integral-intensity changes of clusters yield lifetimes of coupled phonon systems and trace the excitation pathway to surface electronic states. The method is robust to practical limitations (e.g., camera light sensitivity), scales to large datasets, and is directly transferable to other diffraction modalities (ULEED, UTEM, and pump-probe X-ray diffraction), where clustering of intensity evolutions can provide an objective map of structural dynamics.

O 85.6 Thu 16:30 HSZ/0401
ESEM Automation - Agent-Oriented Autonomous Microscopy — •Maurits Vuijk[1], Johannes Zeininger[2], Karsten Reuter[1], Thomas Lunkenbein[3], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]TU Wien — [3]Universität Bayreuth

Are the datasets captured in usual Environmental Scanning Electron Microscopy (ESEM) experiments truly representative? While focusing on a single view or feature, critical events may occur elsewhere on the accessible surface. In addition, effects such as beam damage and inhomogeneous gas concentration introduce further need for more representative surface sampling. Starting from an automation interface to the ESEM, we have built an agent-oriented framework that enables fully autonomous ESEM experiments. To achieve this, the actions normally carried out by the human operator are instead performed by various agents. To this end, a set of agents keep up image quality by controlling brightness and contrast, focus and astigmatism without interrupting the imaging flow. A set of computer vision agents analyze captured images on the fly for interesting features and activity. Using a dynamic priority queue system, high-resolution frames are automatically taken of identified active zones. Each overview image is processed and scored based on activity, feature presence, or other desired qualities. The queue system then assigns an acquisition frequency based on the score, giving priority to more active zones. This gives a full set of overview images and multiple smaller image sets of dynamically identified active areas.

O 85.7 Thu 16:45 HSZ/0401
Image Stacking: A Simple Method to Enhance SNOM Measurements — •Florian Mangold[1], Farid Aghashirinov[1], Enrico Baù[2], Julian Schwab[1], Bettina Frank[1], Andreas Tittl[2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center

SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany — [2]Nano-Institute Munich, Department of Physics, Ludwig-Maximilians Universität München, Germany

Scanning near-field optical microscopy (SNOM) enables optical characterization with spatial resolution far beyond the diffraction limit, making it a powerful tool for studying nanoscale optical and material properties. However, achieving a high signal-to-noise ratio (SNR) in SNOM can be challenging and, depending on the experimental conditions, sometimes not feasible. We present a simple and equipment-free method to enhance SNOM performance by aligning and stacking multiple sequential measurements. This procedure effectively increases the SNR while avoiding drift-induced errors and system alterations. In addition, the stacking process suppresses outliers and isolated noise contributions, further improving data quality. We demonstrate that stacked SNOM measurements can surpass the quality of single measurements under comparable conditions. This straightforward method can be broadly applied to strengthen existing SNOM experiments and opens possibilities for measurements in challenging regimes, including low-signal materials, extended wavelength ranges, and higher-order demodulation schemes where conventional single-shot SNR would be insufficient.

O 86: Surface dynamics

Time: Thursday 15:00–17:45 Location: HSZ/0403

Invited Talk O 86.1 Thu 15:00 HSZ/0403

Ultrafast Dynamics at Surfaces with Machine Learning Surrogates

— •Reinhard Maurer — University of Vienna, AT — University of Goettingen, DE — University of Warwick, UK

Ultrafast dynamics at surfaces (driven by light, electrons, or hyperthermal scattering) involve the concerted motion of electrons and atoms at comparable energy and time scales, giving rise to nonadiabatic effects. Excited electrons drive chemical conversions, induce phase transitions, and mediate energy transfer between adsorbates and surfaces. To reliably predict such effects with scalable, state-of-the-art nonadiabatic dynamics simulations requires the use of accurate and data-efficient high-dimensional machine learning (ML) surrogate models. This includes representations of energy landscapes, but also nonadiabatic couplings or excited-state properties that are required for nonadiabatic simulations. I will present recent strategies to construct high-dimensional ML surrogate models of electronic structure, including active learning and fine-tuning of foundation models that allow us to reduce the required electronic structure data to a few hundred data points per gas-surface dynamics model and even transfer learn across density functional approximations. Electronic properties such as electron-phonon coupling tensors or electronic Hamiltonians can be efficiently represented by encoding physical equivariance properties in the model. I will showcase the utility of the introduced models with recent dynamics applications on reactive molecular scattering and light-driven structural dynamics.

O 86.2 Thu 15:30 HSZ/0403

Ultrafast Structural Dynamics of Layered Material Surfaces

— •Alp Akbiyik[1,2], Felix Kurtz[1,2], Hannes Böckmann[1,2], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, D-37077 Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, D-37077 Göttingen, Germany

Layered materials are promising candidates for studying and applying correlated phenomena, and their carrier dynamics have been extensively investigated, including through ultrafast pump-probe techniques. However, the structural evolution of their surface layers remains poorly accessible. Ultrafast low-energy electron diffraction (ULEED) leverages the surface sensitivity of low-energy electron pulses, with high spatial resolution and temporal resolution down to 1-2 ps. This allows us to monitor the momentum-dependent out-of-plane phonon populations across the Brillouin zone as well as changes in diffraction peak intensities [1,2]. Here, we contrast the phonon equilibration behaviour of transition metal dichalcogenides (TMDCs), such as WTe2, with graphite following electron-phonon coupling.

[1] G. Storeck et al., Structural Dynamics 7, 034304, 2020.

[2] F. Kurtz et al., Nat. Mater. 23, 890-897, 2024.

O 86.3 Thu 15:45 HSZ/0403

Nonadiabatic Energy Loss in Hyperthermal Gas-Surface Scattering: Going Beyond the Mean Field Approximation

— •Ash Baldwin[1] and Reinhard J. Maurer[1,2] — [1]University of Vienna, Vienna, Austria — [2]University of Warwick, Coventry, United Kingdom

Nonadiabatic energy dissipation is known to play a crucial role in hyperthermal scattering at surfaces, leading to electron-hole pair excitation and highly inelastic scattering. For projectiles with unpaired spins, such as hydrogen atoms, hybridisation with the metal surface results in strong non-adiabatic effects driven by a phase transition in its spin-polarisation. It is known that traditional mean-field descriptions of the resultant nonadiabatic dynamics using methods like MDEF and Ehrenfest dynamics break down in the presence of the transition, leading to divergent energy transfer rates and unphysical stopping powers at the location of the spin transition [Box et al. *J. Phys. Chem. Lett.* 15, 51 (2024); Lindenblatt et al. *Phys. Rev. Lett.* 97 (2006)].

Here, we model H/Cu(111) and H/Ag(111) scattering in the presence of on-site correlation in the adsorbate state using the Newns-Anderson Hamiltonian. We go beyond previous works by simulating the dynamics using stochastic trajectory surface hopping methods that capture the coupling between the nuclear and electronic degrees of freedom beyond the mean-field. By systematically classifying scattering regimes, we assess the applicability of mean-field and beyond mean-field methods for predicting nonadiabatic energy loss.

O 86.4 Thu 16:00 HSZ/0403

Manipulation of charge density wave order in 1H-TaS$_2$ to simulate broken lattice degeneracy of misfit layered chalcogenides

— •Laura Pätzold[1], Sandra Sajan[2], Clara Pfister[1,3], Haojie Guo[2], Miguel M. Ugeda[2], and Tim O. Wehling[1,3] — [1]U Hamburg — [2]DIPC San Sebastian — [3]The Hamburg Centre for Ultrafast Imaging

Misfit layer compounds, a class of van der Waals heterostructures comprised of noncommensurate layers, are ideal platforms to explore the influence of broken lattice symmetries and incommensurability on collective electronic phases, such as charge density waves (CDWs). The simulation of these symmetry-broken ground states poses a computational challenge due to large numbers of inequivalent atoms. By employing an electron-lattice downfolding scheme [1] followed by molecular dynamics (MD) simulations, we obtain the (thermo-)dynamics of these systems with the accuracy of full first-principles calculations while reducing the computational cost by several orders of magnitude. Here, we explore CDW control parameters to analyze the influence of the PbS layer in the misfit layer compound (PbS)$_{1.13}$TaS$_2$, where a shift in CDW order accompanied by symmetry breaking is measured in the 1H-TaS$_2$ layer. Simulating charge doping, interlayer hybridization effects via external potentials and frustration effects via the supercell size, we show that only a combination of these effects reproduces the characteristics of the measured structure factor while being thermodynamically stable.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 86.5 Thu 16:15 HSZ/0403

Control and thermal evolution of commensurate charge-density wave order in 1H-NbSe$_2$

— •Clara Pfister[1,2], Alexander Bäder[3,4], Laura Pätzold[1], Tobias Wichmann[3], Felix Lüpke[3,4], Mariana Rossi[5], and Tim O. Wehling[1,2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]The Hamburg Centre for Ultrafast Imaging — [3]Peter-Grünberg-Institut, Forschungszentrum Jülich — [4]II. Physikalisches Institut, Universität zu Köln — [5]MPI für Struktur und Dynamik der Materie, Hamburg

Charge-density waves (CDWs) are symmetry-broken ground states arising from electron-lattice interactions and offer a platform to study tunable ordered phases in quasi two-dimensional materials. Using *ab initio* calculations and a downfolding approach [1], we investigate how biaxial tensile strain and electron doping affect CDW order in 1H-NbSe$_2$. In both cases, a transition from the native 3×3 to a competing 2×2 CDW ground state is induced. The strain-induced 2×2 CDW is supported by experimental data of monolayer 1H-$NbSe_2$ flakes that are rotated with respect to the underlying bulk $NbSe_2$. By constructing phase diagrams, we are able to identify the strain- and doping-induced boundaries between the competing CDW ground states. Moreover, by performing molecular dynamics (MD) simulations, we find that strain-induced 2×2 order persists up to $T_{\mathrm{CDW}} \approx 10$ K, whereas the doping-induced 2×2 CDW is thermally much less stable. Our MD results furthermore suggest that nuclear entropy is the driving mechanism in the melting process of the CDW.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 86.6 Thu 16:30 HSZ/0403

Surface Resonant Raman Scattering of Ag(110) surfaces — Sandhya Chandola[1,2], •Norbert Esser[1], Mohamed Yassine Fatihi[3], and Simone Sanna[3] — [1]Institut für Festkörperphysik,TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 8, 12489 Berlin, Germany — [3]Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

The phonon and electron scattering mechanism on Ag(110) surfaces is investigated using Surface Resonant Raman scattering (SRRS) and Reflectance Anisotropy Spectroscopy (RAS) in ultra-high vacuum (UHV). The surface electronic transition is clearly visible with RAS, with Raman spectra showing surface phonons near the resonant excitation. A low energy peak is also seen, which should be related to the Rayleigh mode at the Brillouin zone edge. This shows that the surface is rough, and that the intensity of this mode depends on the sample treatment. Consequently, RAS together with Raman spectroscopy allows optimization of surface reconstruction and control of surface morphology. By means of first-principles calculations within density functional theory, we demonstrate that the dominant Raman signature is coupled to an electronic transition between localized surface-states (calculated at 1.6 eV). The corresponding surface-localized phonon mode enhances the distance between the topmost surface layers. The combined experimental and theoretical approach to resonant surface Raman spectroscopy establishes a powerful tool for investigating surface vibrational dynamics and electron-phonon interactions.

O 86.7 Thu 16:45 HSZ/0403

Spatiotemporal control of Peierls heterostructures by valley-selective photoswitching — •Hannes Böckmann[1], Jan Gerrit Horstmann[3], Felix Kurtz[1], Manuel Buriks[4], Karun Gadge[4], Salvatore Manmana[4], Stefan Wippermann[5], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, Solids and Nanostructures, University of Göttingen, Germany — [3]Department of Materials, ETH Zurich, Zürich, Switzerland — [4]Institute for Theoretical Physics, University of Göttingen, Germany — [5]Faculty of Physics, Philipps University of Marburg, Germany

Phase competition and coexistence are hallmarks of strongly-correlated materials, promising tunable functionality on the nanoscale. Light allows for tilting the balance between distinct correlated states and phases with a prominent example given by the optical switching of an insulator to a metal. However, optical excitation generally lacks the specificity to select sub-wavelength domains. In this work, we employ valley-selective photodoping of correlated electronic states to drive the domain-specific quench of a textured Peierls insulator. Specifically, we exploit the anisotropic absorption of nanowire domains by tuning both the photon energy and the polarization to the transition matrix elements most strongly coupled to the structural transformation. We find that averting dissipation facilitates domain-specific carrier confinement, control over nanotextured phases, and a prolonged lifetime of the metastable metallic state.

O 86.8 Thu 17:00 HSZ/0403

Surface resonant Raman scattering from coinage metal surfaces — •Mohamed Yassine Fatihi[1], Sandhya Chandola[2,3], Norbert Esser[2,3], and Simone Sanna[1] — [1]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [3]Institut für Festkörperphysik, TU Berlin, 10623 Berlin, Germany

The vibrational characterization of clean metal surfaces has remained largely inaccessible to optical spectroscopy, as Raman scattering from pristine metals is extremely weak and dominated by bulk phonon backgrounds. However, the first direct Raman observation of surface phonons on a Cu(110) single crystal has been recently reported[1]. We explain this Raman activity and predict it for the related Ag(110) surface from first principles, demonstrating by means of atomistic models how tuning the incident photon energy to the surface-state transition induces a striking resonant enhancement of the surface phonon signal. This mechanism selectively amplifies the surface response with respect to the bulk contribution. Our resonant surface phonon Raman approach establishes a powerful probe for investigating surface vibrational dynamics and electron-phonon interactions, creating new opportunities for real-time studies of metallic surfaces under diverse conditions, from ultra-high vacuum to catalytic and electrochemical environments

[1] Denk, M., et al. Phys. Rev. Lett. 128, 216101 (2022).

O 86.9 Thu 17:15 HSZ/0403

Manipulation of Optical Phonons by Thermal Expansion Mismatch in Bi/Si(111) Heterostructures — •Fabian Thiemann, Maja Penkl, and Michael Horn-von Hoegen — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

We investigate how substrate-induced biaxial strain controls the temperature behaviour of the A_{1g} phonon frequency $\Omega(T)$ in epitaxial Bi(111) films on Si(111) in the time domain. Bismuth's anisotropic A7 structure, strong electron-phonon coupling and its Peierls' distortion make the out-of-plane c-axis vibrations highly sensitive to strain. Using *in situ* SPA-LEED and broadband femtosecond transient reflectivity on the same samples, we measured temperature-dependent lattice parameters and coherent-phonon frequencies. Strained Bi films on Si(111) exhibit a larger thermal redshift $\partial\Omega/\partial T$ compared to relaxed bulk or polycrystalline Bi. Applying an extended phonon-shift model reveals that the anharmonic multi-phonon term depends solely on the value of the c-axis lattice parameter. This identifies c-axis expansion as the key structural factor governing the A_{1g} phonon, enabling targeted strain-engineering of phonon properties in bismuth and related anisotropic materials.

O 86.10 Thu 17:30 HSZ/0403

Nested Sampling Simulations of Oxygen Induced Surface Reconstructions on Cu(100) — •Felix Riccius[1,2], Hendrik H. Heenen[1], Jutta Rogal[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG , Berlin — [2]Flatiron Institute, New York

Under operating conditions, catalysts can undergo structural, compositional, and morphological changes, which ultimately dictate their activity and stability. However, extensive sampling of surface configurations at finite temperature and pressure is computationally expensive and non-trivial. To this end, nested sampling simulations can be used to explore the full configuration space, estimate the partition function, and directly access the desired thermodynamic ensemble averages. We here render such simulations tractable by using them in combination with a machine-learning interatomic potential, optimize the code to run efficiently on GPUs, and tailor system specific nested sampling moves. Applied to the early oxidation of Cu(100), the approach correctly captures clean surface configurations at various oxygen coverages and the relative stability of the O adsorption sites as a function of temperature. Moreover, nested sampling successfully predicts the experimentally observed and highly complex $(2\sqrt{2}\times\sqrt{2})$ R45°-O missing-row surface reconstruction and their defect states without any human bias.

O 87: Solid-liquid interfaces: Structure, spectroscopy

Time: Thursday 15:00–17:15 Location: TRE/PHYS

O 87.1 Thu 15:00 TRE/PHYS

Interfacial Enrichment and Reactivity of Organic Molecules in Ionic Liquids — •Alisson Ceccatto Santos[1], Luciano Sanchez Merlinsky[2,3], Luis M. Baraldo[2,3], Federico J. Williams[2,3], Florian Maier[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Departamento de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires — [3]Instituto de Química Física de los Materiales, Medio Ambiente y Energía, CONICET- Universidad de Buenos Aires

Controlling the surface composition of metalloporphyrins in ionic liquids (ILs) is crucial for designing photoactive materials. Here, we investigate the interfacial behavior of zinc-didodecylporphyrin molecules (Zn-DDP) dissolved in the 1-butyl-3-methylimidazolium hexafluorophosphate [C4C1Im][PF6] IL using angle-resolved X-ray photoelectron spectroscopy (ARXPS). Upon mild heating, Zn-DDP undergoes spontaneous demetallation, evidenced by the appearance of aminic (-NH-) and iminic (=N-) nitrogen XPS signals. Our measurements reveal extremely high surface enrichment of porphyrins at the IL/vacuum interface, with the dodecyl chains oriented toward the vacuum. ARXP spectra reveal that the surface enrichment increases with increasing temperature. Our findings provide molecular-level insights to guide the design of photoactive interfaces in IL systems. Acknowledgements: Alexander von Humboldt Foundation for a Humboldt Research Fellowship for postdocs

O 87.2 Thu 15:15 TRE/PHYS

How is the hydrophobic force modified by an oscillation frequency in saline conditions? — •Chiara Wagner, Paul Stöcher, Laura Mears, and Markus Valtiner — Vienna University of Technology, Vienna, Austria

There have been many investigations over the years regarding the mechanism behind the hydrophobic force and over how long a range it can be felt [1]. We present a detailed set of AFM force measurements of hydrophobic SAM modified surfaces, with varying salt concentration and oscillation frequency (0-2kHz). We observe dynamic changes in the force curve characteristics with both salt concentration and oscillation frequency. The changes lead to a reduction of the average force with increasing applied frequency, while multiple distinct characteristic curves are present and enhanced by certain conditions. We also notice changes in the range of the force away from the surface. Altogether, the results we will present bring new insight into the mechanism of hydrophobic interactions.

[1] W. A. Ducker and D. Mastropietro, Current Opinion in Colloid & Interface Science, 2016, 22, 51*58.

O 87.3 Thu 15:30 TRE/PHYS

Interfacial non-Markovian friction determines non-linear spectral shifts at the water-graphene interface — •Johannes Schröter, Louis Lehmann, Shane Carlson, and Roland R. Netz — FU Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin

Understanding the behavior of aqueous interfaces is crucial for various applications. In particular, the graphene water interface plays a key role for energy storage and energy conversion, however, its properties remain poorly understood. Using DFT molecular dynamics simulations we show that the sum-frequency signal of non-hydrogen bonded OH bonds is significantly red-shifted at the water-graphene compared to the water-air interface, in agreement with recent experiments. The red shift is demonstrated to be caused by non-Markovian friction between the graphene surface and interfacial water, which offers a direct method to extract solid-water interfacial friction properties from nonlinear spectroscopy.

O 87.4 Thu 15:45 TRE/PHYS

Structural Stability of NaCl and KCl Cleavage Surfaces in the BMIM-PF6 Ionic Liquid — •Ebru Cihan[1], Natalia Janiszewska[2], Kamil Awsiuk[2], Qingwei Gao[3], Rong An[4], Ronen Berkovich[5], and Enrico Gnecco[2] — [1]TU Dresden, Dresden, Germany — [2]Jagiellonian University, Krakow, Poland — [3]Shanghai University of Electric Power, Shanghai, China — [4]Nanjing University of Science and Technology, Nanjing, China — [5]Ben-Gurion University of the Negev, Beer-Sheva, Israel

An investigation was conducted into the evolution of freshly cleaved NaCl(100) and KCl(100) surfaces exposed to the ionic liquid (IL) 1-butyl-3-methylimidazolium hexafluorophosphate (BMIM-PF6). The surfaces were repeatedly scraped using AFM, resulting in contrasting responses from the two surfaces to the IL. In the case of NaCl, the cleavage step edges are slightly eroded, and the surface is progressively smoothed by the AFM tip. These changes are accompanied by a continuous increase in the friction force. In the case of KCl, a pronounced dissolution of the surface is evident immediately following contact with the IL. The surface is then smeared in the area scratched by the tip and even beyond. An increase in the friction force is also observed but only at the onset of the surface modification process. Crystallites (100-200 nm in size) are observed across the unscratched areas of KCl, but not of NaCl. This result was corroborated by MD simulations and Raman spectroscopy, which revealed that IL exhibits a stronger interaction with the KCl surface, ultimately forming a BMIM-PF6 adlayer. [1] E. Cihan et al., Langmuir 41, 13793 (2025)

O 87.5 Thu 16:00 TRE/PHYS

How Water Controls Ion Adsorption at Aqueous Interfaces via Entropic and Dielectric Interplay — •Florian Altmann[1], Matteo Olgiati[1], Moritz Zelenka[2], Joanna Dziadkowiec[3], Andreas Kretschmer[1], Alper T. Celebi[1], Laura L.E. Mears[1], Ellen H.G. Backus[2], and Markus Valtiner[1] — [1]Vienna University of Technology, Institute of Applied Physics, Wiedner Hauptstrasse 8-10, A-1040, Vienna, Austria — [2]University of Vienna, Faculty of Chemistry, Institute of Physical Chemistry, Währinger Straße 42, 1090 Vienna, Austria — [3]NJORD Centre, Department of Physics, University of Oslo, Oslo 0371, Norway

Ion-specific behavior at aqueous interfaces remains poorly understood. Using Li^+, Ca^{2+}, and Cs^+, we combine quantitative atomic force microscopy on muscovite mica with molecular dynamics simulations and sum-frequency generation spectroscopy to resolve interfacial thermodynamics at molecular resolution. Pair correlation functions link ion-water-surface organization to entropy and electrostatics. Small or highly charged ions compact interfacial water, creating entropic penalties and strong dielectric screening, whereas larger ions deplete interfacial water, lower screening, and promote overadsorption. This interplay between entropy and screening governs inner double-layer formation and provides a molecular framework for ion-specific adsorption in complex electrolytes.

O 87.6 Thu 16:15 TRE/PHYS

Accessing interfaces of ionic liquids in vacuum — •Florian Maier and Hans-Peter Steinrück — Lehrstuhl Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

About one decade ago, the perspective "Surface science goes liquid" described possibilities of investigating surfaces and interfaces of vacuum-stable liquids with surface science tools under ultrahigh vacuum (UHV).[1]

Since then, new experimental concepts and setups have been developed considering the special requirements for handling ionic liquids (ILs) in vacuum in order to push the boundaries of surface science experiments further.

In this presentation, some of our experimental developments including key showcases will be presented demonstrating at which level molecular properties of IL interfaces can be accessed under ultra-clean and well-defined UHV conditions.

References [1] H.-P. Steinrück, 2010, Surf. Sci. 604, 481-484 / DOI: 10.1016/j.susc.2009.12.033.

O 87.7 Thu 16:30 TRE/PHYS

Beyond the Electric Dipole Approximation: Electric and Magnetic Multipole Contributions Reveal Biaxial Water Structure from SFG Spectra at the Air-Water Interface — •Louis Lehmann[1], Maximilian R. Becker[1], Lucas Tepper[1], Alexander P. Fellows[2], Álvaro Díaz Duque[2], Martin Thämer[2], Martin Wolf[2], and Roland R. Netz[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Sum-frequency generation (SFG) analysis has been hindered by the lack of quantitative predictions for higher-order multipole contributions. Magnetic dipole and electric quadrupole terms, though determined by bulk properties, appear in all SFG spectra and obscure connections to interfacial structure. We present a simulation-based framework that predicts all multipole contributions and provides depth-resolved spectra for precise localization of features. Applied to the air-water interface, it reproduces experimental spectra across polarization combinations in both bending and stretching regions. Higher-order multipoles are essential: in the bending band, electric and magnetic dipoles are comparable, while the quadrupole dominates; in the OH-stretch region, the quadrupole accounts for the 3600/cm shoulder. Isolating the true second-order electric-dipole susceptibility reveals pronounced biaxial ordering of interfacial water and enables reliable interfacial structure determination from SFG spectra.

O 87.8 Thu 16:45 TRE/PHYS

Heat transfer across nanometre-sized water meniscus — •Oscar Mateos[1], Ruben Lopez[2], Pablo Martinez[1,3], Guilherme Vilhena[1], Nicolas Agrait[2,4], and Juan Carlos Cuevas[3,4] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049 Madrid, Spain — [2]Departmento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Heat transfer in nanoscale gaps is of key relevance for a variety of technologies. Recent experiments have reported contradictory results shedding doubts about the mechanisms for heat exchange in nanometre-sized gaps. We aim at resolving this controversy by measuring the thermal conductance of gold atomic-sized contacts with a custom-designed scanning tunnelling microscope that incorporates a novel thermal probe, enabling the measurement of thermal and electrical conductance in different transport regimes. When the electrodes are separated by a nanometre-sized gap, we observe thermal signals which cannot be explained with standard heat transfer mechanisms. Through non-equilibrium molecular dynamic simulations, we elucidate that these anomalous signals are due to thermal conduction through water menisci that form between tip and sample under customary operation conditions.

O 87.9 Thu 17:00 TRE/PHYS

Charging dynamics of the electrical double-layer in nanometre sized channels — •Marco Schönig, Serge Lemay, and Marc Koper — Leiden University, Leiden, The Netherlands

Nanoporous electrodes play a crucial role in modern energy storage and conversion technologies. However, despite their ubiquitous usage, the impact of nanoscale geometrical confinement on their electrochemical properties remains poorly understood. This is particularly relevant when the pore dimensions become so confined that the double layers of opposing sides overlap. A key challenge in studying this phenomenon in a systematic manner is the necessary precise control of the experimental dimensions[1]. We aim to bridge this gap by utilizing modern nanofabrication techniques to fabricate model gold slit electrodes[2].

In this contribution, we present the charging behaviour of electrodes with 5 - 20 nm wide slits, under confined and unconfined conditions. We further explore the usage of ATR-IR spectroscopy to probe the electrolyte in the slit electrodes by using micro-grooved Si wafers as substrate[3].

References [1] J. Wordsworth et al. Angew. Chem. Int. Ed. 2022, 61, e202200755; [2] L. Rassaei et al. J. Phys. Chem. C 2012, 116, 10913; [3] T. A. Morhart et al. Anal. Chem. 2017, 89, 11818.

O 88: Catalysis and surface reactions III

Time: Thursday 15:00–17:45 Location: TRE/MATH

O 88.1 Thu 15:00 TRE/MATH

Trapping ionomer for efficient proton exchange membrane fuel cells — •Fanpeng Kong — Harbin Institute of Technology, Harbin, China

Both uniformity of ionomer distribution and adsorption dynamics of side-chain sulfonates are paramount in determining the performance of low Pt-loaded membrane electrode assembly (MEA), particularly at high current densities. However, the heterogeneity of Pt/C leads to strong sulfonate anion adsorption on Pt sites and deleterious ionomer aggregation on the carbon support. Here, we synthesize atomic dipole modulated Pt/C (SCDC-Pt) electrocatalysts for low Pt-loaded MEA. Remarkably,this catalyst delivers a superior peak power density (1.4 W cm-2) and only a 15% of activity loss after 30 000 square-wave cycles. Operando characterization and computational analysis demonstrate that surface charged dipole facilitates homogenous ionomer distribution, while mitigating sulfonate poisoning of Pt. Electrochemical diagnostic technique establishes the low sulfonate coverage (~8%) and local O2 transport resistance (38.6 S m-1).This finding demonstrates the viability of rationally designed high-performance surface composition-homogenization low Pt-loaded MEA.

O 88.2 Thu 15:15 TRE/MATH

Molecular Beam Surface Scattering and PECD to Probe Chirality in Surface Reaction Products — Arved Dorst[1,2], Johannes Diedrich[1,2], Rasika Dissayanake[1,2], and •Tim Schäfer[1,2] — [1]Georg-August-University of Göttingen, Germany — [2]Max-Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

The epoxidation of olefins on Ag/O systems is an important industrial heterogeneous catalytic process. However, the mechanistic details of the surface reaction remain controversial, and it has been highly challenging to reconcile findings obtained under realistic reaction conditions with the highly detailed but static studies performed under ultra-high vacuum (UHV).

An additional level of complexity and opportunity arises when using prochiral olefin molecules. Their epoxidation can yield chiral epoxide products, provided the reaction pathway can be directed toward one enantiomer. In our studies, we combine molecular-beam surface scattering with laser spectroscopy to probe this process. By detecting the photoelectron circular dichroism (PECD) of the reaction products, we are able to determine their absolute chirality.

Our overarching goal is to achieve an atomistic understanding of reaction dynamics on chiral surfaces, ultimately bridging the gap between UHV studies and catalytic behavior under operational conditions.

O 88.3 Thu 15:30 TRE/MATH

From Processes to Mechanisms: Machine-Learning Based Automated Lattice Mapping as Prerequisite to Microkinetic Modeling — •Aditya Kumar[1], Patricia Poths[1], King Chun Lai[2], Christoph Scheurer[1], Sebastian Matera[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computing and Data Facility, Garching

Finding the reaction mechanism of a surface reactive system from first principles is a tedious task requiring a lot of human effort and being affected by human bias. To address these points, we have developed the Automatic Process Explorer (APE), which generates a comprehensive library of elementary reaction steps [1]. With easily thousands of steps identified, their manual assembly into a reaction network as a prerequisite to subsequent microkinetic modeling becomes intractable. To this end, we develop an automated framework that infers an effective lattice onto which all APE-discovered elementary steps may be coarse-grained. In this, atomic configurations from APE are analyzed using density-based hierarchical clustering, creating a fine-to-coarse hierarchy of potential lattice sites. All processes are then mapped onto the lattice as discrete occupation changes and, exploiting symmetry, a network of unique elementary reactions on this lattice is generated. We demonstrate the approach for a large set of elementary processes within the initial oxidation of Pd(100) terrace edges, and discuss the feasibility of subsequent efficient lattice-based microkinetic simulations.

[1] K.C. Lai *et al.*, Phys. Rev. Lett. **134**, 096201 (2025).

O 88.4 Thu 15:45 TRE/MATH

Investigating the Promotion Mechanism of Lanthanum on Cobalt Model Catalysts for Ammonia Production — •Clara C. Aletsee, Lau H. Wandall, Emanuel Biletter, and Ib Chorkendorff — DTU, Copenhagen, Denmark

Developing catalysts for ammonia synthesis under milder conditions than the Haber-Bosch process has gained significant interest. Recent studies demonstrate that usually unreactive magnetic materials, such as cobalt, can be activated for NH_3 synthesis by adding lanthanum.(1,2) According to theoretical calculations, this is attributed to not only an electrostatic, but also a beneficial spin promotion effect.(3) Herein, we examine the role of the promoter form on the catalytic performance. For this, either metallic La or La_2O_3 was deposited on a stepped Co(10-115) single crystal surface via e-beam evaporation. Additionally, mass-selected Co nanoparticles were deposited on two different magnetron-sputtered film supports: LaN and La_2O_3. All catalysts were characterized by X-ray photoelectron spectroscopy and low-energy ion scattering before and after reaction, and their activity was measured between 350-500°C at 1 bar in a UHV-compatible cell.(4) We show that Co/La_2O_3 exhibits the same activity as the LaN supported catalyst system at 350°C, but the stability decreases at higher temperatures.

References: (1) K. Zhang et al., Science 383, 1357 (2024). (2) T. N. et al., Nature 583, 391 (2020). (3) A. Cao et al., Nat Commun. 13 (2022). (4) K. Zhang et al., Rev. Sci. Instrum. 94, 114102 (2023).

O 88.5 Thu 16:00 TRE/MATH

Bridging the Pressure and Materials Gaps in NO Adsorption on Ceria — •Lukas Bolz[1], Ali Essa[1], Zairan Yu[1], Alexei Nefedov[1], Julia Vecchietti[2], Adrian Bonivardi[3], Yuemin Wang[1], and Christof Wöll[1] — [1]Insitute of Functional Interfaces, KIT, Eggenstein-Leopoldshafen, Germany — [2]Instituto de Desarrollo Tecnológico para la Industria Química, UNL, Santa Fe, Argentina — [3]Facultad de Ingenieria, UBA, Buenos Aires, Argentina

Nitric oxide (NO) is well known to have adverse effects on human health and the environment. One effective approach to decrease its emission is the selective catalytic reduction of NO over metal oxide surfaces. Understanding the reaction mechanisms, by tracking the structural changes of the active sites and intermediates as a function of reaction atmosphere and temperature, is crucial. Here, we present results on UHV-IRRAS and FTIRS as well as in situ/operando DRIFTS studies at atmospheric pressures and elevated temperatures to investigate the interaction between NO and ceria (CeO_2). A reliable assignment of the IR bands observed in the complex DRIFTS spectra was achieved based on accurate references obtained for NO molecules adsorbed on single crystal surfaces and nanocrystalline powders, thereby bridging the material and pressure gap for oxidic catalysts. The combined results enabled the tracking of facet-dependent surface transformations, the adsorption and reaction of NO, and the formation of intermediates such as nitrous oxide (N_2O). This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 426888090 - SFB 1441, project B03 and A04.

O 88.6 Thu 16:15 TRE/MATH

Competing reaction pathways in decomposition of 2-propanol over V-doped Co3O4(111) model catalyst: a mechanistic study. — •Patrick Hubert[1], Jan Smyczek[1], Maximilian Galinski[1], Lina Marquardt[1], Justin Girschik[1], Philipp Fredersdorff[1], Paul Fröhlich[1], Bernd Hartke[1], Guntram Rauhut[2], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 1, 24118 Kiel, Germany. — [2]Insitute of Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany.

This study investigated catalytic decomposition of 2-propanol over $Co_3O_4(111)/Au(111)$ and $VO_x/Co_3O_4(111)/Au(111)$ model catalysts to unravel competing reaction pathways toward acetone or propene. Ultra-high vacuum (UHV) surface science techniques were employed, including scanning-tunneling microscopy (STM), molecular-beam methods, infrared reflection absorption spectroscopy (IRAS), and temperature-programmed desorption (TPD). The $VO_x/Co_3O_4(111)/Au(111)$ surface exhibits structures with V^{3+}, V^{4+} adsorption sites and vanadyl groups (V=O). TPD measurements showed propene desorption at 480 K from 2-propanol adsorbed at 100 K on surfaces exceeding 0.6 ML VO_x coverage. At 180 K, 2-propanol dissociatively adsorbs on VO_x, consuming vanadyl groups during OH deprotonation, forming tilted 2-propoxy with surface-proximal methyl groups. At 400 K, a second intermediate forms via C-O bond scission and methyl deprotonation. IR spectra suggest this intermediate is a surface-bound propene-derived species.

O 88.7 Thu 16:30 TRE/MATH

Beyond U-Ce charge transfer: stabilization of Ce^{3+} states in epitaxial $Ce_{1-x}U_xO_2$ films grown on Ru(0001) — •Carlos Morales[1], Rudi Tschammer[1], Thomas Gouder[2], Hicham Idriss[3], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology, Cottbus, Germany — [2]European Commission, Joint Research Centre (JRC), Karlsruhe, Germany — [3]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Cerium oxide (CeO_2) stands out among reducible metal oxides for its stability and activity. Yet, promoting Ce^{3+} active states requires high energy. The conversion of Ce^{4+} to Ce^{3+} at lower temperatures for the thermochemical splitting of H_2O or CO_2 can be enhanced by doping ceria with other elements. Particularly, ceria mixing with uranium has been proven successful: substituting a fraction of Ce^{4+} by U^{4+} results in a charge transfer that promotes the formation of Ce^{3+} and U^{5+} states. We have explored the redox properties of 8 nm thick epitaxial (111)-oriented $Ce_{1-x}U_xO_2$ on Ru(0001). In line with previous studies focused on polycrystalline powders, the as-grown films exhibit a high Ce^{4+} to Ce^{3+} conversion, with a maximum reduction corresponding to approximately 20 % of U content. However, the concentration of Ce^{3+} states and oxygen is higher than predicted by density function theory (DFT) calculations for various U contents and spatial ordering. The observed behaviour could be likely related to the lattice distortion caused by the significant difference in the ionic radii of Ce^{3+} and U^{5+}. This effect has not been considered before in $Ce_{1-x}U_xO_2$ mixed oxides.

O 88.8 Thu 16:45 TRE/MATH

Product Selectivity in Fischer-Tropsch Synthesis — •Benjamin Rasmus Grimm, Luis Antonio Cipriano Marcos, Oliver Christensen, and Jens Kehlet Nørskov — DTU Physics, Kongens Lyngby, Denmark

The product selectivity and activity of Fischer-Tropsch synthesis (FTS) is important for producing synthetic fuels and chemicals from natural gas, coal, or biomass. Some catalysts generate mainly undesired methane, whereas others show higher selectivity toward longer hydrocarbons. In this study, density functional theory (DFT) is employed to calculate the activity- and selectivity-determining reaction steps and energy barriers of FTS on cobalt-based catalysts. Reaction rates and product selectivities are then evaluated using a microkinetic model that incorporates the rate- and selectivity-determining steps of the FTS mechanism. To describe the catalyst as realistically as possible, adsorbate coverage and migration effects under experimental conditions are taken into account. Finally, strategies to improve reaction rates and selectivity are discussed.

O 88.9 Thu 17:00 TRE/MATH

Low-Temperature CO2 Methanation over Ni/Ce-Sm Oxide Catalysts — •Rachow Fabian, Sichen Liu, Evgenia Charlafti, Raquel Sánchez-Barquilla, and Jan Ingo Flege — Brandenburg University of Technology, Cottbus-Senftenberg, Germany

Nickel catalysts on doped ceria are attractive for CO_2 methanation due to their redox flexibility and potential for improved efficiency and stability. In this work, we investigate Ni supported on mixed Ce–Sm oxides with Ce:Sm ratios of 3:1, 2:1, and 1:1. The catalysts are tested as powders in a fixed-bed flow reactor between 250 and 400°C and benchmarked against a conventional Ni/Al_2O_3 catalyst. Among the compositions, the Ce:Sm ratio of 2:1 shows the highest CO_2 conversion, with a pronounced enhancement in low-temperature activity compared to Ni/Al_2O_3. To relate performance to material properties, we combine X-ray diffraction (XRD), temperature-programmed reactivity (H_2-TPR), Raman spectroscopy, high-resolution transmission electron microscopy (HRTEM/EDX), as well as in-situ X-ray absorption near-edge spectroscopy (XANES) under reaction conditions, elucidating how Sm incorporation and Ce:Sm ratio influence the structural and redox characteristics of the oxide support, oxygen vacancy formation, and Ni dispersion, which together govern catalytic activity and stability. To assess practical applicability and scale-up, the optimized Ni/Ce–Sm (2:1) oxide formulation is deposited on Al_2O_3 spheres and evaluated under conditions representative of packed-bed operation with a limited amount of active material, revealing high conversion and stable, efficient operation in low-temperature CO_2 methanation.

O 88.10 Thu 17:15 TRE/MATH

Heteroepitaxial growth of Sm_2O_3 nanoislands on Cu(111) — •Björn Riedel[1], Raquel Sánchez-Barquilla[1], Lars Buss[1], Iulia Cojocariu[2], Tevfik Onur Mentes[2], Andrea Locatelli[2], and

Jan Ingo Flege[1] — [1]Brandenburg University of Technology, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste, Basovizza, Italy

Doping of CeO_2 with samarium can significantly influence its redox behavior by promoting the formation and stabilization of reduced Ce^{3+} species. Yet, studies of well-defined samaria model systems grown on single-crystal surfaces are scarce, leading to a lack of combined structural and spectroscopic studies and, hence, a gap in understanding the relationship between samaria's structure and its chemical behavior. We have investigated hexagonal and monoclinic Sm_2O_3 nanoislands grown on Cu(111) using a multi-method approach with high structural and chemical sensitivity, employing low-energy electron microscopy (LEEM), micro-spot diffraction (μLEED) and intensity-voltage LEEM in combination with X-ray absorption spectroscopy photoemission electron microscopy (XAS-PEEM). To study the influence of different structures and phases on the chemical behavior of Sm_2O_3 islands, we have examined their redox properties under reducing (H_2) and oxidizing (O_2) conditions. The results indicate a highly dynamic system that can be readily adjusted by varying the conditions during deposition, such as growth temperature and oxygen partial pressure.

O 88.11 Thu 17:30 TRE/MATH

Surface Modifications in Complex Mixed Oxide Activation for the Selective Oxidation of Hydrocarbons — •Kyeonghyeon Nam[1], L. Masliuk[1], T. Jones[1], Y. Song[1], A. Trunschke[1], R. Schlögl[1], T. Lunkenbein[1,2], K. Reuter[1], and C. Scheuer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Calcination (thermal activation) is crucial for metal-oxide catalysts, enhancing activity and durability by preparing surface morphology and active sites. However, thermal treatment also induces dynamic surface changes, such as defect formation, reconstruction, and grain reorientation, complicating the continuous monitoring of a catalyst's surface. Here, identical-location STEM imaging of a ternary M1 (Mo,V)O_x catalyst reveals that the (hk0) surface undergoes pronounced modification under calcination and oxidative dehydrogenation (ODH) conditions. The surface evolution is modeled using machine learning force fields. Molecular dynamics (MD) simulations reproduce the reconstruction of extended M1 regions from MoO_2-like motifs, as well as mass transport within the pentagonal motif that further activates the catalyst. Experimentally observed catalytic activity changes can be assigned to the presence of highly charged surface metal centers via DFTB Mulliken charge analysis. These surface transformations strongly influence the catalytic properties of ternary M1 catalysts, suggesting potential applications in improving catalytic performance through controlled surface modifications.

O 89: Spins on surfaces at the atomic scale II

Time: Thursday 15:00–18:00 Location: WILL/A317

O 89.1 Thu 15:00 WILL/A317

Magnetization Curves of Antiferromagnetic Spin Chains: Probing the Quantum to Classical Crossover — •Henrik Lichtl[1,2], Lukas Veldman[1,2], Nicolaj Betz[1,2], Johannes Schust[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss- Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna.

As the size of a magnetic structure increases it undergoes a transition from a quantum system to a classical magnet, yet the evolution of the magnetization behavior at this crossover is largely unexplored. Here we introduce an approach to record high-speed magnetization curves in a scanning tunneling microscope (STM), reaching magnetic field sweep rates of up to 40kT/s. We analyze the statistics of the transitions between the two antiferromagnetic ground states of antiferromagnetic Fe spin chains on a Cu2N surface, which allows us to distinguish between quantum and classical regimes in their magnetization curves. Quantum signatures diminish rapidly with size of the chain, where chains longer than five atoms already show characteristics of classical nanoscale magnets. Accessing such high-speed magnetization curves at the atomic scale brings concepts originally developed for bulk materials into the STM, offering insight into how quantum spins interact with their environment during the quantum-to-classical transition.

O 89.2 Thu 15:15 WILL/A317

Optimizing On-Surface Quantum Spins for Quantum Information Processing — •Denis Jankovic[1,2], Hoang-Anh Le[1,2], Saba Taherpour[1,3], and Christoph Wolf[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Departement of Physics, Ewha Womans University, Seoul, Republic of Korea

The bottom-up engineering of quantum-coherent spins on surfaces with STM enables atomically precise quantum logic in on-surface qubits, and atomic-scale multi-qubit devices.

We use optimal control on an open-system model of exchange-coupled surface spins to counter decoherence, static coupling, and imperfect initialization, identifying high-fidelity gates compatible with current ESR-STM constraints.

Finally, building on advances in electrically driven nuclear spins, we will outline ongoing experiments using lanthanides on surfaces, where ESR-STM manipulates hyperfine-coupled nuclear-spin manifolds as on-surface qudits.

O 89.3 Thu 15:30 WILL/A317

Spin Lifetime Engineering using Superconducting Surfaces — •Máté Stark, Luise Renz, Jonas Arnold, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Extending the spin lifetime (T_1) and decoherence time (T_2) of atomic and molecular spins is central to realizing quantum-coherent spin systems on surfaces studied by scanning tunneling microscopy (STM). For instance, previous studies have demonstrated that T_1 can be extended to nanoseconds for Fe-OEP-Cl on superconducting Pb(111) to milliseconds for Fe on MgO/Ag(001) by exploiting superconducting protection or electronic decoupling, respectively [1,2].

Building on these concepts, we aim here to combine protection by a superconducting gap and insulating decoupling layers to explore and control spin lifetimes of single FePc spins. By switching from the normal-conducting into the superconducting state we discuss how superconductivity as well as decoupling from the substrate and tip govern the lifetime and dynamics of molecular spin excitations. We show first results using all electric pump-probe spectroscopy, which are performed in a home-built dilution refrigerator scanning tunneling microscope operating at 50 mK. [1] Nat. Phys. 9, 765 (2013) [2] Nat. Phys. 13, 403 (2017)

O 89.4 Thu 15:45 WILL/A317

Bottom-up realization of band structure using arrays of individual Cs atoms on InSb(110) — •Niek M.M. Aarts, Kira Junghans, Roel Burgwal, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud Universiteit, Nijmegen, Netherlands

The combination of atomic manipulation and scanning tunneling spectroscopy has become a powerful platform for quantum simulation of electronic structure. The approach is based on the atomically precise placement of atoms and the flexibility to realize structures with a variety of shapes and symmetry. Inherent to this approach is role of finite size effects in the tailored electronic structure. This plays an integral role in understanding the influence of various interactions, like spin-orbit interactions, or electron-electron interactions, on any potential quantum phase of matter to be simulated.

Here, we study the evolution of the electronic structure as a function of lattice size, using the recently discovered quantum simulator platform of Cs on InSb(110). Using STM, we start by studying structures that exhibit atomic like states and expand these structures into the molecular limit. We study the changes in the localized states and the symmetry of the responsible wavefunctions. We then quantify the increase of states as the number of sites in the system increases, and band structure emerges. We also discuss the role of the size of the artificial atomic sites. This extension of the Cs/InSb(110) quantum simulator to larger systems enables the study of artificial band structure in the presence of strong SOC.

O 89.5 Thu 16:00 WILL/A317

Crystal field manipulation of magnetic atoms on an insulating surface — •Julian Zeitler[1], Johannes Schust[1], Nicolaj Betz[1,2], Lara Mezger[1], Lukas Veldman[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Philip Willke[5], Sebastian Loth[1,2], and Susanne Baumann[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna. — [5]Karlsruhe Institute of Technology, Physikalisches Institut.

The magnetic behavior of ions in solid-state materials is predominantly driven by their immediate atomic-scale environment. The specific arrangement of surrounding charges creates a crystal field (CF), which alters and mixes the electronic states. For magnetic atoms on insulating thin films, this CF is strongly influenced by the atom's adsorption site on the underlying lattice. Using combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM), we investigate the CF influence on magnetic atoms on thin-film MgO and use tip-atom forces to precisely reposition the atoms within their binding sites, thereby tuning the CF. We quantify changes of the local binding geometry by combining our measurements with multiplet calculations. Our measurements pave the way for harnessing magneto-elastic effects in individual atoms either by manipulating their magnetic properties via electric fields or local forces, such as mechanical strain.

O 89.6 Thu 16:15 WILL/A317

Topological End States of Chiral Graphene Nanoribbons on Proximitized Superconducting Au (111) — •Trisha Sai[1], Frederik Bauer[1], Stefano Trivini[1], and Jose Ignacio Pascual[1,2] — [1]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Graphene nano-structures may host localized magnetic moments characterized by their geometry, heteroatom substitution, topological frustration, or bulk-boundary correspondence. However, observation of their open-shell configuration via on-surface synthesis can be inhibited due to charge transfer. This is in the case of (3, 2, 8) chiral graphene nanoribbons (chGNRs) synthesized on Au(111), whose symmetry-protected topological end states (SPTES) are quenched due to electron depopulation. In this work, we synthesize (3, 2, 8) chGNRs on thin films of Au (111) grown on a superconducting Nb (110) single crystal. Through controlled deposition of monolayers of Au, we observe a modulation in the surface state of Au (111), thereby a reduction in the work function of the resulting platform. Moreover, the substrate is also complemented with proximity induced superconductivity. Low-Temperature scanning tunneling spectroscopic (STS) measurements reveal that the SPTES of (3, 2, 8) chGNRs are retained in a mixed-valence regime where their spectral weight is distributed between an in gap Yu-Shiba-Rusinov (YSR) state and an orbital state close to Fermi energy. In case of a depopulated terminus, the YSR states are weak and suppressed while the orbital state is more pronounced.

O 89.7 Thu 16:30 WILL/A317

Confinement-modulated spin-orbit coupling tuned with atomic-scale gating fields — •Hermann Osterhage, Julian H. Strik, Anna M. H. Krieg, Ivan Ado, Mikhail Titov, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

In 2D, inversion symmetry breaking combined with a sizeable potential gradient leads to the well-known Rashba spin-orbit coupling (SOC), locking the spin and momentum. Using potential gradients to induce SOC is not limited to the Rashba case, but may be extended to lower dimensional structures, such as quantum dots. However, tuning SOC in these limits is challenging: it requires potential gradients that are comparable to the size of the confined structure itself.

Here, we demonstrate a new type of SOC, akin to the Rashba effect, where large potential gradients are formed within an atomically patterned quantum dot. Using low-temperature scanning tunnelling microscopy and spectroscopy we create quantum dots of various shapes and sizes by patterning individual Cs ions on the surface of InSb(110). We find that we can tune the confinement potential, as shown by the presence of multiple localized states. In addition, by probing the resultant multiplet structure, we identify zero-field splittings within a given quantum dot that are induced by the geometry of the potential. We also discuss the magnetic field dependence of this level structure and explain the findings based on the 8-band Kane model.

[1] E. Sierda et al, Science 380, 1048 (2023).

O 89.8 Thu 16:45 WILL/A317

Tuning the Kondo temperature of MoS$_2$ mirror twin boundaries on graphene — •Tfyeche Y. Tounsi[1], Kuber Vyas[1], Camiel van Efferen[1], Affan Safeer[1], Achim Rosch[2], Jeison Fischer[1], Thomas Michely[1], Theo A. Costi[3], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

In scanning tunneling spectroscopy, the dI/dV signatures of the Kondo effect in MoS$_2$ mirror twin boundaries (MTBs) are the zero-bias resonance peak, in addition to the impurity levels [1]. The experimental data give access to the Anderson model parameters; The splitting U of the non-degenerate states, the impurity orbital's position ϵ with respect to E$_F$, and the impurity level's bare width γ_0.

In this work, we compare the Kondo temperature T$_K$ measured in MTBs of MoS$_2$ grown on three different substrates. In the case of MoS$_2$ / Graphene (Gr) / Ir (111), T$_K$ was in the range [10^{-4} K, 10^{-10} K] [1]. By intercalating with a single layer of Eu under Gr, we have noticed a decrease of γ_0, leading to a drop in T$_K$. The third system, MoS$_2$ / Gr / Ir (110), T$_K$ increased significantly to the range [1 K, 10 K]. This enabled us to study the Kondo effect at the boundary between the weakly screened magnetic state above T$_K$ and the Kondo singlet state below T$_K$.

References: [1] C. van Efferen et al, Nat. Phys. 20, 82-87 (2024).

O 89.9 Thu 17:00 WILL/A317

Statistical analysis of electron-induced switching of a spin-crossover complex — •Jonas Fussangel[1], Björn Sothmann[1], Sven Johannsen[2], Sascha Ossinger[3], Felix Tuczek[3], Richard Berndt[3], Jürgen König[1], and Manuel Gruber[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spin-crossover complexes switch between two spin states, but the microscopic pathway remains unclear. Using low-temperature STM, electron-induced switching of [Fe(H$_2$B(pz)(pypz))$_2$] on Ag(111) has opened new perspectives for understanding the switching mechanisms. Current time traces show two levels matching the spin states. An analysis of waiting-time distribution yields switching rates whose voltage dependence is explained by a simple model where transient molecular charging triggers switching. Comparing experiment and theory provides previously inaccessible estimates of LUMO energies [1]. The approach offers new insights into the switching mechanism and predicts higher switching rates when the molecule is electronically decoupled from the substrate, e.g., by introducing an ultrathin insulating layer.

[1] J. Fußangel et al., *arXiv*: 2506.13373 (2025)

O 89.10 Thu 17:15 WILL/A317

Decoupling strategies for YPc$_2$ molecular spin qubit platforms on metal surfaces — Franklin H. Cho[1,2], Soyoung Oh[1,2,3], Dan Chi Nguyen[1,2], Jinjoo Lee[1,2], We-hyo Soe[1,2], Luciano Colazzo[1,2], Jisoo Yu[1,2], Pierre Josse[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], Christoph Wolf[1,2], and •Fabio Donati[1,2] — [1]IBS Center for Quantum Nanoscience, South Korea — [2]Ewha Womans University, South Korea — [3]The Clarendon Laboratory, University of Oxford, The United Kingdom

Yttrium phthalocyanine double-decker (YPc$_2$) is an appealing building block for surface spin-qubit architectures due to its delocalized $S = 1/2$ radical and planar structure [1]. Here, we investigated the morphology, electronic structure, and spin properties of single- and multi-layer YPc$_2$ on Cu(111) single crystals and on zinc phthalocyanine (ZnPc) grown on Cu(111). Low temperature scanning tunneling microscopy reveals the molecular layer structure and the variation of its electronic configuration when directly adsorbed on Cu(111) versus on a ZnPc decoupling layer [2]. X-band electron spin resonance using our custom-built surface-sensitive spectrometer [3] shows that the YPc_2 radical is preserved on ZnPc but quenched upon direct contact with Cu(111). Density functional theory attributes this quenching to the hybridization of molecular orbitals with the substrate electrons. Our study highlights the necessity of suitable decoupling layers to preserve radical spins near metallic surfaces. [1] F. Branzoli et al., Phys. Rev. B 83, 174419 (2011). [2] S. Oh et al., Nanoscale 17, 22163 (2025). [3] F. H. Cho et al., Rev. Sci. Instrum. 95, 063904 (2024).

O 89.11 Thu 17:30 WILL/A317

Inelastic Zoo: Spin, Vibrational, and Orbital Excitations in Conductance Spectra — •Arnab Banerjee, Richard Berndt, and Alexander Weismann — Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany

First-principle predictions of excitation energies and cross sections in inelastic tunneling spectroscopy are challenging, making it difficult to assign experimental features to specific excitations. There is a need for a reliable identification of conductance features. We investigated the spin-1/2 molecule cobaltocene on superconducting Pb(110) and use Yu-Shiba-Rusinov states combined with a superconducting tip to detect a large number of sharp spectral features. From a peak shape analysis, we find the coexistence of spin, vibrational, and orbital excitations within a single conductance spectrum.

O 89.12 Thu 17:45 WILL/A317

Current-induced Electron Spin Polarization in Magnetic Molecules — •Paul Greule, Wantong Huang, Máté Stark, Kwan Ho Au-Yeung, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron spins of single molecules offer a promising platform for quantum information processing. To harness such spins as functional qubits, efficient initialization is essential. Electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) has emerged as a powerful technique to probe molecular spins at the atomic scale. Using this technique, it has been shown that a spin-polarized tunnelling current can polarize the nuclear spin of a single Cu atom [1]. In this talk, we show that this concept can be transferred to the electron spin of molecules: Using Fe-FePc complexes with an electron spin of S=1/2 [2], we build molecular dimers. Here, the first complex serves as a readout and pumping system, while the energy-level occupation of the second complex is probed and manipulated. The exchange interaction between them enables remote spin-pumping, where angular momentum is transferred. Controlling the spin-polarized tunnel current via the bias voltage allows us to tune the spin polarization of the second complex remotely. Our findings establish an all-electrical technique to initialize molecular spin qubits and provide insights for enhanced control schemes. [1] K. Yang et al., Nat Nano 2018, 13, 1120-1125 [2] W. Huang et al., Nat Commun 2025, 16, 5208

O 90: Members' Assembly of the Vacuum Science and Technology Divison (VA)

Time: Thursday 17:15–18:15 Location: HSZ/0401

All members of the Vacuum Science and Technology Division are invited to participate.

O 91: Members' Assembly

Time: Thursday 19:00–19:30 Location: HSZ/AUDI

All members of the Surface Science Division are invited to participate.

O 92: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: HSZ/AUDI

Contributed Post-Deadline Talks

O 93: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Friday 9:30–12:00 Location: HSZ/0201

O 93.1 Fri 9:30 HSZ/0201

Identifying Electronic Doorway States in Secondary Electron Emission — •Anna Niggas[1], Maosheng Hao[2], Peter Richter[3], Felix Blödorn[1], Florian Simperl[1], Alessandra Belissimo[4], Joachim Burgdörfer[2], Thomas Seyller[3], Wolfgang Werner[1], Florian Libisch[2], and Richard A Wilhelm[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute for Theoretical Physics, TU Wien, Vienna, Austria — [3]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Photonics, TU Wien, Vienna, Austria

Secondary electron emission following low-energy (<200 eV) electron impact is fundamental to particle-solid interactions but remains incompletely understood. While high-energy electrons are described by reflected primaries undergoing inelastic losses, the low-energy (<20 eV) region is often considered featureless. Coincidence spectroscopy has revealed hidden structures, notably the 3.3 eV X peak in graphite arising from plasmon excitation and interlayer-state hybridisation. Following that, we have measured low-energy secondary electrons from graphite and quasi-freestanding single- and bilayer graphene, enabling a controlled transition from bulk to two-dimensional systems. We observe layer-dependent features and, supported by density functional theory, attribute them to Feshbach-type resonances of quasi-bound above-vacuum states coupling to the continuum. The strong 3.3 eV resonance appears only in systems with five or more layers [1].

[1] A. Niggas et al., Phys. Rev. Lett. 135, 166401 (2025)

O 93.2 Fri 9:45 HSZ/0201

A novel approach to depth-resolved magnetic spectoscopy: grazing-incidence XMCD — •Umut Parlak[1], Katharina Wehrstein[1], Pia Maria Düring[1], Oliver Rehm[1], Endrit Kusari[1], David Capalbo[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [3]Peter Grünberg Institut, PGI-6, Research Centre Jülich, 52425, Jülich, Germany

Magnetic depth profiling plays a key role in understanding inter- and intra-layer magnetic coupling mechanisms in multilayer thin films. We employ a synchrotron-based photoelectron spectroscopy approach (P22 beamline, DESY) to measure x-ray magnetic circular dichroism with depth-resolution taking EuO thin films grown on heavy metal (HM) underlayers as prototype sample. The presence of HM underlayer enables the near-total reflection x-ray excitation, where the incident and reflected x-rays interfere at the grazing angles forming high-intensity nodal points. The depth-resolution is achieved by probing at angles between 0.2 and 1°, i.e., tuning the position of the nodal points. Simulations of the x-ray intensity profile at these low angles allow us to optimize the MBE-grown MgO/EuO/HM trilayer structure for accessing both the upper and lower interfaces. Our results reveal the distribution of Eu^{2+} and Eu^{3+} ions throughout the EuO layer, which form ferromagnetic and paramagnetic oxides, respectively. The valency profile of the Eu ions directly aligns with the magnetic asymmetry profile.

O 93.3 Fri 10:00 HSZ/0201

Experimental Verification of the d-band Center Model in Au/Pt Systems: A Low-Energy XPS Study — •Justyna Piwowar[1,2,3] and Adam Lewera[3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Faculty of Chemistry, University of Warsaw Pasteura 1 02-093 Warszawa

This work presents an experimental verification of the relationship between electronic structure and electrocatalytic properties in Pt-based materials, specifically critically evaluating the d-band center theory. Using Au-modified Pt as a model system, surface electronic properties were probed via X-ray Photoelectron Spectroscopy (XPS). We demonstrate that employing low-energy X-ray sources (Zr Mγ, 151 eV) provides superior surface sensitivity compared to standard sources (~1500 eV), allowing for the detection of subtle surface electronic shifts otherwise masked by bulk signals.

We observed a nonlinear evolution of electronic properties in Au/Pt thin films, specifically in core-level binding energies, which correlates with synergistic catalytic activity in formic acid oxidation. Detailed analysis of the valence band spectra reveals that significant modifications in the Density of States (DOS) near the Fermi level can occur even when the calculated shift in d-band center is negligible, due to spectral redistribution on both sides of the centroid. These findings indicate that the d-band center parameter alone may be insufficient to describe complex electronic structure modifications.

O 93.4 Fri 10:15 HSZ/0201

Spin Polarization of Photoelectrons Excited by Deep-UV Pulses with Orbital Angular Momentum — •Paul Valerian Möllers, Ruwen Quenter, and Helmut Zacharias — Center for Soft Nanoscience, Universität Münster

It is well known that circularly polarized light can excite longitudinally spin-polarized photoelectrons from centrosymmetric crystal surfaces [1]. The light carries an angular momentum of $\pm\hbar$, and the selection rules dictate that the photoexcitation occurs into final states with a specific total angular momentum. In the presence of spin–orbit interaction, states with different total angular momenta are energetically separated, and the excited electrons can exhibit a net spin imbalance. Light with helical wave fronts carries orbital angular momentum as a degree of freedom that is independent of its polarization and not limited to $\pm\hbar$ [2]. As the light always acts on the orbital electron angular momentum during photoexcitation, it appears plausible to assume that the optical orbital angular momentum could translate into a nonzero photoelectron spin polarization. This hypothesis has yet to be tested experimentally. We present preliminary results of spin-resolved photoemission measurements on Cu(111) and Au(111) surfaces that address this issue. [1] G. Borstel, M. Wöhlecke, Phys. Rev. B 26, 1148-1155 (1982) [2] S. S. R. Oemrawsingh et al., Appl. Opt. 43, 688-694 (2004)

O 93.5 Fri 10:30 HSZ/0201

Imaging stripe dynamics in superconducting nickelate — •Uladzislau Mikhailau[1], Luke C. Rhodes[1], Matthias Hepting[2], Masahiko Isobe[2], Pascal Puphal[2], and Peter Wahl[1,3] — [1]University of St Andrews, St Andrews, United Kingdom — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [3]Physikalisches Institut, Universitat Bonn, Germany

In the Hubbard model, there is a competition between charge localization due to Coulomb repulsion and delocalization due to the energy reduction from electrons hopping between sites. When both tendencies are equally strong, a unique correlated stripe order can be stabilized [1]. Such a state is known to be realized in lightly doped high temperature superconducting cuprates and in nickelates.

Our STM investigation shows that commensurate stripe order forms in the metallic state of the recently discovered high-temperature superconductor $La_4Ni_3O_{10}$. Quasi-1D channels of delocalized charge appear as solitonic domain walls in charge density probed by STM. Interestingly, electrons tunnelling from the tip can induce local stripe fluctuations, pointing at the weak pinning of the order to the lattice.

Observation of stripe orders in normal states of high temperature cuprates and nickelates suggests shared correlated physics as a precursor to high-temperature superconductivity in both systems. Such experimental evidence is a valuable foundation for investigations into the mechanism of high-temperature superconductivity in both systems.

[1] J. Zaanen and O. Gunnarsson. Phys. Rev. B, 40(10):7391-7394 (1989).

O 93.6 Fri 10:45 HSZ/0201

Surface Rashba effect influence on bulk states: test case on Au(111) — •Laurent Nicolaï[1], Ján Minár[1], Christine Richter[2,3], Olivier Heckmann[2,3], Laxman Nagi Redi[2,3], Sourour Ayari[1], Aki Pulkkinen[1], Mauro Fanciulli[2,3], and Karol Hricovini[2,3] — [1]University of West-Bohemia in Pilsen, Czeck Republic — [2]CY Cergy Paris Université, France — [3]Université Paris-Saclay, CEA, France

Au(111) crystals are commonly used in the Photo-emission Spectroscopy field to calibrate instruments. When coming to spin-resolved ARPES, one uses the well-known surface states, spin-split due to the Rashba effect [1,2], as a reference. Au(111) being a centro-symmetric material, it is commonly assumed that bulk sates are spin degenerate. However, we here present measurements attesting a spin polarisation of bulk states within the valence band. The measurements are complemented with ab-initio calculations confirming the existence of bulk states' spin polarisation on a fundamental level.

[1] Yu A. Bychkov and E. I. Rashba, J. of Phys. C: Sol. St. Phys., 17:6039-6045, 1984 [2] S LaShell et al. , Phys. Rev. Lett. 77 3419, 1996

O 93.7 Fri 11:00 HSZ/0201

calcQPI - a tool to simulate quasiparticle interference — •Peter Wahl[1,2], Luke Rhodes[1], and Carolina de Almeida Marques[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom — [2]Physikalisches Institute, Universität Bonn

Quasiparticle interference imaging (QPI) is a powerful tool to study the low energy electronic structure of quantum materials and one of a few methods that can provide phase-sensitive information about the superconducting order parameter of unconventional superconductors, but the interpretation of QPI often requires complex modelling. This talk introduces calcQPI[1,2] as a new tool for the realistic simulation of QPI measurements. CalcQPI allows for the calculation of QPI from tight-binding models for a wide range of quantum materials, including magnetic materials, topological insulators and unconventional superconductors. I will give an overview of its capabilities and a few examples of how it can be applied to real materials.

[1] P. Wahl, L.C. Rhodes, C.A. Marques, calcQPI: A versatile tool to simulate quasiparticle interference, SciPost Phys. Codebases 61 (2025). [2] P. Wahl, L.C. Rhodes, C.A. Marques, Codebase release 1.0 for calcQPI, SciPost Phys. Codebases 61-r1.0 (2025).

O 93.8 Fri 11:15 HSZ/0201

Defect-driven polarity compensation on weakly polar $BaTiO_3$ (001) and $SrTiO_3$ (001) surfaces. — •Darin Joseph[1], Llorenç Albons[4], Florian Ellinger[2], Michele Reticcioli[2,3], Martin Setvin[4], and Cesare Franchini[1,2] — [1]University of Bologna, Italy — [2]University of Vienna, Austria — [3]CNR-SPIN, L' Aquila, Italy — [4]Charles University, Prague , Czech Republic

$BaTiO_3$ (001) and $SrTiO_3$ (001), commonly classified as Tasker Type I and nonpolar, exhibit surface instability, as evidenced by A-site (Ba/Sr) adatoms and vacancies on cleaved surfaces observed in experiments. Density Functional Theory (DFT) calculations revealed the work function variation between the TiO_2 and AO terminations and an electric field in the vacuum of asymmetric slabs, which are typically associated with polar surfaces. Our study reveals that both perovskites exhibit weak polar stacking along the crystallographic axis, leading to surface charges on the pristine terminations and creating an unfavorable electrostatic environment. Our analysis shows that the experimentally observed A-site defects act as compensation mechanisms by counterbalancing these charges to restore charge equilibrium. Charge compensation occurs at 12.5% Sr adatom and 12% vacancy coverage for $SrTiO_3$ and at approximately 12-13% defect concentration for $BaTiO_3$. These theoretical values are consistent with the experimental defect concentrations.

O 93.9 Fri 11:30 HSZ/0201

3D Mapping of Photoelectron Diffraction Patterns at Very

Low Energies — •O. Tkach[1], T.-P. Vo[2], D. Biswas[3], J. Liu[3], O. Fedchenko[1,4], T.-L. Lee[3], J. Minár[2], H.-J. Elmers[1], and G. Schönhense[1] — [1]Univ., Mainz — [2]Univ. of West Bohemia, Czech Republic — [3]Diamond Light Source, UK — [4]Goethe Univ. Frankfurt

The full-field recording architecture of momentum microscopes (MMs) efficiently captures the (E,k) valence band structure along with the corresponding dichroism and spin texture [1]. Here, we apply the same approach to photoelectron diffraction (PED) in the low-energy range. Capturing PED in a solid angle up to 2π, including the corresponding core-level CDAD [2] reveals a wealth of structure far beyond that of standard PED measurements. The experiments are compared with calculated three-dimensional (E,k_x,k_y) patterns obtained via one-step photoemission calculations using the PED implementation [3] within the SPRKKR package. Calculated results over a wide range of kinetic energies (106 – 1036 eV) for the Ge 3d core level reveal striking patterns that change rapidly with photon energy. The high-energy end provides insight into bulk (Kikuchi-) diffraction, while the lower end with its high surface sensitivity yields structural information about the surface. This is indicative of the transition from a localized core level to an itinerant, time reversed LEED photoemission final state. In general, these results bridge the gap between PED analysis and electronic structure investigations.

[1] Medjanik et al. Nat. Mater 16, 615 (2017); [2] Tkach et al. Ultramic. 250, 113750(2023); [3]Vo et al. npj Comput. Mater.11, 159(2025)

O 93.10 Fri 11:45 HSZ/0201

Shaping Surface States: The Art of Designing Quantum Corrals — •Nadine Egger, Simon B. Hollweger, and Oliver T. Hofmann — Institute of Solid State Physics, TU Graz, Austria

Quantum corrals enable precise control over electron behavior on surfaces and can be designed to carry out tasks such as atomic-scale logic operations. However, determining the optimal corral shape and the precise placement of the individual building blocks is a nontrivial task. To address this, we introduce a simulation-based framework that automatically designs corral geometries to achieve specific functionalities. The approach combines surface-state electron simulations with an optimization algorithm that identifies not only the number of atomic building blocks required but also their optimal arrangement on the surface. As a first application, the framework is applied to design corrals capable of performing basic logic operations, such as AND or NOT gates. Beyond these examples, this method offers a versatile path toward creating atomically precise nanostructures with customized functional properties, paving the way for future developments in quantum device engineering.

O 94: Oxides and insulators: Adsorption and reaction of small molecules

Time: Friday 9:30–12:30 Location: HSZ/0204

Invited Talk O 94.1 Fri 9:30 HSZ/0204

Surface Chemistry on Copper Oxides — •Dario Stacchiola — Brookhaven National Laboratory, Upton NY, 11720, USA

The chemical and electronic properties of copper combined with its large natural abundance lend this material to impact a wide range of technological applications, including heterogeneous catalysis. The reactivity of copper in its Cu1+ oxidation state makes this specific state relevant in various chemical reactions, but the facile redox properties of copper make the isolation of individual states for fundamental studies difficult. I will present our work on model systems including Cu2O/Cu(111) films, bulk Cu2O crystals and copper-based mixed-oxides used to study the interaction of Cu1+ with small molecules making use of in-situ surface science techniques. Advantages and disadvantages of each system are discussed and exemplified through case studies of chemical adsorption and reactivity studies

O 94.2 Fri 10:00 HSZ/0204

Calculating vibrational bands for formic acid on magnetite surfaces — •Gregor Vonbun-Feldbauer — Institute for Interface Physics and Engineering, TU Hamburg, Germany — Institute of Surface Science, Helmholtz-Zentrum hereon, Germany

Understanding the adsorption properties of organic molecules on oxide surfaces, such as their adsorption geometry, is crucial for optimising processes in various applications, ranging from heterogeneous catalysis to hybrid nanocomposites. In this study, the adsorption of formic acid on magnetite surfaces (001), (111) and (112) is examined using Density Functional Theory (DFT). The vibrational properties are then calculated and compared with experimental infrared spectroscopy data for single crystalline surfaces and nanoparticles. This enables adsorption geometries and modes to be identified.

O 94.3 Fri 10:15 HSZ/0204

Thermal CO_2 Activation and Carbonate Formation on $Fe_2O_3(012)$ — •Johannes Filzmoser, Moritz Eder, Florian Kraushofer, Jiri Pavelec, and Gareth Parkinson — Vienna University of Technology, Austria

The adsorption of CO_2 on hematite α-$Fe_2O_3(012)$ has been investigated in ultra-high vacuum (UHV) using temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS). CO_2 adsorption on this surface exhibits complex behavior, resulting in multiple desorption features in TPD. For coverages up to one molecule per unit cell (0.5 molecules per Fe^{2+} cation), two desorption features centered around 150 K and 220 K increase concurrently with increasing coverage. IRAS shows that this behavior originates from a thermally activated conversion of weakly bound, physisorbed CO_2 into surface carbonate (CO_3^{2-}) species at temperatures above 100 K, a process that directly competes with molecular desorption. By supplying CO_2 at temperatures just below the carbonate desorption temperature, higher carbonate coverages can be obtained. These findings contribute to our understanding of CO_2 activation on $Fe_2O_3(012)$ and will be a prerequisite for surface reaction studies.

O 94.4 Fri 10:30 HSZ/0204

Redox dynamics of $Co_3O_4(111)$ during H_2S adsorption and decomposition — Jonas Hauner[1], Tomáš Skála[2], Nataliya Tsud[2], Fernando Stavale[3], •Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Charles University, Prague, Czech Republic — [3]Brazilian Center for Research in Physics, Rio de Janeiro, Brazil

The redox interactions between transition metal oxides and sulfur-containing compounds play a key role in catalytic processes and gas sensing technologies. We investigated the redox dynamics of $Co_3O_4(111)/Ir(100)$ model catalysts in response to the adsorption and decomposition of hydrogen sulfide (H_2S) using synchrotron radiation photoelectron spectroscopy (SRPES). Upon adsorption, H_2S partially dissociates to form a variety of species including sulfites, sulfides, chemisorbed H_2S, hydroxyl and sulfhydryl groups. Subsequent annealing in ultrahigh vacuum induces desorption and conversion of adsorbed species to sulfates. These transformations are accompanied by temperature-dependent redox processes which can be monitored as a function of Co^{3+}/Co^{2+} ratio. The obtained insights into H_2S–Co_3O_4 redox interactions offers a foundation for the rational design of cobalt oxide catalysts and sensors for H_2S detection and abatement.

O 94.5 Fri 10:45 HSZ/0204

Characterization of CO_2 adsorption configurations on stoichiometric, reduced and hydroxylated In_2O_3 — •Sarah Tobisch[1], Andreas Ziegler[2], Sarah Horak[1], Marco Knapp[1], Michele Riva[1], Michael Schmid[1], Ulrike Diebold[1], Bernd Meyer[2], and Margareta Wagner[1] — [1]TU Wien, Vienna, Austria — [2]FAU-Erlangen-Nürnberg, Erlangen, Germany

CO_2 reduction to methanol is a promising pathway towards a more circular economy, converting CO_2 into valuable fuels and feedstock for the chemical industry. In_2O_3-based catalysts have gained lots of attention in recent years due to their high selectivity towards methanol synthesis. Since catalytic reactions typically take place at the interface, it is important to understand how CO_2 molecules interact and adsorb on the surface on an atomic level.

In this work, the adsorption of CO_2 molecules was studied on three different $In_2O_3(111)$ surfaces: stoichiometric, reduced, and hydroxylated. We present atomically resolved non-contact AFM images which allow for the identification of the adsorption sites of all individual molecules. The CO_2-saturated, stoichiometric $In_2O_3(111)$ shows long range order, albeit breaking the three-fold symmetry of the surface. Missing contrast inversion in nc-AFM combined with XPS measurements result in the identification of physisorbed and carbonate species. DFT calculations confirm adsorption sites and orientation of the individual molecules. CO_2 shows similar motifs on the reduced surface but partly displaces the In adatoms. On the hydroxylated surface, the OH groups block adsorption of CO_2 and long-range order is not observed.

O 94.6 Fri 11:00 HSZ/0204

How chirality controls catalysis: Spin-dependent effects in the catalytic OER from first-principles — •Suryansh Suryansh[1], Rafael Gutiérrez[1], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,2] — [1]Institute of Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden 01062, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062, Dresden, Germany

The evolution of a mixture of unpolarized electrons into an ensemble of spin-polarized electrons after passing through a chiral molecule such as DNA, proteins, or peptides is a well-established phenomenon attributed to the chiral-induced spin selectivity (CISS) effect. This effect has important implications for electrochemical water-splitting. Experiments have shown that chiral molecules enhance the oxygen evolution reaction (OER) by controlling the spin of electrons at the electrode surface when the electrode is coated with a monolayer of chiral molecules, a film of chiral polymer, or a chiral inorganic oxide. This enhancement is associated with facilitating the singlet-to-triplet spin transition of oxygen at the interface. However, the microscopic origin and physical mechanisms behind CISS-based water-splitting remain unclear. In this work, we investigate the electronic and magnetic properties of ferrimagnetic surfaces functionalized with chiral and achiral molecules using first-principles calculations. We compute the reaction energy barriers of the individual OER steps and analyze the spin-polarized electronic states near the Fermi level, providing theoretical insights into the mechanisms underlying spin-assisted water-splitting.

O 94.7 Fri 11:15 HSZ/0204

Tailoring the OER activity of Co_3O_4 surfaces by Mn and V-doping: insights from DFT+U calculations — •Palani Muthu Kumar and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The rational design of efficient electrocatalysts for sustainable energy conversion demands an atomistic understanding of how surface modifications influence the overall activity. Here we present a detailed DFT+U investigation of Mn- and V-doping on the oxygen evolution reaction (OER) activity at Co_3O_4 surfaces. Mn-doping at the surface octahedral sites on both A- and B-terminated $Co_3O_4(001)$, reduces the OER activity. Conversely, V-doping demonstrates termination-dependent behaviour: at the B-termination, V^{5+} in a surface octahedral site reduces the overpotential at Co_{oct} from 0.48 V to 0.43 V. At the A-termination, V^{4+} in a subsurface octahedral site leads to the lowest overpotential of 0.18 V at Co_{tet} reaction site, reversing the intrinsic activity trend where pristine Co_{tet} sites (0.74 V) are less active than Co_{oct2} (0.55 V) sites. For most studied cases, the deprotonation of *OH to *O is the potential-determining step. The enhanced catalytic activity of the V-doped A-termination originates from the modification of surface Co^{3+}(IS) to Co^{2+}, weakening the *OH binding energy and lowering the PDS by 0.56 eV. These findings show that selective doping effectively tunes electrocatalyst performance. The scope of the investigation is further extended to the $Co_3O_4(111)$ surface, thereby broadening the understanding of facet-dependent effects.

O 94.8 Fri 11:30 HSZ/0204

Towards Understanding the Photoreactivity of SrTiO3 through Studies in Ultra-High Vacuum — •Anna Lemperle, Philip Petzoldt, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Strontium titanate is renowned for its photocatalytic water splitting capabilities. However, the catalytic mechanism remains elusive. A promising approach to obtain insights into structure-reactivity relations is to investigate well-defined single crystal model catalysts under ultra-high vacuum conditions. This contribution discusses first results on the thermal and photoreactivity of water and oxygen on the bare strontium titanate (100) surface. Experiments combining temperature programmed desorption and studies under illumination point to a high importance of the dynamic behaviour of bulk and surface oxygen for the reactivity of strontium titanate (100).

O 94.9 Fri 11:45 HSZ/0204

Methanol photodecomposition on $TiO_2(110)$ under UV illumination studied with vibrational SFG spectroscopy in ambient conditions — •Milad Salarinasab[1], Julian Andreas Hochhaus[1], Anas Akhtar[2], Kristina Tschulik[2], Carsten Westphal[1], Zhe Wang[1], and Ahmed Ghalgaoui[1] — [1]Department of Physics, TU Dortmund University, Otto-Hahn-Str. 4a, Dortmund, 44227, Germany — [2]Analytical chemistry II, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany.

Methanol is widely used as a model system for photocatalysis on TiO_2 surfaces, but many earlier investigations were performed in UHV and therefore do not reflect real catalytic conditions. To address this gap, we studied methanol photodecomposition on $TiO_2(110)$ under realistic ambient conditions using vibrational sum frequency generation (SFG) spectroscopy. By recording spectra in the C-H stretch region, we followed CH_3, CH_2, and methoxy species during UV illumination and monitored how these surface species evolve in real time.

The SFG signals show clear differences from the reaction pathways commonly described in vacuum studies. Most importantly, we identify a new photodecomposition route that becomes active only under realistic conditions combined with UV excitation. This finding provides new insight into methanol chemistry on $TiO_2(110)$ and helps connect surface science studies with photocatalytic behavior in practical environments.

O 94.10 Fri 12:00 HSZ/0204

Bridging the Gap: Interpreting Photocatalysis Under Ambient Conditions Based on Findings from Surface Science — •Martin Tschurl, Philip Petzoldt, Lucia Mengel, Paula Neumann, Anna Lemperle, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

The interpretation of heterogenous photocatalytic reactions is usually closely linked to electrochemistry. Based on a qualitative, exclusively thermodynamic picture, it normally focuses on the properties of photon-generated charge-carriers. However, some years ago in ultra-high vacuum (UHV) studies, we discovered that for the heavily studied Pt-titania system, a fundamentally different reaction mechanism governs the photocatalytic conversion of alcohols. This mechanism underscores the critical role of surface chemistry - an aspect often neglected in the interpretation of applied photocatalysts. In this presentation, we will interpret systems operating under ambient conditions based on insights gained from UHV experiments. This way, we also demonstrate merit of surface science studies for a comprehensive understanding of photocatalysis.

O 94.11 Fri 12:15 HSZ/0204

Molecular Dynamics Simulation of Impingment of Atomic Oxygen on Alumina and Silica Surfaces — Stephen Hocker, Hansjörg Lipp, Aahmed Kassem, Ricco Isele, Leonidas Simitsis, and •Johannes Roth — Institute for Functional Matter and Quantum Technologies (FMQ), University Stuttgart, Germany

Atomic oxygen (AO) impinging on satellite surfaces in very low earth orbit (VLEO) transfers momentum and energy, leading to material degradation and drag forces. To be able to counteract these effects, we investigate the impact mechanisms of AO on alumina (Al2O3) and silica (SiO2) surfaces. In this talk we give an overview of our activities: Using molecular dynamics (MD) simulations with classical force fields, we study material stability, angular distributions of reflected particles, and adsorption rates. Our findings indicate that bare Al2O3 does not degrade under AO impacts but accumulates oxygen due to adsorption processes. The angular distribution of reflected particles is highly dependent on the surface structure and the angle of incidence, with a higher ratio of specular reflection observed on smoother surfaces and at larger incidence angles. This is confirmed by the few experimental results available. We further present first results of the impingement of AO on SiO2 surfaces obtained with the same method. Here we study especially the influence of different interactions. The talk is completed with an outlook on the role of specific interactions in general.

O 95: 2D Materials: Stacking and heterostructures (joint session O/HL/TT)

Time: Friday 9:30–12:30 Location: HSZ/0401

O 95.1 Fri 9:30 HSZ/0401

A new fabrication method for metal intercalated epitaxial graphene devices — •Marc Bothe[1], Stefan Wundrack[1,2], Marcelo Jaime[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Hans Werner Schumacher[1], Andrey Bakin[2], and Teresa Tschirner[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany

Epitaxial graphene grown on silicon carbide is a promising platform to achieve metal intercalation. It enables the creation of two-dimensional metal layers that are encapsulated and protected by graphene. However, the use of metal intercalated graphene samples for lithographic device fabrication presents two critical challenges. First, solvents used in the lithography process lead to the deintercalation of the metal atoms. Second, the presence of lattice defects in the graphene - necessary for the intercalation process - compromises the structural and electronic integrity of the device. We present a novel fabrication method that solves these problems. In our approach, the graphene devices are first pre-structured using lithography and subsequently intercalated. This is made possible by a spatial separation on the sample between the device structures and the intercalation origin and by intercalation channels that can guide the intercalation front reliably to the devices. We demonstrate this method on gallium intercalated epitaxial graphene Hall bars that exhibit superconducting behaviour.

O 95.2 Fri 9:45 HSZ/0401

Anisotropic Strain Observation in Naturally Occurring Buckling on Twisted Bilayer Graphene: A Nano-Raman Study — •Gustavo Soares[1], Rafael R. Barreto[1], Rafael Nadas[1], Kenji Watanabe[2], Takashi Taniguchi[2], Leonardo C. Campos[1], Luiz G. Cancado[1], and Angelo Malachias[1] — [1]Physics Department, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, 31270-901, Brazil — [2]National Institute for Materials Science, Tsukuba, Ibaraki, 3050047, Japan

This work investigates naturally occurring buckling and its relation with anisotropic strain relaxation in twisted bilayer graphene (tBG). In the tBG system a twist angle is imposed to influence graphene structural and electronic properties. Such condition directly implies in the occurrence of biaxial in-plane strain, with usual observation of buckled/wrinkled localized regions where the tBG morphology is no longer planar. Using tip-enhanced Raman spectroscopy, we conducted high-resolution mapping to analyze variations in Raman bands associated with twist angle variation and strain effects. Our findings reveal that localized strain gradients, modulated by twist angle variations, induce deterministic buckling in graphene layers, evidencing distinct uniaxial and biaxial strain regions. Finite element modeling further supports these observations, showing that buckling can store elastic energy sufficient to overcome usual tBG-substrate adhesion forces.

O 95.3 Fri 10:00 HSZ/0401

Kirkendall Voids in Monolayer $\mathbf{Mo_xTa_yS_2}$ Alloys on Au(111) — Kai Mehlich[1], Thais Chagas[1], Francis H. Davies[2,3], Alessia Bardazzi[1], Catherine Grover[1], Arkady V. Krasheninnikov[3], and •Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen, Germany — [2]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter, EX4 4QL United Kingdom

During the growth of monolayer MoS_2-TaS_2 heterostructures, we observe the Kirkendall effect: Diffusing vacancies agglomerate in MoS_2, forming what are commonly termed Kirkendall voids - here manifesting as holes in the 2D layer. This phenomenon has not been previously reported in systems with reduced dimensionality.

We prepare the lateral heterostructures by reactive molecular beam epitaxy on chemically inert and weakly interacting Au(111). First, compact MoS_2 cores are grown. In a second step, TaS_2 is added in a sulfur-rich environment at elevated temperatures which promotes diffusion at the interface. The resulting heterostructures exhibit characteristic 2D Kirkendall holes surrounded by a $Mo_xTa_yS_2$ alloy region. These findings reveal defect-mediated processes in low-dimensional systems and open new avenues for designing 2D lateral heterostructures with intricate morphologies.

O 95.4 Fri 10:15 HSZ/0401

Designing 2D Non-van der Waals Heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Heterostructure interfaces created by stacking two-dimensional (2D) materials offer a pathway to realizing advanced electronic and magnetic functionalities at the nanoscale. In this work, we present a high-throughput screening of non-van der Waals (non-vdW) 2D heterostructures; including sandwich-like stacking. Non-van der Waals 2D materials can be obtained by both top-down exfoliation as well as bottom-up growth approaches of non-layered bulk crystals [1]. Our approach uses the AFLOW-Hetbuilder - a newly developed tool for stacking 2D systems based on the coincidence lattice algorithm [2-4].

We investigate interfacial binding effects across a wide range of heterobilayers [5] and sandwich-like systems, analyzing their structural, electronic, and magnetic characteristics such as hybrid interface bands and robust magnetic coupling. Furthermore, we compare the binding energetics of non-vdW and conventional vdW heterostructures. The tunable interfacial properties of non-vdW 2D heterostructures provide a versatile platform for advanced functionalities with potential applications in electronics, spintronics, and the energy sector [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989, (2022).
[2] D.S. Koda *et al.*, J. Phys. Chem. C **120**, 10895, (2016).
[3] https://zenodo.org/record/4721346 .
[4] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[5] A. Nihei, *et al.*, arXiv DOI: 10.48550/arXiv.2503.12209 (2025).

O 95.5 Fri 10:30 HSZ/0401

Second-Order Nonlinear Imaging for Probing 2D van der Waals Structures — •Tao Yang[1], Ben John[1], Kyoung P. Lee[2], Nasim Mirzajani[1], Martin Wolf[1], Xiaoqin Li[2], Martin Thaemer[1], Alexandar Paarmann[1], Niclas S. Mueller[3], and Alexander P. Fellows[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas at Austin, Austin, USA — [3]Freie Universitaet Berlin, Berlin, Germany

Twisted and stacked multi-layer architectures offer new opportunities for tailoring the electronic and optical properties of two-dimensional (2D) van der Waals materials. Reliable determination of crystal structure, stacking sequence, and twist angle is therefore crucial. Second-order nonlinear optical microscopy, including second-harmonic and sum-frequency generation (SHG and SFG, respectively), provides high sensitivity to crystal symmetry and orientation in noncentrosymmetric lattices. Recently, we employed heterodyne-detected vibrational SFG microscopy to probe the local structure of hexagonal Boron Nitride (hBN) monolayers with sub-micron resolution. By employing our developed azimuthal-scanning approach, we fully resolved the crystallographic structure and edge termination in monolayer flakes. Here, we extend these measurements to multi-layer hBN structures, using the same azimuthal-scanning approach in a newly developed SHG microscope to gain insight into their different stacking configurations. Our results highlight second-order nonlinear microscopy as a powerful tool for quantitative structural analysis in 2D materials and for future studies of moiré and twisted heterostructures.

O 95.6 Fri 10:45 HSZ/0401

Moiré-Driven Electronic Modulations in Weakly Coupled h-BN/Graphite — •Fábio J. R. Costa[1,2,7], Daniel Arribas[2], Thiago G. L. Brito[2], Tin S. Cheng[3], Jonathan Bradford[3], Amelia Thompson[3], Alex Saywell[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergey V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Luiz F. Zagonel[1], Klaus Kuhnke[2], Klaus Kern[2,6], and Anna Rosławska[2] — [1]University of Campinas, Brazil — [2]Max-Planck-Institut für Festkörperforschung, Germany — [3]University of Nottingham, UK — [4]Laboratoire Charles Coulomb, France — [5]Institut Universitaire de France, France — [6]EPFL, Lausanne, Switzerland — [7]Current address: Université de Strasbourg, CNRS, IPCMS, Strasbourg, France

Van der Waals materials and their heterostructures offer exciting opportunities for next-generation nanophotonic and electronic technologies. Their electronic and optical properties can be modulated by moiré superlattices that emerge when mismatched layers are stacked together. Hexagonal boron nitride (h-BN) is a key platform in this context, yet the influence of moiré patterns on weakly interacting h-BN interfaces remains underexplored. Here[1], we use scanning tunneling microscopy to resolve large moiré superlattices in h-BN/graphite and uncover pronounced nanoscale modulations of the electronic landscape, despite their weak interlayer interactions. These findings position moiré engineering in h-BN as a powerful tool to tailor local functionalities in van der Waals heterostructures. Ref.: 1. Fábio J. R. Costa *et al.* ACS Nano 2025 19 (40), 35528-35538

O 95.7 Fri 11:00 HSZ/0401

μ-ARPES study on the fine electronic structure of misfit layer compound (PbSe)1.16(TiSe2)2 — •haruki muramatsu[1], natsuki mitsuishi[2,3], teppei ueno[4], kenichi ozawa[5], kaya kobayashi[4,6], and kyoko ishizaka[1,2] — [1]Dept. of Appl. Phys. & QPEC, Univ. of Tokyo — [2]CEMS, RIKEN — [3]Grad. Sch. Sci., Nagoya Univ. — [4]Dept. of Physics, Okayama Univ. — [5]KEK-PF — [6]RIES, Hokkaido Univ.

Misfit layered compounds have been attracting significant attention due to their lattice mismatches and resultant two-dimensional electronic structures reminiscent of van der Waals heterostructures. One such compound, (PbSe)1.16(TiSe2)2, consists of alternating stacking of PbSe monolayers (NaCl-type, four-fold symmetry) and TiSe2 bilayers (CdI2-type, three-fold symmetry). To elucidate its electronic structure, we performed μ-ARPES measurements by carefully distinguishing the cleavage surface terminations. In the presentation, we will discuss the novel electronic states reflecting the natural incommensurate heterostructure as well as charge density wave in the buried TiSe2 bilayer.

O 95.8 Fri 11:15 HSZ/0401

Twisted NbSe$_2$ heterostructures — •Alexander Bäder[1,2], Clara Pfister[3,4], Tobias Wichmann[1,5], Laura Pätzold[3,4], Tim O. Wehling[3,4], and Felix Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]I. Institute of Theoretical Physics, U Hamburg — [4]The Hamburg Centre for Ultrafast Imaging — [5]Institut für Experimentalphysik IV A, RWTH Aachen

We fabricated monolayers (MLs) of the van der Waals material NbSe$_2$ that are rotated with respect to the underlying bulk NbSe$_2$ using our developed ultra-high vacuum (UHV) stacking technique. These heterostructures were characterized through the use of scanning tunneling microscopy and spectroscopy at a base temperature of 1.4 K. The MLs realize a variety of twist angles relative to the underlying bulk lattice, with the lowest observed twist angle being 10°. The MLs display the coexistence of charge density waves (CDW) and moiré effects: In the absence of strain, the MLs develop a 3×3 CDW, however the application of strain through interfacial disorder results in a 2×2 CDW state, supported by theoretical calculations. Compared to isolated MLs the superconducting order parameter is enhanced due to the proximity effect from the underlying bulk.

O 95.9 Fri 11:30 HSZ/0401

band structure and charge density wave in a natural van der Waals heterostructure 4Hb-TaSe2 — •fumihiko kimura[1], tomoki maeda[2], natsuki mitsuishi[3,4], kazuki okada[2], takuya nomoto[5], kenichi ozawa[6], masahiro naritsuka[3], tetsuo hanaguri[3], shunsuke kitou[7], yuiga nakamura[8], taka-hisa arima[3,7], takao sasagawa[2], and kyoko ishizaka[1,3] — [1]Quantum-Phase Electronics Center & Department of Applied Physics, The University of Tokyo — [2]Laboratory for Materials and Structures, Science Tokyo — [3]RIKEN CEMS — [4]Graduate School of Science, Nagoya University — [5]Department of Physics, Tokyo Metropolitan University — [6]Institute of Materials Structure Science, High energy Accelerator Research Organization (KEK) — [7]Department of Advanced Materials Science, The University of Tokyo — [8]Japan Synchrotron Radiation Research Institute (JASRI), SPring-8

4Hb-TaSe2 is a natural van der Waals heterostructure charge density wave (CDW) material consisting of alternative stacking of monolayer 1T-TaSe2 (Mott insulator with Star-of-David CDW) and monolayer 2H-TaSe2 (superconductor with 3 by 3 CDW). Although transport measurements have suggested the existence of multiple CDWs, the details of the CDW and electronic structures remain unclear. In this study, we directly observed the electronic structure of 4Hb-TaSe2 by micro-focused angle-resolved photoemission spectroscopy with careful selection of the surface terminations. We discuss the temperature dependent electronic structure with comparison to the CDW structures obtained by scanning tunneling microscopy and X-ray diffraction.

O 95.10 Fri 11:45 HSZ/0401

Coexisting charge density waves in twisted NbSe2 bilayers — •Christopher Tat Shun Cheung[1], Zachary A. H. Goodwin[2], Yixuan Han[3], Jiong Lu[3], Arash A. Mostofi[1], and Johannes Lischner[1] — [1]Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K. — [2]Institute for Functional Intelligent Materials, National University of Singapore, Singapore 117544, Singapore — [3]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Twisted bilayers of semiconducting transition metal dichalcogenide (TMD) monolayers have been studied extensively. In contrast, twisted bilayers composed of metallic monolayers, such as NbSe2, remain less understood.

Monolayer NbSe2 can host different types of charge density waves (CDWs), in which the Nb atoms move away from their high-symmetry positions. In twisted bilayer NbSe2, identifying CDWs in relaxed structures is challenging because atomic relaxations occur both because of CDW formation and also because of the moiré pattern.

We have carried out large-scale first-principles calculations using density functional theory to study the moiré relaxations and CDWs in twisted bilayer NbSe2. We have developed methods for revealing the CDWs, and for locally classifying the type of CDW. We find that different types of CDWs coexist in the moiré unit cell due to the interactions with strain induced by moiré relaxations [1].

[1] Cheung et al, Nano Lett. 2024, 24, 12088-12094.

O 95.11 Fri 12:00 HSZ/0401

MicroARPES studies of contact doping of monolayer transition metal dichalcogenides by RuCl3 — •Thomas Nielsen[1], Edvard Solbrekken[1], Alfred J. H. Jones[1], Zhihao Zhiang[1], Chakradar Sahoo[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jill A. Miwa[1], Søren Ulstrup[1], Christian Overby[1], and Christian V-B. Fokdal[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan

Placing van der Waals materials into contact with α-RuCl$_3$ has recently emerged as a method of modulating their electronic structures. The proximity to α-RuCl$_3$ has been observed to produce strong hole doping in the van der Waals material, and this has been established as a method to create better electrical contacts in transistor devices based on monolayer transition metal dichalcogenides (TMDs). Here, we use the microARPES endstation at the ASTRID2 synchrotron light source at Aarhus University in Denmark to study the valence bands and core levels of semiconducting monolayer TMDs in proximity to α-RuCl$_3$. We observe a large valence-band shift of $0.7-0.8$eV indicating strong hole doping. α-RuCl$_3$ is highly sensitive to the temperatures and chemicals typically used in the dry-transfer fabrication procedures of van der Waals heterostructures. How the degradation of α-RuCl$_3$ affects the proximity-induced doping of the TMD is discussed based on the ARPES measurements.

O 95.12 Fri 12:15 HSZ/0401

STEM Investigation of Entropy Forbidden Ordering in CVD Grown WSe$_2$-MoSe$_2$ Alloys — •Max Bergmann[1], Matvei Kislitsyn[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

2D transition metal dichalcogenides have gained significant interest due to their optoelectronic properties, which can be tailored by structural variation. However, controllable production, namely growth, of such tailored structures still remains a key challenge towards large-scale production. In this study, we show lateral heterostructures of 2D MoSe$_2$ and WSe$_2$, grown on a SiO$_2$ TEM grid by chemical vapor deposition, that at the interface show a highly ordered structure of W and Mo atoms at the TMD positions, as observed by scanning transmission electron microscopy. This is in contrast to *ab initio* calculations, which ascribe unordered alloys as the preferred configuration, since entropy is the main driving force compared to formation enthalpy. We link this unexpected phenomenon to the initial nucleation of the material on a clean $MoSe_2$ crystal edge, present before the alloy growth, together with special precursor chemistry. Furthermore, we show *ab initio* results in conjunction with the special quasirandom structure method on the bandstructure and optical properties of this structure.

O 96: Plasmonics and nanooptics: Fabrication, characterization and applications

Time: Friday 9:30–12:30 Location: HSZ/0403

O 96.1 Fri 9:30 HSZ/0403

How to fix silver for plasmonics ? — •Jonas Graf[1], Björn Ewald[1], Leo Siebigs[1], Cheng Zhang[2], Achyut Tiwari[3], Max Rödel[1], Sebastian Hammer[1], Vladimir Stepanenko[4], Frank Würthner[4], Bruno Gompf[3], Bert Hecht[2], and Jens Pflaum[1] — [1]Experimental Physics 6, Univ. Würzburg, 97074 Würzburg — [2]Experimental Physics 5, Univ. Würzburg, 97074 Würzburg — [3]1. Physikalisches Institut, Univ. Stuttgart, 70569 Stuttgart — [4]Institute for Organic Chemistry, Univ. Würzburg, 97074 Würzburg

Silver (Ag) is an ideal plasmonic material for applications in the visible regime, but its use is hindered by poor chemical stability and structural quality of thermally evaporated thin films and nanostructures. Here, we present a simple approach to overcome these limitations by alloying Ag thin films with small amounts of gold (Au) through thermal co-evaporation. We analyzed $Ag_{100-x}Au_x$ thin films with Au contents ranging from 5 to 20 at.% with respect to their surface and bulk crystal quality, optical properties and chemical stability. Remarkably, already $Ag_{95}Au_5$ thin films exhibit a drastically enhanced chemical stability and excellent plasmonic properties outperforming pure Ag. This is related to the high film quality achieved without metallic wetting layers, epitaxial substrates or template stripping. As a proof of concept, we fabricate $Ag_{95}Au_5$ plasmonic nanoantennas demonstrating excellent long-term durability over one month under ambient conditions. Our approach thus demonstrates a simple and effective strategy to overcome the general limitations of Ag in plasmonic applications. B. Ewald et al., ACS Photonics 2025, DOI: 10.1021/acsphotonics.5c01659

O 96.2 Fri 9:45 HSZ/0403

Topological quasiparticles in a bucket: water waves as an experimental platform for emulating optical nearfields — •Alexander Neuhaus, Pascal Dreher, Philipp Gessler, Michael Horn-von Hoegen, Karin Everschor-Sitte, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

Optical near fields can host a variety of topological quasiparticles, including merons, skyrmions, skyrmion bags and optical vortices, but their nanometric spatial scales and femtosecond time dynamics make them difficult to access experimentally. Modern techniques, such as time resolved photoemission microscopy or nearfield scanning optical microscopy can image these field configurations, but they are both experimentally challenging. Here, we demonstrate a much simpler 3d printed experiment that can be used as a model system to emulate the behavior of optical nearfields with capillary-gravity water waves. Although water waves and surface polaritons are vastly different wave phenomena, the displacement vector field in the water can be described by surface wave equations that are similar to the equations used to describe surface polaritons. We reconstruct the displacement field of the water wave by fast checkerboard decomposition of videos of the water wave propagation. Water-wave experiments yield the same topological quasiparticles as observed in optical nearfields, yet they do so in seconds instead of hours of experimental time.

O 96.3 Fri 10:00 HSZ/0403

Layer-Resolved Optical Metrology of MoS_2 Using Surface Plasmon Resonance Imaging — •Priyanka Thawany[1,2], Hesam Amiri[1], Lina Jäckering[2], Andrei Vescan[3], Thomas Taubner[2], Sven Ingebrandt[1], and Vivek Pachauri[1] — [1]Institute of Materials in Electrical Engineering 1 (IWE1), RWTH Aachen University — [2]I. Institute of Physics (IA), RWTH Aachen University — [3]Compound Semiconductor Technology, RWTH Aachen University

Conventional techniques such as scanning probe microscopy, Raman spectroscopy [1], ellipsometry [2], and terahertz microscopy [3] provide crucial information on optical and electronic parameters of 2D materials. However, they remain limited in measurement speed and spatial coverage for large-area characterization. To address these limitations, we demonstrate the use of surface plasmon resonance imaging (SPRi) as a complementary wide-field technique for mapping few-layer MoS_2 stacks. Thickness-dependent shifts in the SPR resonance angle and corresponding reflectance contrast allow clear discrimination of atomic-layer regions, consistent with theoretical predictions for MoS_2 optical permittivity changes. SPRi therefore offers a rapid, scan-free approach for real-time metrology of few-layer MoS_2, and similar measurements on other 2D materials show the same suitability for rapid optical characterization. [1] Malard et al., *Phys. Chem. Chem. Phys.* **23**, 23428 (2021). [2] Amiri et al., *Nano Trends* **111**, 100130 (2025). [3] Whelan et al., *Sci. Rep.* **14**, 3163 (2024).

O 96.4 Fri 10:15 HSZ/0403

Launching and confining In-Plane Hyperbolic Phonon Polaritons in α-MoO_3 with In_3SbTe_2 nanostructures — •Umberto Saldarelli[1], Lina Jäckering[1], Lukas Conrads[1], Matthias Wuttig[1], Pablo Alonso-González[2,3], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Department of Physics, University of Oviedo — [3]Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo)

Alpha-phase molybdenum trioxide (α-MoO_3), a van der Waals material, supports in-plane hyperbolic phonon polaritons (HPPs) with high confinement, low losses, and extremely directional propagation [1]. Rapid prototyping of nanostructures for tailoring polaritons can be achieved with the plasmonic phase-change material In_3SbTe_2 (IST) [2], switchable between amorphous and crystalline phases via laser-induced heating. This has been already shown for programmable resonator structures within hBN [3]. Here we combine α-MoO_3 with IST. We use scattering-type scanning near-field optical microscopy (s-SNOM) to explore HPP launching by antennas of different orientations. Next, we optically program a circular launching structure to focus polaritons. Finally, adding a second focusing disk and reconfiguring the disk distance, we tailor field enhancement and confinement. Our results enable rapid design of reconfigurable structures and provide an all-optical material platform for controlling in-plane HPPs. [1] Ma et al. *Nat.* **562**, 557-562, (2018) [2] Conrads et al. *Opt. Mat. Expr.* **15**, 2664-2687, (2025) [3] Jäckering et al. *Nano Lett.* **25**, 15809, (2025)

O 96.5 Fri 10:30 HSZ/0403

Nanoscale Optical Readout of Antiferromagnetic Order by Photocurrent Nanoscopy — •Dario Siebenkotten[1], Anna Schmid[2], Dinghe Dai[1], Joao Godinho[2], Sam Fairman[1], Arne Hoehl[1], Tomas Janda[2], Tomas Ostatnicky[3], Bernd Kästner[1], and Jörg Wunderlich[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [3]Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

Antiferromagnets are prime candidates for next-generation spintronic technologies as they allow for rapid switching and miniaturization compared to ferromagnets. However, readout of their magnetic state remains an open challenge, as their vanishing net magnetisation suppresses conventional magnetic readout schemes. Therefore, new mechanisms are required to measure the state of antiferromagnetic domains, which are often confined to the nanoscale. Here, we report on the experimental observation of a previously only theoretically predicted light-induced, Néel-order-dependent transverse photocurrent that we refer to as the optical nonlinear anomalous Hall effect. We demonstrate the effect by nanoscale imaging of the photocurrent generated in PT-symmetric CuMnAs cross-bar devices by mid-infrared near fields at the apex of a sharp metal tip. We exclude purely thermal mechanisms by showing that the photocurrent reverses sign when the Néel vector is rotated by 180° via current-induced switching of nanoscale antiferromagnetic domains of a few hundred nanometers in size, consistent with a time-reversal-odd nonlinear anomalous Hall photocurrent.

O 96.6 Fri 10:45 HSZ/0403

Plasmonic Effects in a honeycomb metasurface of Ag Nanotriangles and Nanoholes — •Paul-G. Nitsch[1], Paul

Oleynik[1], Markus Ratzke[1], David Stolarek[2], Jon Schlipf[2], Oliver Skibitzki[2], Rudi Tschammer[3], Carlos Morales[3], Jan I. Flege[3], Christian Wenger[2], and Inga A. Fischer[1] — [1]Experimentalphysik und funktionale Materialien, BTU-CS, Cottbus, Germany — [2]IHP - Leibniz- Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [3]Angewandte Physik und Halbleiterspektroskopie, BTU-CS, Cottbus, Germany

Coupled lattices of metal nanoparticle and nanohole arrays can support spectrally narrow plasmonic resonances with potential applications, e.g., in biosensing. In nanohole arrays, the interplay of surface plasmon polaritons at metal-dielectric interfaces and Rayleigh anomalies can lead to Fano resonances, whose spectral positions are well described by Bragg coupling conditions. For nanoparticle arrays with small interparticle distances, the coupling of neighboring particles via their overlapping evanescent fields leads to resonances, whose dispersion relation has been described by tight-binding models. Here, we investigate resonances in coupled nanoparticle and nanohole lattices both experimentally and in simulation. We show that a variation in angle of incidence can be used to tune mode coupling and present results on the detection of near-surface refractive index changes with high sensitivities and figures-of-merit in our samples.

O 96.7 Fri 11:00 HSZ/0403

Hybrid Gold–Vanadium-Dioxide Tunable Plasmonic Devices — Rostislav Řepa, Jiří Kabát, Jiří Liška, Peter Kepič, Michal Horák, Tomáš Šikola, and •Vlastimil Křápek — Brno University of Technology, Brno, Czechia

Vanadium dioxide (VO_2) exhibits a metal-insulator transition near room temperature, which can be exploited in tunable plasmonic devices with compelling functions. However, devices based solely on VO_2 suffer from a large optical absorption and low chemical stability of VO_2 [1].

We present a hybrid material platform that combines high-quality crystalline self-assembled VO_2 nanoparticles [2] with lithographically defined gold nanostructures in a lateral arrangement In this way, we benefit from both the tunability of VO_2 and the high conductivity of gold. The lateral arrangement minimizes the amount of VO_2 and thus contributes to the high quality of the devices.

We demonstrate two tunable plasmonic devices based on the abovementioned material platform: (1) Electric-magnetic switches, in which either an electric or magnetic hot spot is formed, following a design from Ref. [3]. (2) Resonance-energy switches, in which the spectral profile of the scattering or absorption is controlled, with possible applications in selectively-enhanced photoluminescence.

[1] Krpenský et al., Nanoscale Adv. **6**, 3338–3346 (2024).
[2] Horák et al., arXiv:2408.11972.
[3] Křápek et al., Nanophotonics **9**, 623–632 (2020).

O 96.8 Fri 11:15 HSZ/0403

Phonon Polariton Materials Discovery from First Principles — Elena Gelzinyte[1], Giulia Carini[1], Niclas S. Mueller[1], Martin Wolf[1], Karsten Reuter[1], •Johannes T. Margraf[2], Alexander Paarmann[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Phonon Polaritons (PhPs), quasi-particles that arise from strong coupling between infrared photons and optical lattice vibrations, are promising in nanophotonic applications for highly directional and confined light propagation with low optical loss [1]. So far, PhP studies have been mostly focused on a few canonical materials, and the trends in the material space that influence the emergence and properties of PhPs remain largely unexplored. To consider the suitability of various polar crystals for the formation of PhPs, we compute the infrared permittivity functions [2] of 3,000 materials in the JARVIS-DFT database [3]. We then categorize these compounds by their normalized light-matter coupling strength and Reststrahlen band width, whereby we also decompose these in terms of individual phonon mode contributions. A broad range of materials emerges with comparable or better properties than those of typically studied PhP compounds. Using orthorhombic PbO, monoclinic TiO_2, and trigonal $CdCN_2$ as representative examples, we validate our approach and discuss the PhP property trends that allow to identify and design promising PhP candidates.
[1] E. Galiffi *et al.*, Nat. Rev. Mater. **9**, 9 (2024).
[2] X. Gonze and C. Lee, Phys. Rev. B **55**, 16 (1997).
[3] K. Choudhary *et al.*, npj Comput. Mater. **6**, 1 (2020).

O 96.9 Fri 11:30 HSZ/0403

Infrared beam-shaping via geometric phase metasurfaces with the plasmonic phase-change material In_3SbTe_2 — •Lukas Conrads, Florian Bontke, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Conventional optical elements are bulky and limited to specific functionalities, contradicting the increasing demand of miniaturization and multi-functionalities. Optical metasurfaces enable tailoring light-matter interaction at will, especially important for the infrared spectral range which lacks commercially available beam-shaping elements. While the fabrication of those metasurfaces usually requires cumbersome lithography techniques, direct laser writing promises a simple and convenient alternative. Here, we exploit the non-volatile laser-induced insulator-to-metal transition of the plasmonic phase-change material In_3SbTe_2 (IST) [1,2] for optical programming of large-area metasurfaces for infrared beam-shaping. We tailor the geometric phase of metasurfaces with rotated crystalline IST rod antennas to achieve beam steering, lensing, and beams carrying orbital angular momenta. Finally, we investigate multi-functional and cascaded metasurfaces exploiting enlarged holography, and design a single metasurface creating two different holograms along the optical axis. Our approach facilitates fabrication of large-area metasurfaces within hours, enabling rapid-prototyping of customized infrared meta-optics for sensing, imaging and quantum information.[3] [1] Heßler et al. *Nat. Com.* **12**, 924 (2021) [2] Conrads et al. *Opt. Mat. Ex.* **15**, 2664-2687 (2025) [3] Conrads et al. *Nat. Com.* **16**, 3698 (2025)

O 96.10 Fri 11:45 HSZ/0403

Ab Initio Theory of Chemical Interface Damping of Surface Plasmons — •Jordan Edwards[1], Johannes Lischner[1], Andrei Stefancu[2], Wenxuan Tang[3], Ming Fu[3], Ross Schofield[3], Toby Millard[3], Rupert Oulton[3], Pilar Carro[4], Naomi Halas[5], Peter Nordlander[5], and Emiliano Cortes[2] — [1]Imperial College London, London, United Kingdom — [2]Ludwig-Maximilians-Universität (LMU), Munich, Germany — [3]Imperial College London, London, United Kingdom — [4]University of Laguna, La Laguna, Spain — [5]Rice University, Houston, United States

Metallic nanostructures support surface plasmons, collective electron oscillations that give rise to unique optical properties. Molecular adsorption can strongly modify plasmon behaviour; for example, experiments showing that functionalisation reduces their propagation length, a phenomenon is known as chemical interface damping (CID). However, the origin behind CID remains debated, with two proposed mechanisms being: (1) excitation of electron-hole pairs involving the adsorbate orbitals, and (2) electronic scattering by adsorbate-induced dipoles.

To investigate the physical origin of CID, we perform first-principles density-functional theory calculations for different molecules adsorbed on Au(111) surfaces. We calculate the density of states projected onto the adsorbate orbitals to analyse surface-plasmon decay channels associated with mechanism (1). We also use cluster models of the surface to investigate mechanism (2). These results are compared to experimental measurements, offering insights into the origin of CID.

O 96.11 Fri 12:00 HSZ/0403

Tailoring hyperbolic phonon polaritons in hexagonal boron nitride with the phase-change material In_3SbTe_2 — •Lina Jäckering, Aaron Moos, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Polaritons in van-der-Waals materials (vdWM)[1] promise high confinement and multiple tailoring options by resonators and launching structures which conventionally require cumbersome lithography techniques. Optical programming of phase-change materials (PCMs) offers fast and reconfigurable fabrication of these structures. As the plasmonic PCM In_3SbTe_2 (IST) can be switched between a dielectric and metallic phase, IST is promising for nanophotonics[2], especially for optical programming of metallic launching structures to tailor and confine polaritons in vdWM. Here, we combine the vdWM hexagonal boron nitride (hBN) with IST.[3] We optically program circular resonators for hBN's phonon polaritons into IST through the hBN flake. We investigate the polariton resonators with near-field optical microscopy. Demonstrating the reconfigurability, we decrease the resonator diameter to increase the confinement up to $\lambda/39$ and achieve a quality factor of 72. Finally, we fabricate a focusing structure for hBN's polaritons whose focal point we reconfigure. We promote IST as a versatile platform for rapid prototyping of polariton optics in various vdWM such as α-MoO_3, β-Ga_2O_3 and $MoOCl_2$. [1] Basov et al. Science **354**, 6309 (2025) [2] Conrads et al. Opt. Mater. Express **15**, 2664 (2025). [3]

Jäckering et al. Nano Letters **25**, 15809 (2025).

O 96.12 Fri 12:15 HSZ/0403

Self-assembled dielectric network metamaterials based on vanadium oxide — •Marcello Pozzi[1], Jeremi Setz[1], Noel von Wattenwyl[1], Georg Haberfehlner[2], Arnold Müller[3], Ralph Spolenak[1], and Henning Galinski[1] — [1]Laboratory for Nanometallurgy, ETH Zürich, Switzerland — [2]FELMI-ZFE, TU Graz, Austria — [3]Laboratory of Ion Beam Physics, ETH Zürich, Switzerland

Among scalable optical nanomaterials, network metamaterials stand out because of their large-area compatibility, versatility and low footprint. These systems are created by self-assembly in a reaction-diffusion process called "chemical dealloying", resulting in complex network structures with broadband optical response driven by plasmonic mode equipartition [1]. Typical network metamaterials consist of noble metallic elements and show plasmonic behavior. Here we propose a material system that extends the design space of network metamaterials to dielectrics. Using magnetron co-sputtering of aluminum-vanadium followed by chemical dealloying, we fabricate network metamaterials based on vanadium oxide. Through the combination of Rutherford backscattering spectroscopy (RBS) and focused ion beam (FIB) tomography we analyze the dynamics of pattern formation, while the light-matter interaction is studied combining full-wave simulations and various spectroscopy techniques. Finally, we determine the degree of hyperuniformity of the dielectric networks by measuring the scaling behavior of the volume fraction variance of the systems.

[1] Adv. Optical Mater. 2023, 11, 2300568

O 97: Solid-liquid interfaces: Reactions and electrochemistry III

Time: Friday 9:30–12:30 Location: TRE/PHYS

Invited Talk O 97.1 Fri 9:30 TRE/PHYS

Questions of Selectivity in Electrocatalysis — •Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Heterogeneous electrocatalysis is at the heart of developing sustainable energy technologies. The rational design of suitable electrocatalysts, however, depends on a deeper understanding of the underlying reaction mechanisms. Product selectivity, in particular, remains poorly understood and cannot be rationalized by popular thermodynamic models that currently define the state-of-the-art in computational electrocatalysis. In this talk, I will address a number of possible scenarios as to why this may be while challenging prevalent mechanistic assumptions. Atomistic models, based mainly on density-functional theory, will explore microscopic reaction mechanisms to demonstrate effects due to the local field at the electrical double layer, the delicate kinetic competition between electrochemical and non-electrochemical reaction steps, as well as the key role of mesoscopic mass transport. The emerging insight adds to our fundamental understanding of electrocatalysis and supports ongoing efforts toward optimal process design.

O 97.2 Fri 10:00 TRE/PHYS

Mechanism of Fe(II) Chemisorption on Hematite(001) Revealed by Machine Learning Molecular Dynamics — •Kit Joll[1], Philipp Schienbein[1,2], Kevin Rosso[3], and Jochen Blumberger[1] — [1]Department of Physics and Astronomy and Thomas Young Centre, University College London, London WC1E 6BT, United Kingdom; — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany; Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — [3]Pacific Northwest National Laboratory, Richland, Washington 99354, United States;

Understanding ion adsorption at mineral-water interfaces is key to explaining geochemical processes such as redox cycling, dissolution, and crystal growth. However, probing these reactions experimentally at atomic resolution remains challenging. Here, we employ reactive neural network potential molecular dynamics (NNP-MD) with umbrella sampling and reactive flux transition state theory to simulate the chemisorption of aqueous Fe^{2+} on hematite(001) at density-functional theory (DFT) accuracy and nanosecond time scales. We identify a dissociative mechanism for Fe^{2+} water-ligand exchange and multiple stable surface complexes, nonadsorbed, physisorbed, monodentate, and tridentate chemisorbed species, along the adsorption pathway. The overall process is exergonic, in contrast to previous classical force-field predictions. These results demonstrate how machine-learning potentials bridge the accuracy of ab-initio methods with the sampling efficiency of classical molecular dynamics, providing new atomistic insight into reactive processes at oxide-water interfaces.

O 97.3 Fri 10:15 TRE/PHYS

How to Best Achieve a Steady State: Comparison of Different Methods to Acquire Tafel Plots — •Maren-Kathrin Heubach and Gregory Jerkiewicz — Department of Chemistry, Queen's University, Kingston, Canada.

The performance of an electrocatalyst is typically characterized by Tafel plots, which show a natural logarithm of the current density of a reaction as a function of the overpotential. Hereby, the exchange current density and the Tafel slope can be determined, giving insights into the mechanism of the electrocatalytic reaction. Even though Tafel plots are widely used, there is a large variety in performing the measurements to create Tafel plots.

In this contribution, we will discuss and compare several approaches to achieve the closest approximation to the desired steady state. These approaches will be showcased with the benchmark system of a polycrystalline Pt sample in an aqueous sulphuric acid solution.

O 97.4 Fri 10:30 TRE/PHYS

Exploring the Surface Structure of Ni Anodes and the Role of pH for Alkaline Oxygen Evolution Using SERS — •Justus Leist, Annika Neufischer, Roman Jocher, Benjamin Schilling, Timo Jacob, and Albert Engstfeld — Ulm University, Institute of Electrochemistry, Ulm, Germany

Sustainable hydrogen can be generated by electrochemical water splitting, but the process is typically limited by the sluggish kinetics of the oxygen evolution reaction (OER) at the anode. To avoid reliance on noble-metal catalysts such as Ir and Ru, Ni-based catalysts have attracted considerable interest due to their abundance and efficiency. Under OER conditions, where the Ni anode surface is accepted to be NiOOH, Raman spectroscopy enables *in situ* monitoring of both the surface structure and possible OER intermediates. In this work, using Surface-enhanced Raman spectroscopy (SERS) combined with DFT, we challenge the assumed presence of NiOOH under OER conditions.[1]

To probe the atomic composition of the oxidized Ni anodes, isotope-labelled Raman experiments were performed, revealing the absence of hydrogen in the lattice. The presence of NiO*, rather than NiOOH, is further supported by DFT-calculated spectra. Additionally, we illustrate that a band previously attributed to an OO- species is more likely related to overtones. By varying the pH from alkaline to near-neutral conditions, we examine the impact of pH on the Raman spectra during the OER and discuss these changes in relation to the vibrational Stark effect and possible OER intermediates.

[1] J. Leist et al. *ChemRxiv* DOI: 10.26434/chemrxiv-2025-jb73p

O 97.5 Fri 10:45 TRE/PHYS

Optimizing oxygen vacancies through grain boundary engineering to enhance electrocatalytic nitrogen reduction — •Xiu Zhong[1], Fu Yang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany — [2]School of Environmental and Chemical Engineering, Jiangsu University of Science and Technology, Zhenjiang, Jiangsu 212100, China

This study develops an efficient N2-reduction catalyst by in-situ anchoring ultrafine MoO2 nanograins on N-doped carbon fibers. Optimized thermal treatment generates abundant grain boundaries that increase oxygen-vacancy concentration, enhance electron transfer, and create highly active N2-trapping sites. The optimal MoO2/C700 catalyst delivers superior performance, achieving an NH3 yield of 173.7 μg h-1 mgcat -1 and a Faradaic efficiency of 27.6% at -0.7 V vs. RHE in 1 M KOH. In-situ XPS and DFT confirm the electronic-structure modulation and strong N2-oxygen-vacancy interaction, revealing electron transfer between adsorbed nitrogen and Mo(IV). Correlating activity with interfacial effects further clarifies the origin of enhancement. The catalyst also shows stable operation for 60 h, demonstrating the promise of grain-boundary engineering to boost oxygen vacancies for efficient and sustainable electrochemical ammonia synthesis.

O 97.6 Fri 11:00 TRE/PHYS

Investigating the Role of Nuclear Quantum Effects at Zinc Oxide-Water Interfaces with High-Dimensional Neural Network Potentials — •Jan Elsner[1,2] and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Zinc oxide is a promising material for sustainable hydrogen production via catalytic water splitting. The interface of ZnO with water exhibits complex dynamical behaviour, including water dissociation and recombination, as well as long-range proton transport. Previous studies [1] have elucidated these mechanisms using High-Dimensional Neural Network Potentials (HDNNPs), which enable simulations at the system sizes and timescales needed for statistically converged interfacial properties. However, the validity of the classical approximation for atomic nuclei in such systems, particularly for describing interfacial proton transfer (PT), remains poorly understood. Here, we employ a new efficient parallel implementation of path-integral molecular dynamics with HDNNPs [2] to investigate the role of nuclear quantum effects (NQEs) at the ZnO-water interface. We show that NQEs significantly lower free energy barriers for PT, and discuss the resulting implications for the interfacial dynamics of the system.

[1] Quaranta V., Hellström M., Behler J., J. Phys. Chem. Lett. 2017, 8, 1476-1483

[2] Shiga M., Elsner J., Behler J., Thomsen B., J. Chem. Phys. 2025, 163, 134119

O 97.7 Fri 11:15 TRE/PHYS

Linking Water Structure to Proton-Coupled Electron Transfer at Metal Interfaces — •Julius Lonnes[1,2], Nicolas G. Hörmann[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG — [2]Technische Universität München

Understanding the kinetics of interfacial electrochemical reactions is essential for optimizing technologies such as fuel cells and batteries. To this end, the interfacial water structure plays a key role in determining the effects of pH and electrolyte cations on reaction rates, yet the mechanistic link between water arrangement and reaction barriers remains unclear. By examining the acidic Volmer step on Pt(111) and tuning the hydrogen-bond network surrounding the proton, we uncover how interfacial solvation modulates electrochemical activation barriers. We find that proton stability at the metal-water interface strongly influences the barrier height, a relationship that can be rationalized with Hammond's postulate:[1] variation in electrochemical potential shifts the transition state position along the reaction coordinate, altering its sensitivity to local solvation structure. We establish that interfacial solvation is a decisive factor in determining electrochemical activation energies, advancing fundamental understanding of proton-coupled electron transfer at charged interfaces.

[1] G.S. Hammond, J. Am. Chem. Soc. **77**, 334 (1955).

O 97.8 Fri 11:30 TRE/PHYS

Understanding of degradation of catalyst/semiconductor interfaces — Sergej Levashov[1], Tim Rieth[1,2], Ian D. Sharp[1,2], and •Johanna Eichhorn[1] — [1]TUM School of Natural Sciences, TU Munich — [2]Walter Schottky Institute, TU Munich

The performance of photoelectrochemical (PEC) materials are governed by interfacial processes where atomic structure, electronic states, and chemical reactions meet. Local defects and dynamic surface transformations at the nanoscale can dominate charge transfer and often trigger degradation under operating conditions. Accessing such mechanisms requires in-situ/operando techniques that probe interfacial structure and dynamics with nanoscale resolution. We employ in situ scanning probe microscopy to study the interfacial stability of TiO2/Pt photocathodes by monitoring local surface transformations and detachment events during operation. Pt catalysts are deposited on conformal TiO2 coatings either by sputtering, yielding continuous films, or by atomic layer deposition (ALD), forming discrete nanoislands and enabling atom-efficient utilization of precious metals. Under PEC conditions, both architectures show comparable onset potentials and saturation current densities, yet chronoamperometry reveals an enhanced long-term stability for the nanostructured ALD-Pt electrodes. We attribute this contrasting behavior to different bubble formation and detachment dynamics at the catalyst-semiconductor interface. These nanoscale insights highlight the importance of interfacial and morphological engineering, as well as the necessity of controlling reaction processes, to achieve durable and efficient PEC material systems.

O 97.9 Fri 11:45 TRE/PHYS

An Analytical Description for Atomic Diffusion involved Peaks in Cyclic Voltammograms: the Reversible Place-Exchange on Pt(111) — Jon Bjarke Valbaek Mygind[1], Francesc Valls Mascaró[2], Gerard J. Verbiest[3], and •Marcel J. Rost[4] — [1]Catalan Institute of Nanoscience and Nanotechnology, Campus UAB, Barcelona, Spain — [2]Faculty of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [3]Department of Precision and Microsystems Engineering, Delft University, Delft, The Netherlands — [4]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Cyclic voltammetry (CV) is one of the most powerful tools for the experimental investigation and characterization of electron transfer processes in electrochemistry. As the unique electrochemical fingerprint of a particular system is given by specific (current) peaks in the cyclic voltammogram, it is not surprising that great effort is done to understand, describe, and model these peaks. However, the underlying thermodynamic and kinetic processes make this a difficult task, especially when features in the fingerprint change with the applied CV sweep rate. Here we show, on the example of the reversible Place-Exchange peak, a precursor in the electrochemical oxidation of the Pt(111) surface, that a combination of a Frumkin isotherm followed by an Arrhenius (atomic) diffusion process delivers a rather good description. We present an analytical theory that fits all peaks of all CVs, measured with different sweep rates, with only six fit variables. These variables deliver hard quantitative thermodynamic values.

O 97.10 Fri 12:00 TRE/PHYS

Machine Learning the Energetics of Electrified Solid-Liquid Interfaces — •Nicolas Bergmann[1], Nicéphore Bonnet[2], Nicola Marzari[2], Karsten Reuter[1], and Nicolas G. Hörmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Theory and Simulation of Materials, EPFL, Lausanne

Machine learning interatomic potentials (MLIPs) accelerate many aspects of computational chemistry. However, MLIPs fail to describe the biases introduced at applied potential conditions for typical electrocatalytic systems, where effects of the inner double layer play a critical role [1]. Here, we present the "Response Analysis in z-ORientation" (RAZOR) model [2], which machine-learns the work function, the first-order energy change to bias charges q. RAZOR is stabilized by additionally learning the atomic force derivative to q, equivalent to Born effective charges. The approach extends MLIPs to the variable charge case, by adding bias-induced energy and force changes to traditional zero-bias MLIPs. This enables large-scale molecular dynamics simulations at finite bias. We demonstrate RAZOR's capabilities by investigating OH adsorption on Cu(100) and explicit Pt(111)-H_2O interfaces, faithfully recreating *ab initio* and experimental results.

[1] N. Bergmann *et al.*, J. Chem. Theory Comput. **19**, 8815 (2023).

[2] N. Bergmann *et al.*, Phys. Rev. Lett. **135**, 146201 (2025).

O 97.11 Fri 12:15 TRE/PHYS

Entropy-Enthalpy Relationships in Heterogeneous Electrocatalysis: A Case Study of the Hydrogen Evolution Reaction — •Andrew J. Wong, Barbara Sumić, Elias Diesen, Nicolas G. Hörmann, Hendrik H. Heenen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Temperature is a key parameter in industrial electrolyzers. And yet, the vast majority of mechanistic lab-scale studies ignores temperature variations by operating at room temperature. This is surprising since existing experimental evidence has shown that even modest heating can significantly affect the rate and selectivity of electrocatalytic reactions. Understanding the origin of such effects is crucial for advancing fundamental electrocatalysis and exploiting temperature as a control parameter. Here, we explore temperature effects on the hydrogen evolution reaction (HER) by developing a simple mean-field microkinetic model based on first-principles energetics. An Arrhenius analysis on the HER rates across different metal catalysts reveals distinct entropy-enthalpy correlations, reflected in the apparent activation enthalpy and entropy-dependent prefactor. Despite the simplicity of our model, these trends are in remarkable qualitative agreement with experiments. A degree of rate control analysis explains the kinetic fingerprints in terms of a change in the rate-determining step, inducing a shift in kinetic regime. We thus conclude that the enthalpy-entropy compensation effect is explained, at least to a first approximation, by the surface kinetics. Our work overall highlights the subtle interplay between temperature, applied potential, and catalyst reactivity.

O 98: Ultrafast electron dynamics at surface and interfaces IV

Time: Friday 9:30–12:15 Location: TRE/MATH

Invited Talk O 98.1 Fri 9:30 TRE/MATH

Electron-phonon interactions in the time domain: from non-equilibrium phonon dynamics to theoretical spectroscopy — •Fabio Caruso — University of Kiel, Germany

First-principles simulations of electron-phonon interactions (EPI) are key to clarifying the microscopic origin of the ultrafast electron and phonon dynamics revealed by pump-probe experiments in crystalline solids [1]. In this talk, I will discuss recent advances in ab-initio simulations of the EPI and their application to light-driven electron and lattice dynamics. Building on recent progress in many-body theory and software, predictive atomistic simulations of complex non-equilibrium phenomena have now become feasible. I will highlight, in particular, non-thermal phonon populations [2], coherent phonons [3], and ultrafast polaron formation as representative examples. This progress forms the basis for a strong synergy between ab-initio theory and experimental ultrafast science.

[1] F. Caruso et al., J. Phys. Mater. **9**, 012501 (2025).
[2] Y. Pan et al., ACS Nano **19**, 11381 (2025).
[3] C. Emeis et al., Phys. Rev. X **15**, 021039 (2025).

O 98.2 Fri 10:00 TRE/MATH

Coherent phonon control beyond amplitude saturation in a sliding ferroelectric — •Jan Gerrit Horstmann[1,2], Christoph Emeis[3], Andrin Caviezel[1], Quintin Meier[4], Nicolas Wyler[1], Thomas Lottermoser[1], Fabio Caruso[3], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, Zurich, 8093, Switzerland — [2]University of Würzburg, Institute of Physical and Theoretical Chemistry, Am Hubland, 97074 Würzburg, Germany — [3]Institute of Theoretical Physics and Astrophysics, Kiel University, Leibnizstraße 15, Kiel, 24118, Germany — [4]Institut Néel, C.N.R.S-Université Grenoble Alpes, BP 166, Grenoble, 38042, France

Intense optical excitation can drive quantum materials into regimes where the usual linear relation between photo-excited carriers and lattice-driving forces no longer applies. Using time-resolved second-harmonic generation, we observe that the interlayer sliding phonon governing sliding ferroelectricity in WTe_2 saturates and even decreases at high single-pulse fluence. Density functional theory traces this nonlinearity to band-specific electron-phonon coupling that produces competing lattice forces. By dividing the same total fluence into two well-timed pulses, we avoid populating counteracting electronic states and achieve significantly larger coherent phonon amplitudes. The resulting enhanced sliding motion reveals anharmonic phonon coupling far from equilibrium and shows that nonlinear limits in driven solids can be overcome through temporal shaping of the optical excitation.

O 98.3 Fri 10:15 TRE/MATH

Ultrafast x-ray sonography: A novel technique to spatially resolve phase heterogeneity on picosecond timescales — •Maximilian Mattern[1], Angel Rodriguez-Fernandez[2], Roman Shayduk[2], Wonhyuk Jo[2], Vojtech Uhlir[3], Jon Ander Arregi[3], Anders Madsen[2], Daniel Schick[1], and Jan-Etienne Pudell[2] — [1]Max-Born-Institut, Germany — [2]European XFEL, Germany — [3]CEITEC BUT, Czech Republic

Laser-induced heterogeneities play an important role for ultrafast dynamics especially of first-order phase transitions due to the phase coexistence during nucleation. However, their probing on picosecond time and nanometer length scales is challenging.

To address this challenge, we introduce ultrafast X-ray sonography. It combines well-established ultrafast hard-X-ray diffraction with a propagating strain pulse as a universal and non-invasive structural marker. The signatures of the strain pulse in the phase-specific lattice dynamics localizes the different phases in both space and time. This non-invasive pump-probe technique can follow the coherent growth and stochastic nucleation of structural domains on picosecond timescales with almost no requirements for sample preparation and is broadly applicable to a broad class of materials, provided that the coexisting phases exhibit distinguishable diffraction signatures. As a benchmark, we apply this approach to the antiferromagnetic-to-ferromagnetic magneto-structural phase transition in FeRh and identify the ferromagnetic phase to nucleate at the surface as columnar domains of approximately 30nm diameter.

O 98.4 Fri 10:30 TRE/MATH

Ultrafast energy flow among electrons and phonons in a Pb/Si nanoscale heterosystem — •Christian Brand[1], Mohammad Tajik[1], Tobias Witte[1], Laurenz Rettig[2], Birk Finke[1], Björn Sothmann[1], Uwe Bovensiepen[1], and Michael Horn-von Hoegen[1] — [1]Department of Physics, University of Duisburg-Essen, Germany — [2]Department of Physical Chemistry, Fritz Haber Institute, Germany

Microscopic excitations in condensed matter interact on ultrafast time scales. In this study, we employed time-resolved photoelectron spectroscopy and ultrafast electron diffraction to probe the spatially confined dynamics of electrons and phonons in ultrathin epitaxial Pb films on Si(111) subsequent to fs-laser excitation. Spatial confinement is crucial here, as without it, the energy flow into the unexcited bulk would obscure the transient dynamics and prevent targeted investigation. Electrons dissipate their excess energy within 400 fs, while lattice vibrations gradually build up over 3-8 ps. During this time gap, energy is transiently stored in high-frequency phonon modes, as captured by a three-temperature model. The transient electron temperature provides direct experimental access to the occupation of these phonons after equilibration at $\approx 3\,\mathrm{ps}$. Subsequent excitation of low-frequency phonons and full lattice thermalization at $\approx 20\,\mathrm{ps}$ are governed by anharmonic phonon-phonon coupling within the Pb film.

O 98.5 Fri 10:45 TRE/MATH

Ultrafast manipulation of topological transport properties in Td-MoTe2 via coherent phonon excitation — •Huimin Wang[1], Matthew Day[2,3], Juan Aranzadi[1], James McIver[2,3], and Michael Sentef[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]Department of Physics, Columbia University, New York, NY, USA. — [3]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany

Ultrafast control of topological properties in quantum materials has emerged as a promising route toward dissipative-free and fast optoelectronic functionalities. In type-II Weyl semimetals such as Td-MoTe*, selective photoexcitation of coherent phonons offers an efficient non-thermal pathway to drive topological phase transitions by modifying lattice symmetry. Yet the microscopic origin of the laser-induced interlayer shear mode*central to this process*remains unclear, with both electron*phonon coupling (EPC) and strong phonon anharmonicity expected to contribute. Here, using real-time TDDFT combined with non-adiabatic molecular dynamics, we map out the excitation pathways of this shear mode under varying photon energies, polarizations, and field strengths. We reveal cooperative EPC and phonon*phonon mechanisms that enable control of the phonon phase and amplitude. The resulting lattice dynamics induce shifts of Weyl node positions and associated nonlinear photocurrents, providing insight into observed ultrafast Hall responses.[1]Nature 565, 61*66 (2019). [2]Nat. Commun., vol. 12, p. 1885, 2021.[3]Phys. Rev. X, vol. 9, no. 2, p. 021036, 2019.

O 98.6 Fri 11:00 TRE/MATH

Competition of electron-electron and electron-phonon scattering in thermalization of laser-excited electrons — •Christopher Seibel, Tobias Held, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

When an ultrashort laser pulse irradiates a metal, electrons are excited to a state of strong nonequilibrium. According to the common picture, they thermalize subsequently towards a hot Fermi distribution on a femtosecond timescale and transfer energy to the still cold lattice on a picosecond timescale. Often these two processes are considered to be independet and driven by different interactions. Electron-electron scattering is considered responsible for the thermalization, whereas electron-phonon scattering is considered responsible for the energy transfer to the lattice. However, there are indications that these two processes influence each other and can act on similar timescales.

We use a kinetic description based on full Boltzmann collision integrals to trace the dynamics of the electron distribution during the thermalization after ultrashort laser excitation. We show that electron-electron and electron-phonon scattering have different effects on the distribution, which both lead to thermalization. Comparing various excitation fluences, we find that the thermalization times of the two processes exhibit an opposite fluence dependence and can become comparable for weak excitations.

O 98.7 Fri 11:15 TRE/MATH

Interfacial charge dynamics in hybrid plasmonic-excitonic nanostructures — •Tommaso Pincelli[1], Alessandro De Vita[1], Gian Marco Pierantozzi[2], Manuel Izquierdo[3], Pavel Trofimov[4], Trideep Kadwe[4], Hélène Seiler[4], Niclas S. Müller[4], Caterina Cocchi[5], Laurenz Rettig[6], Martin Wolf[6], Ralph Ernstorfer[1], and Giancarlo Panaccione[2] — [1]Technische Univ. Berlin — [2]IOM - CNR — [3]EuXFEL — [4]Freie Univ. Berlin — [5]Fredrich Schiller Univ. Jena — [6]Fritz Haber Inst. - MPG

Hybrid interfaces that merge plasmonic surfaces with 2D semiconductors are pivotal in energy materials research, allowing to tailor local fields and functionalize charge-transfer excitations. In this work, we exfoliate few-layer WSe_2 on a plasmonic lattice of nanostructured Au in UHV. Angle-resolved reflectivity reveals a rich photonic band structure matching finite-element calculations. Using time and angle resolved photoemission spectroscopy (trARPES), we observe an ultrafast quench of excitonic signatures and hints of rapid interfacial charge transfer. Angle-integrated trPES at higher photon energies allows access to the buried interface by tracking shallow core levels. Notably, the plasmonic lattice induces a pronounced slowing of Au 4f peak shifting dynamics compared with unpatterned Au, suggesting a bottleneck in the interfacial charge transfer. These results highlight the potential of hybrid interfaces as flexible platforms for engineering optoelectronic responses at ultrafast timescales. We acknowledge the Energy Materials community proposal collaboration, the teams of SXP@EuXFEL and HEXTOF@FLASH.

O 98.8 Fri 11:30 TRE/MATH

Non-equilibrium electron dynamics in antenna-reactor plasmonic photocatalysts — •Henry T. Snowden[1] and Reinhard J. Maurer[1,2] — [1]University of Warwick, UK — [2]University of Vienna, AT

Antenna-reactor nanoparticles are a promising form of plasmonic photocatalyst, combining strong light absorption and high catalytic activity. A key materials design question is the correct nanoparticle geometry with proposals ranging from core-shell structures to nanoalloys. Optimal photocatalysts combine strong light absorption, effective carrier transport, and long carrier lifetime. Here, we study the non-equilibrium electron dynamics after pulsed laser excitation using the Athermal Electron Model (AthEM), which explicitly considers thermal and non-thermal electrons in contact with a phonon bath, and a laser source term. Electron-electron scattering effects are considered at the level of the relaxation time approximation. We investigate how athermal electron-hole pair distributions evolve in different classes of promising materials according to the interplay of electron-electron and electron-phonon scattering. Based on our findings, we propose optimal materials compositions and photocatalyst geometries.

O 98.9 Fri 11:45 TRE/MATH

Influence of sulphur vacancies on ultrafast charge separation in WS2-graphene heterostructures — •Johannes Gradl[1], Niklas Hofmann[1], Leonard Weigl[1], Camilla Coletti[2], Raül Perea-Causín[3], Ermin Malic[4], and Isabella Gierz[1] — [1]University of Regensburg, Regensburg, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy — [3]AlbaNova University Center, Stockholm, Sweden — [4]University of Marburg, Marburg, Germany

Ultrafast charge separation following photoexcitation, commonly observed in van der Waals heterostructures, is a key process for future optoelectronic devices that rely on the conversion of light into electricity. While electron and hole transfer rates are largely determined by band alignment and interlayer hybridization, recent experiments have revealed that defects critically affect the lifetime of the charge-separated state [1][2]. A microscopic understanding of defect-assisted charge transfer, however, remains elusive. We disentangle the role of sulphur vacancies on ultrafast charge separation and recombination in WS2-graphene heterostructures by (i) systematically increasing the defect density and (ii) switching the defect-assisted charge transfer channel on and off. Using time-resolved ARPES, we probe the resulting charge-transfer dynamics on ultrafast time scales directly in the band structure.

[1] Phys. Rev. Lett. 127, 276401, (2021)
[2] Sci. Adv. 7, eabd9061, (2021)

O 98.10 Fri 12:00 TRE/MATH

Formation and thermalization of non-equilibrium excitonic occupations — •Paul Werner[1], Wiebke Bennecke[1], Jan Philipp Bange[1], Giuseppe Meneghini[2], David Schmitt[1], Marco Merboldt[1], Anna Seiler[1], AbdulAziz AlMutairi[3], G. S. Matthijs Jansen[1], Junde Liu[1], Daniel Steil[1], Stephan Hofmann[3], R. Thomas Weitz[1], Ermin Malic[2], Stefan Mathias[1], and Marcel Reutzel[3] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany — [3]Department of Engineering, University of Cambridge, United Kingdom

Upon optical excitation, bright excitons can scatter into lower energy, potentially dark, exciton states. In these formation and relaxation processes, non-equillibrium exciton populations play a major role, but remain largely elusive because they are inaccessible by most spectroscopic methods. In this work we provide direct access to the formation and thermalization of non-equilibrium exciton states in 2H-homobilayer MoS_2. Using time-resolved momentum microscopy and microscopic many-particle calculations, we reveal the fingerprint of non-equillibrium exciton distributions and quantify their formation and relaxation timescale [1].

[1] Werner *et al.*, arXiv:2505.06074 (2025).

O 99: Spins on surfaces at the atomic scale III

Time: Friday 9:30–12:30 Location: WILL/A317

O 99.1 Fri 9:30 WILL/A317

Measuring magnetic exchange forces of individual quantum spins — •Nicolaj Betz[1,2], Lukas M. Veldman[1,2], Milton Aguliar[3], Eric Lutz[3], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany. — [3]University of Stuttgart, Institute for Theoretical Physics, Stuttgart, Germany

Dynamics of single atomic spins are governed by interactions with the spins immediate, i.e. atomic scale environment. In that, spin-polarized scanning tunnelling microscopy (STM) can give access to some of these interactions, e.g. those between coupled spins, and it can also be used to detect the dynamics in form of individual spin switches. Atomic force microscopy (AFM) on the other hand, gives access to atomic-scale forces, for example the magnetic exchange interaction [1,2]. Here, we show magnetic exchange force detection on a dynamically switching single Fe atom on MgO/Ag(100). We can tune this spin to undergo a ground state reversal as a function of exchange interaction with the tip. We find that the switching spin interacts strongly with the AFM cantilever. Thus, access to these forces provides a new avenue to study dynamically switching single atomic quantum spins revealing information about the interplay between an atom's interactions and the dynamics of the spin.

[1] N. Hauptmann et al., Nat. Com. 11, 1197 (2020).
[2] U. Kaiser et al. Nature 446, 522-52 (2007).

O 99.2 Fri 9:45 WILL/A317

Tip induced f-π interaction of $YbPc_2$ Molecules utilizing STM — •Jonas Arnold[1], Kwan Ho Au-Yeung[1], Wantong Huang[1], Eufemio Moreno Pineda[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Mario Ruben[2], and Philip Willke[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Individual molecules constitute excellent building blocks for quantum technologies thanks to their small size, reproducibility and the benefit of self assembly. A promising class are rare-earth bis-phthalocyanine complexes (1). In this work, we investigate $YbPc_2$ molecules using a mK- scanning tunneling microscope (STM) to identify potential indicators of a magnetic signature. In the gas phase, the $YbPc_2$ molecule is expected to exhibit a radical spin localized at its ligands, an f-shell electron spin S = 1/2 as well as a nuclear spin (I = 1/2 and 5/2) for certain isotopes. Thus, this system is a potential candidate for a spin cascade (1). We perform measurements on self-assembled multi-layer islands of $YbPc_2$ on Ag(001) and MgO/Ag(001). We find that the proximity of the STM tip changes the spin state of the molecule by tuning states close to the Fermi level (2). We identify the emerging spectral features close to zero bias as inelastic electron tunneling excitations that result from the combined f-π system. This mechanism can be found for the first, second and third molecular layer on Ag(001) as well as MgO/Ag(001). (1) Wernsdorfer, W. et al., Adv. Mat., 2019, 31(26), 1806687. (2) Liao, X. et al., Nat. Com., 2025, 16(1), p.6263.

O 99.3 Fri 10:00 WILL/A317

Quantifying the interplay between atomic-scale magnetism and Josephson transport atom-by-atom — •Zhengyuan Liu, Sebastian Scherb, Manuel Steinbrecher, Nadine Hauptmann, and Alexander Khajetoorians — IMM, Radboud University Nijmegen, the Netherlands

Josephson transport can locally be affected by the presence of magnetic moments in the junction. For example, it was shown that the individual magnetic impurity, and the Yu-Shiba-Rusinov (YSR) excitations they induce in the superconductor can be used to induce a superconducting diode effect [1]. Furthermore, an intrinsic phase shift of π in its ground state can exhibit when a ferromagnetic layer with certain thickness is introduced in the Josephson junction, known as the π-junction [2]. Here, we study the effect of individual and coupled magnetic atoms on the Josephson transport between a superconducting tip and superconducting surface, using scanning tunneling microscopy. We study the evolution of the YSR states going from an individual impurity to a magnetic nanostructure. We correlate this evolution to changes in the Josephson junction properties locally, by using spatially-dependent I-V spectroscopy. We also review the local diode effect induces in these structures. [1] Trahms, M et al. Nature 615, 628*633 (2023). [2]Ryazanov et al. Phys. Rev. Lett. 86, 2427 (2001)

O 99.4 Fri 10:15 WILL/A317

Exchange-field model for electron spin resonance scanning tunneling microscopy — •Christoph Wolf[1,2], Jose Reina-Galvez[3], Xue Zhang[4], Jan Martinek[5], and Nicolas Lorente[6] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [4]Institute of Molecular Physics, Polish Academy of Science, Smoluchowskiego 17, 60-179 Poznan, Poland — [5]Spin-X Institute, China University of Technology, Guangzhou, China — [6]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Spain

Since the first experimental demonstration of electron spin resonance in a scanning tunneling microscope the understanding of how spin transitions are driven by oscillating electric fields has gone through several evolutions. In this talk, I will show how an exchange-field model can explain the magnetoelectric coupling between the electric field and a spin impurity. This model is based on an Anderson impurity model and non-equilibrium transport using magnetic electrodes. When the hopping between a magnetic electrode and the impurity is modulated on resonance with the Zeeman splitting one obtains an effective magnetic field that can coherently drive the spin. The sign and magnitude of the exchange field depends on the applied DC bias which gives full control over the position of the resonance and potentially can be used for DC-based quantum-logic operations.

O 99.5 Fri 10:30 WILL/A317

Revealing spatial inhomogeneities in superconducting 2H-NbS_2 using magnetic sensor atoms — •Werner M.J. van Weerdenburg, Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — FachbereichPhysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) are an interesting material class in which multiple quantum phases such as charge-density-wave (CDW) order, superconductivity and pair-density-wave order may coexist [1]. Within the family of superconducting TMDCs, 2H-NbS_2 stands out as the only material that does not develop a CDW phase, but this interpretation is challenged in the presence of defects, since the material is very close to a lattice instability [2,3].

Here, we present how magnetic adatoms on a superconducting TMDC substrate can be used to investigate spatial inhomogeneities of 2H-NbS_2. By manipulating an individual Fe atom between binding sites with the tip of a scanning tunneling microscope, we probe the Yu-Shiba-Rusinov (YSR) states and their response to surface variations with high energy resolution. The sensitivity of YSR states to the crystal field, density of states and disorder allows us to analyze the relation between the YSR energies and the properties of the substrate, and to find indications of local charge-density-wave nucleation around intrinsic defects.

[1] Liu et al., Science **372**, 1447-1452 (2021); [2] Heil et al., PRL **119**, 087003 (2017); [3] Wen et al., PRB **101**, 241404 (2020)

O 99.6 Fri 10:45 WILL/A317

Magnetic quantum corrals on a proximity-superconducting Rashba surface alloy — •Jinkyung Kim, Harim Jang, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, D-20355, Germany

Quantum corrals can confine and resonate surface-state electrons at discrete eigenenergies. When coupled to superconducting substrates, quantum corrals can be used to sculpture Yu-Shiba-Rusinov (YSR) in-gap states as well as spin-degenerate Andreev bound states, referred to as Machida-Shibata (MS) states, due to proximity-induced Cooper pairing [1,2]. Here, we investigated quantum corrals crafted from Fe atoms on a proximity-superconducting BiAg2/Ag/Nb(110) heterostructure. Multiple in-gap states emerge with similar numbers of antinodes as in the eigenmode closest to the Fermi energy. They show an almost perfect spatial antiphasing between the particle- and hole-like components, reminiscent of long-range YSR states of individual magnetic atoms [3]. By further studying how these in-gap states evolve with corral size and the 3d metal atom species, our work characterizes the interplay between YSR and MS states within the quantum corral. [1] L. Schneider et al., Nature 621, 60-65 (2023) [2] K. Ton That et al., Nat. Phys. (2025) https://doi.org/10.1038/s41567-025-03109-y [3] H. Jang et al., arXiv:2506.17414 (2025)

O 99.7 Fri 11:00 WILL/A317

Spin and Charge States of Open-Shell Nanographenes over Functional Substrates — •Francisco Romero-Lara, Trisha Sai, Katerina Vaxevani, Dongfei Wang, Jon Ortuzar, Leonard Edens, Stefano Trivini, Fabian Schulz, and Jose Ignacio Pascual — CIC nanoGUNE, 20018 San Sebastián, Spain

Atomically precise open-shell nanographenes are platforms hosting spin states, which can be manipulated by local probes and by tuning their local environment. Here, we present the fabrication of aza-triangulenes-based nanostructures over two novel substrates with potential control over their charge and spin state: a rare-earth-gold alloy monolayer and a superconducting surface. The aza-triangulene platforms can host several weakly interacting spin states and a doublet ground state sensitive to Jahn-Teller distortion. We use scanning tunnelling microscopy to resolve their Kondo and spin excitation spectrum. We also resolve the presence of Yu-Shiba-Rusinov (YSR) states inside the proximity gap on the superconducting surface. Owing to an inhomogeneous local contact potential difference, the nanographenes on rare-earth-gold alloy surfaces appear with varying charge states depending on their adsorption site, which is also translated into variations of the spin ground state. Over a superconducting substrate, sub-gap spectral maps reveal with high precision their YSR excitations. They are interpreted based on a model theory as reflecting, in some cases, Jahn-Teller distortions. Overall, our results highlight the potential of unconventional substrates for on-surface nanographene synthesis and for tailoring and probing their intrinsic spin states.

O 99.8 Fri 11:15 WILL/A317

Extracting mechanical work from quantum spin switching of a single atom — Nicolaj Betz[1,2], Lukas M. Veldman[1,2], Milton Aguilar[3], Eric Lutz[3], Susanne Baumann[1], and •Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart — [3]University of Stuttgart, Institute for Theoretical Physics

Stochastic dynamics are ubiquitous in atomic-scale systems, often arising from dissipative processes through which energy is lost to the environment. Harnessing such dynamics to perform work is at the heart of molecular motors and quantum heat engines. Here, we demonstrate that a single magnetic atom can function as an electric motor that converts spin excitations into mechanical oscillations of a macroscopic cantilever. We couple an Fe atom on MgO/Ag(100) via magnetic exchange interaction to the tip of a combined atomic force (AFM) and scanning tunneling microscope (STM) at milli-Kelvin temperatures. Current-induced inelastic electron tunneling induces cyclic spin switching, creating an alternating exchange force that transfers energy between the quantum spin and the AFM cantilever with a power output sufficient for free-running operation. This single-atom electric motor bridges the quantum-classical divide and provides a platform for studying energy transfer in hybrid quantum-classical systems.

O 99.9 Fri 11:30 WILL/A317

Tuning the magnetic excitation of a single atom by local gating — •Anna M. H. Krieg, Hermann Osterhage, Julian H. Strik, Niels P. E. van Mullekom, Ben Verlhac, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

The description of single-atom magnetism depends on the interplay of various degrees of freedom and the balance of different interactions. This includes the interplay between the orbital, spin and charge degrees of freedom, as well as the balance between spin-orbit coupling, hybridization, and different exchange interactions, such as Hund's and Kondo exchange. To date, the strategy to change the magnetic behavior of a single atom is to explore different atom/surface combinations. However, in this way, nearly all these parameters are fixed by the material system and when changing the material system, the entire set of parameters changes. Here, we tune the local electrostatic potential in order to modify the magnetic excitations and tunneling transport of individual Fe atoms. We start with Fe atoms on the surface of InSb(110), and characterize its magnetic excitations as a function of magnetic field. We then harness a newly developed quantum simulator platform, based on patterning Cs atoms on the surface of InSb. We show that by varying the local density of Cs on InSb, we can tune the magnetic excitation of an individual Fe atom. These results serve as a starting point to develop quantum simulation to study magnetic models in which the spin, charge, and orbital degree of freedom can be tuned.

O 99.10 Fri 11:45 WILL/A317

Spin dynamics of atomic defects in monolayer MoS_2 — •Johanna Matusche[1,2], Kwan Ho Au-Yeung[1,2], Wantong Huang[1,2], Paul Greule[1,2], Jonas Arnold[1,2], Lovis Hardeweg[1,2], Máté Stark[1,2], Luise Renz[1,2], Affan Safeer[3], Daniel Jansen[3], Jeison Fischer[3], Thomas Michely[3], Wolfgang Wernsdorfer[1,2], Christoph Sürgers[1,2], Johannes Schwenk[1,2], Wouter Jolie[3], and Philip Willke[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Köln, Germany

Scanning tunneling microscopy (STM) combined with electron spin resonance (ESR) has enabled coherent control of single ad-atoms and single molecules on surfaces [1]. Additionally, recent studies have revealed that defects in monolayer MoS_2 exhibit well-defined spin signatures [2]. In this talk, we combine these two advances for individual point-like defect spins in monolayer MoS_2 on graphene/Ir(111): First, we focus on stochastic resonance spectroscopy (SRS) [3] to periodically drive rapid transitions between spin states. This allows to identify the main relaxation mechanisms and to determine the T_1 relaxation times. Second, pulsed ESR enables coherent control of the defect spins via Rabi and Ramsey sequences, which provides direct access to their T_2 coherence times. [1] K. Yang et al., Science, 366, 509-512 (2019). [2] S. Trishin et al., Phys. Rev. B, 108, 165414 (2023) [3] N. Betz et al., arXiv:2412.12647 (2025).

O 99.11 Fri 12:00 WILL/A317

Following Spin Interactions into a Chemical Bond Formation — •Dmitriy Borodin[1], Merve Ercelik[1], Andres Pinar Sole[1], Shadi Fatayer[2], Harald Brune[3], Christoph Wolf[1], Franz J. Giessibl[4], Fabio Donati[1], and Andreas Heinrich[1] — [1]IBS Center for Quantum Nanoscience, Seoul, South Korea — [2]KAUST, Thuwal, Saudi Arabia — [3]EPFL, Lausanne, Switzerland — [4]University of Regensburg, Regensburg, Germany

Exchange interactions are essential for the formation of chemical bonds between atoms and dictate the electronic structure of molecules. In a condensed-matter system, a manifold of exchange mechanisms coexist, ultimately defining the local magnetic structure and phase stability. A particularly interesting interaction occurs between transition metal atoms and rare earth elements, where the nature of magnetic coupling in their alloys remains not fully understood. In this work, we use low-temperature scanning probe microscopy to follow the spin interactions between a tip and an adatom on a surface into a chemical bond. By controlling atom-tip separations on the picometer scale, we continuously tune interaction energies and observe spin pairing between the adatom and the magnetic tip, a situation that is reminiscent of covalent bond formation.

O 99.12 Fri 12:15 WILL/A317

Dark state formation in a zero-field split molecular triplet — •Maria Steiner and Andrea Donarini — Institute of Theoretical Physics, Regensburg University, Regensburg, Germany

In analogy to atomic physics [1], we propose a protocol to prepare and probe a dark state in a single molecule. To this end, we coherently manipulate with a multifrequency magnetic field a three-level system in the V-configuration. Thus, within a density-matrix formalism for open systems, we extend existing protocols developed to probe Rabi oscillations in ESR-AFM on pentacene [2]. The dissipative dynamics of the reduced density matrix are interpreted in terms of multipole expansion and visualized using three intertwined Bloch spheres. We consider a molecule with a zero-field splitting of the first excited triplet. This splitting typically arises from the spatial anisotropy of the frontier orbitals and the spin dipole-dipole interaction between the unpaired electrons. Pentacene is an archetypal example, which, in addition to these properties, also exhibits anisotropic decay to the ground state singlet [3] and thus enables experimental readout of the occupied state [2]. We consider both ideal scenarios and realistic parameterization for ESR-AFM on pentacene to model the expected dark state signature.

[1] Arimondo and Orriols, Lett. al Nuovo Cim. **17**, 333 (1976).
[2] Sellies et al., Nature **624**, 64 (2023).
[3] Peng et al., Science **373**, 452 (2021).

O 100: Closing Talk Steinrück

Time: Friday 13:15–14:00 Location: TRE/PHYS

Topical Talk O 100.1 Fri 13:15 TRE/PHYS

Ionic Liquid Surface Science — •Hans-Peter Steinrück — Friedrich-Alexander-Universität Erlangen-Nürnberg

Traditional surface science is often limited to solids, due to the high vapor pressure of conventional liquids or solvents. Quite recently, low-vapor-pressure liquids such as ionic liquids (ILs) or liquid metal alloys have received significant attention as they offer new concepts in catalysis. This contribution focuses on ILs, which are liquid salts with melting points below 100 °C, often even below room temperature. Since their physical and chemical properties can be tailored over a wide range, they represent a fascinating class of liquid materials with interesting applications. Two important concepts in catalysis are the Supported Ionic Liquid Phase (SILP) and Solid Catalyst with Ionic Liquid Layer (SCILL) concepts. In both, a high surface area solid substrate is covered with a thin IL film. In SILP, the film contains a homogeneously dissolved transition metal complex; in SCILL, the film modifies catalytically active surface sites at the catalyst. The interfaces of the IL are thus of critical importance. Due to their extremely low vapor pressure, ILs can be investigated in great detail under well-defined ultrahigh vacuum conditions using surface science methods like angle-resolved XPS, STM, AFM and molecular beam techniques. In this presentation, both the IL/vacuum and the IL/support interfaces are addressed. In the first example, the buoy concept will be introduced, that is, the tailored enrichment of metal complexes at the liquid/vacuum interface. The second example addresses the modification of the properties of single crystal surfaces by an ultrathin IL film.